Full wwPDB X-ray Structure Validation Report (i)

Sep 9, 2023 – 03:39 PM EDT

PDB ID	:	4I9H
Title	:	Crystal structure of rabbit LDHA in complex with AP28669
Authors	:	Zhou, T.; Stephan, Z.G.; Kohlmann, A.; Li, F.; Commodore, L.; Greenfield, M.T.; Shakespeare, W.C.; Zhu, X.; Dalgarno, D.C.
Deposited on	:	2012-12-05
Resolution	:	2.17 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

The following versions of software and data (see references (i)) were used in the production of this report:

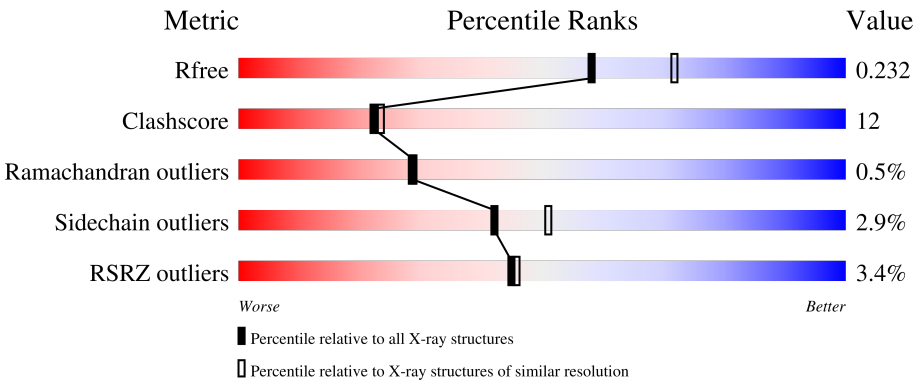
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.35.1
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35.1

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.17 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	6864 (2.20-2.16)
Clashscore	141614	7689 (2.20-2.16)
Ramachandran outliers	138981	7564 (2.20-2.16)
Sidechain outliers	138945	7564 (2.20-2.16)
RSRZ outliers	127900	6738 (2.20-2.16)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5% The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	331	2% 75% 23% • •
1	B	331	4% 80% 17% • •
1	C	331	3% 78% 19% • •
1	D	331	2% 78% 21% •
1	E	331	4% 77% 21% •

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Mol	Chain	Length	Quality of chain
1	F	331	4% 77% 20%
1	G	331	3% 74% 22%
1	H	331	4% 74% 21%

2 Entry composition (i)

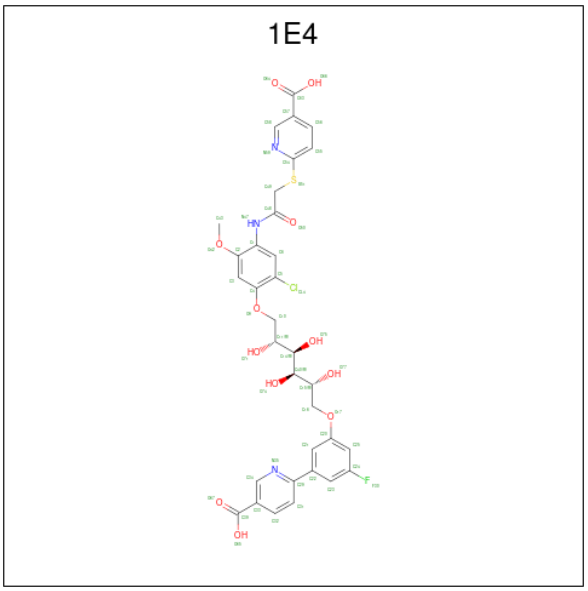
There are 3 unique types of molecules in this entry. The entry contains 21086 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called L-lactate dehydrogenase A chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	325	2511	1607	431	459	14	0	0	0
1	B	327	2528	1616	436	462	14	0	0	0
1	C	328	2532	1618	436	464	14	0	0	0
1	D	331	2559	1633	441	471	14	0	0	0
1	E	331	2559	1633	441	471	14	0	0	0
1	F	329	2540	1622	437	467	14	0	0	0
1	G	324	2502	1602	429	457	14	0	0	0
1	H	329	2546	1626	439	467	14	0	0	0

- Molecule 2 is 1-O-[3-(5-carboxypyridin-2-yl)-5-fluorophenyl]-6-O-[4-({[(5-carboxypyridin-2-yl)sulfanyl]acetyl}amino)-2-chloro-5-methoxyphenyl]-D-mannitol (three-letter code: 1E4) (formula: $C_{33}H_{31}ClFN_3O_{12}S$).



Mol	Chain	Residues	Atoms							ZeroOcc	AltConf
			Total	C	Cl	F	N	O	S		
2	A	1	51	33	1	1	3	12	1	0	0
2	B	1	51	33	1	1	3	12	1	0	0
2	C	1	51	33	1	1	3	12	1	0	0
2	D	1	51	33	1	1	3	12	1	0	0
2	E	1	51	33	1	1	3	12	1	0	0
2	F	1	51	33	1	1	3	12	1	0	0
2	G	1	51	33	1	1	3	12	1	0	0
2	H	1	51	33	1	1	3	12	1	0	0

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
3	A	67	67	67	0	0
3	B	59	59	59	0	0
3	C	47	47	47	0	0
3	D	49	49	49	0	0

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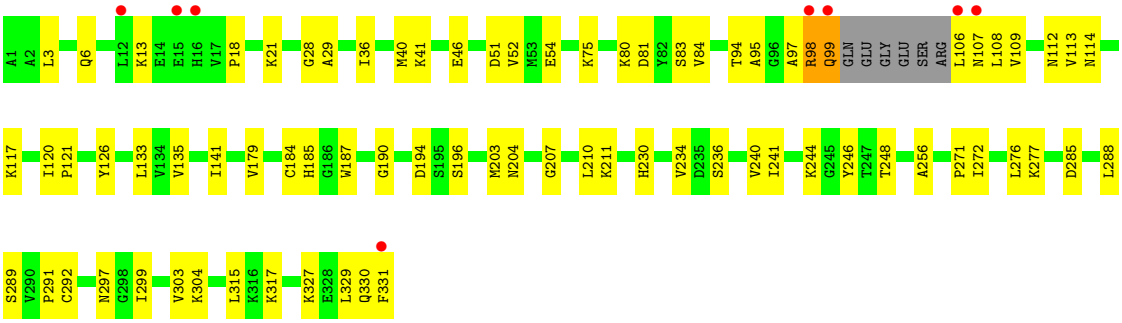
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
3	E	37	37	37	0	0
			Total	O		
3	F	39	39	39	0	0
			Total	O		
3	G	57	57	57	0	0
			Total	O		
3	H	46	46	46	0	0

3 Residue-property plots (i)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density (RSRZ > 2). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

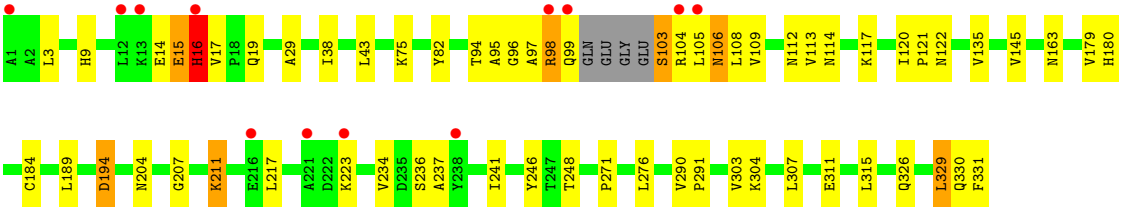
• Molecule 1: L-lactate dehydrogenase A chain

Chain A:



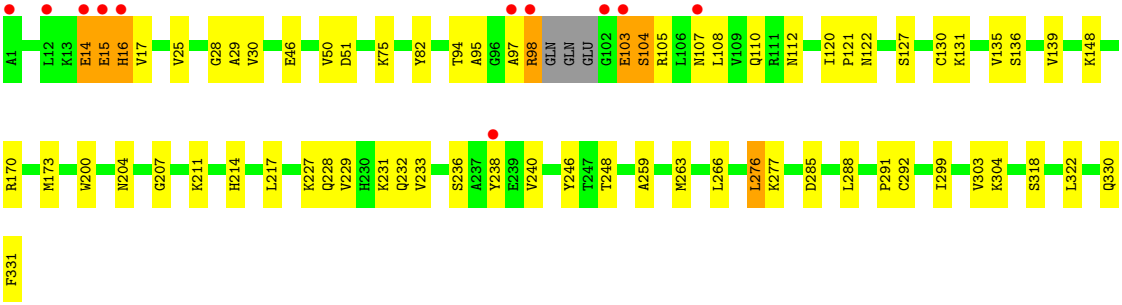
• Molecule 1: L-lactate dehydrogenase A chain

Chain B:



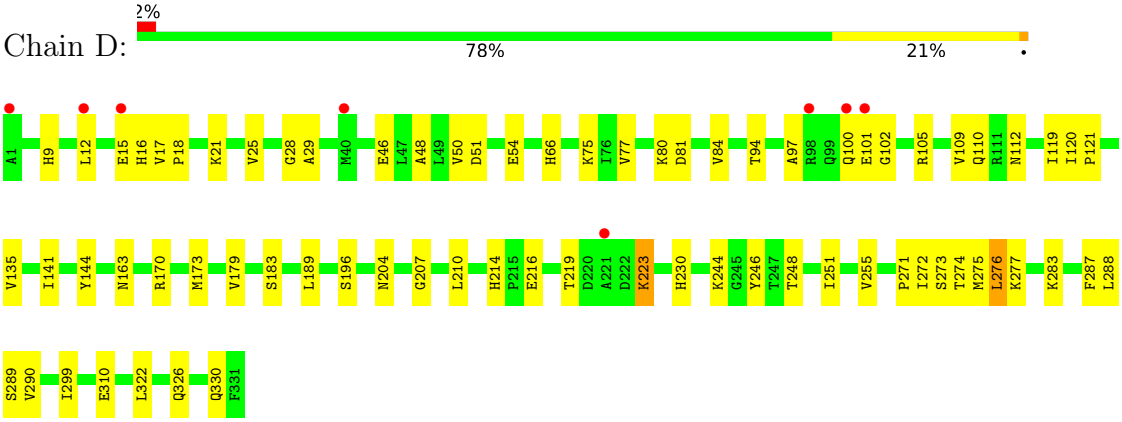
• Molecule 1: L-lactate dehydrogenase A chain

Chain C:



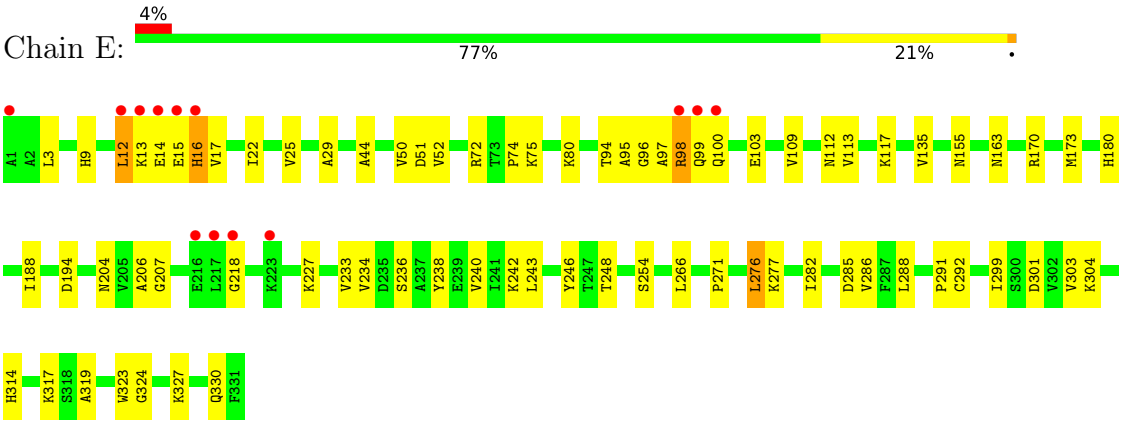
• Molecule 1: L-lactate dehydrogenase A chain

Chain D:



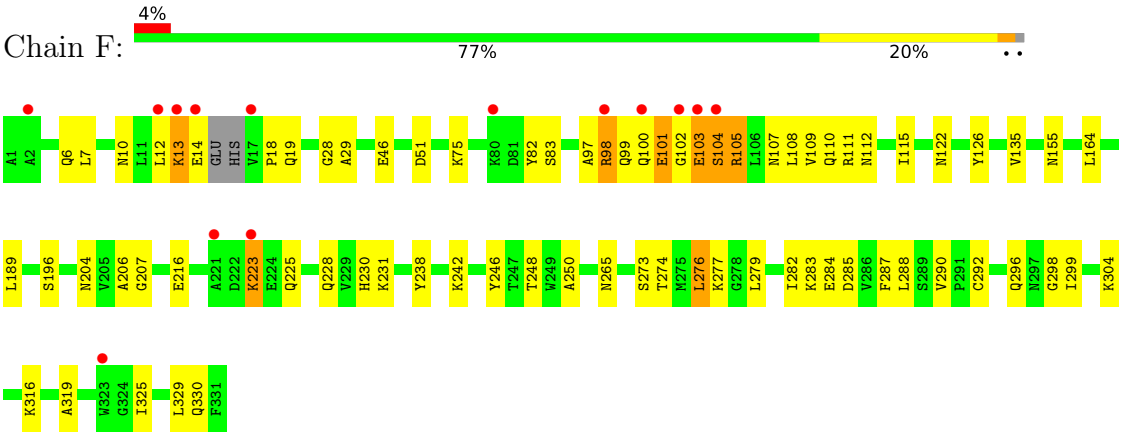
• Molecule 1: L-lactate dehydrogenase A chain

Chain E:



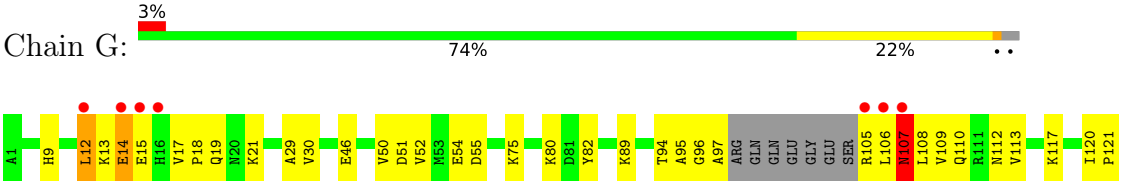
• Molecule 1: L-lactate dehydrogenase A chain

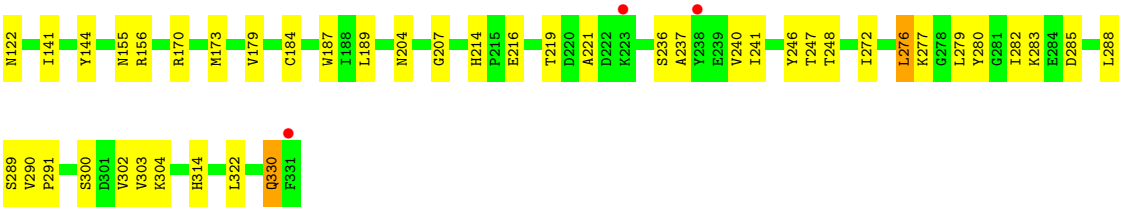
Chain F:



• Molecule 1: L-lactate dehydrogenase A chain

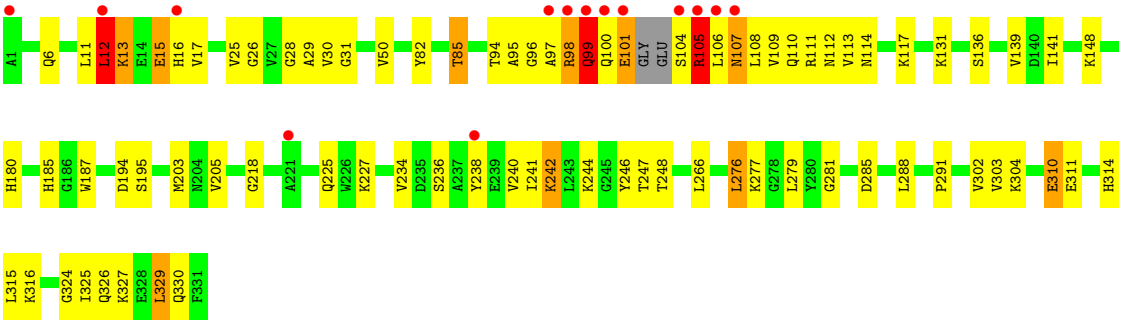
Chain G:





• Molecule 1: L-lactate dehydrogenase A chain

Chain H:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	83.87Å 139.69Å 138.81Å 90.00° 94.43° 90.00°	Depositor
Resolution (Å)	50.00 – 2.17 49.17 – 2.17	Depositor EDS
% Data completeness (in resolution range)	92.1 (50.00-2.17) 91.8 (49.17-2.17)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.57 (at 2.16Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.207 , 0.243 0.197 , 0.232	Depositor DCC
R_{free} test set	8378 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å^2)	32.0	Xtriage
Anisotropy	0.288	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.36 , 41.8	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	21086	wwPDB-VP
Average B, all atoms (Å^2)	36.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.31% of the height of the origin peak. No significant pseudotranslation is detected.*

[1]Intensities estimated from amplitudes.

[2]Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: 1E4

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\#\|Z\| >5$	RMSZ	$\#\|Z\| >5$
1	A	0.31	0/2556	0.49	0/3457
1	B	0.31	0/2573	0.50	0/3479
1	C	0.30	0/2577	0.48	0/3484
1	D	0.30	0/2605	0.48	0/3523
1	E	0.29	0/2605	0.47	0/3523
1	F	0.29	0/2584	0.47	0/3493
1	G	0.30	0/2547	0.49	0/3445
1	H	0.30	0/2591	0.49	0/3503
All	All	0.30	0/20638	0.48	0/27907

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand.A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	B	0	2
1	G	0	2
1	H	0	4
All	All	0	8

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (8) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	15	GLU	Peptide
1	B	16	HIS	Peptide

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Mol	Chain	Res	Type	Group
1	G	105	ARG	Peptide
1	G	107	ASN	Peptide
1	H	105	ARG	Peptide
1	H	12	LEU	Peptide
1	H	15	GLU	Peptide
1	H	99	GLN	Peptide

5.2 Too-close contacts (i)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2511	0	2597	55	0
1	B	2528	0	2615	60	0
1	C	2532	0	2616	57	0
1	D	2559	0	2639	64	0
1	E	2559	0	2639	64	0
1	F	2540	0	2625	68	0
1	G	2502	0	2589	73	0
1	H	2546	0	2629	76	0
2	A	51	0	29	5	0
2	B	51	0	29	6	0
2	C	51	0	29	8	0
2	D	51	0	29	4	0
2	E	51	0	29	6	0
2	F	51	0	29	4	0
2	G	51	0	29	8	0
2	H	51	0	29	6	0
3	A	67	0	0	1	0
3	B	59	0	0	1	0
3	C	47	0	0	0	0
3	D	49	0	0	0	0
3	E	37	0	0	1	0
3	F	39	0	0	0	0
3	G	57	0	0	0	0
3	H	46	0	0	0	0
All	All	21086	0	21181	489	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including

hydrogen atoms). The all-atom clashscore for this structure is 12.

All (489) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:104:SER:HA	1:F:107:ASN:HB2	1.35	1.06
1:E:29:ALA:HB1	1:E:248:THR:HG21	1.44	0.99
1:H:29:ALA:HB1	1:H:248:THR:HG21	1.42	0.98
1:F:29:ALA:HB1	1:F:248:THR:HG21	1.45	0.98
1:G:29:ALA:HB1	1:G:248:THR:HG21	1.44	0.98
1:H:97:ALA:H	1:H:112:ASN:HD21	1.11	0.97
1:D:29:ALA:HB1	1:D:248:THR:HG21	1.44	0.96
1:E:97:ALA:H	1:E:112:ASN:HD21	1.14	0.96
1:E:98:ARG:H	1:E:98:ARG:HE	0.98	0.94
1:C:29:ALA:HB1	1:C:248:THR:HG21	1.46	0.94
1:H:110:GLN:HE22	1:H:330:GLN:H	1.09	0.92
1:D:97:ALA:H	1:D:112:ASN:HD21	1.18	0.91
1:C:304:LYS:HD2	1:D:9:HIS:HB2	1.54	0.90
1:B:29:ALA:HB1	1:B:248:THR:HG21	1.51	0.89
1:D:110:GLN:HE22	1:D:330:GLN:H	1.18	0.89
1:C:98:ARG:HH21	1:C:98:ARG:HG3	1.39	0.88
1:A:29:ALA:HB1	1:A:248:THR:HG21	1.53	0.87
1:E:98:ARG:HE	1:E:98:ARG:N	1.73	0.87
1:C:276:LEU:HD21	1:C:288:LEU:HB2	1.55	0.86
1:B:29:ALA:HB1	1:B:248:THR:CG2	2.07	0.85
1:B:97:ALA:H	1:B:112:ASN:ND2	1.75	0.85
1:H:97:ALA:H	1:H:112:ASN:ND2	1.74	0.84
1:G:97:ALA:H	1:G:112:ASN:HD21	1.21	0.84
1:A:97:ALA:H	1:A:112:ASN:HD21	1.27	0.83
1:E:9:HIS:HB2	1:F:304:LYS:HD2	1.60	0.82
1:E:276:LEU:HD21	1:E:288:LEU:HD12	1.63	0.81
1:E:29:ALA:HB1	1:E:248:THR:CG2	2.12	0.80
1:G:9:HIS:HB2	1:H:304:LYS:HD2	1.63	0.79
1:C:97:ALA:H	1:C:112:ASN:HD21	1.30	0.79
1:F:29:ALA:HB1	1:F:248:THR:CG2	2.13	0.79
1:B:95:ALA:HA	2:B:401:1E4:H3	1.64	0.78
1:F:28:GLY:HA3	2:F:401:1E4:O74	1.83	0.78
1:B:97:ALA:H	1:B:112:ASN:HD21	1.32	0.78
2:B:401:1E4:H8	3:B:501:HOH:O	1.84	0.77
1:A:304:LYS:HD2	1:B:9:HIS:HB2	1.66	0.77
1:C:28:GLY:HA3	2:C:401:1E4:O74	1.84	0.77
1:C:110:GLN:HE22	1:C:330:GLN:H	1.29	0.77
1:E:97:ALA:H	1:E:112:ASN:ND2	1.82	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:216:GLU:O	1:D:219:THR:HG22	1.86	0.76
1:G:219:THR:HG23	1:G:221:ALA:H	1.49	0.76
1:C:29:ALA:HB1	1:C:248:THR:CG2	2.14	0.76
1:C:211:LYS:HD3	1:C:217:LEU:HB3	1.65	0.76
1:D:97:ALA:H	1:D:112:ASN:ND2	1.82	0.76
1:A:297:ASN:OD1	1:B:14:GLU:HG2	1.85	0.76
1:B:15:GLU:HB3	1:B:16:HIS:HD2	1.51	0.75
1:F:276:LEU:HD21	1:F:288:LEU:HD12	1.68	0.75
1:D:276:LEU:HD21	1:D:288:LEU:HB2	1.67	0.75
1:H:95:ALA:HA	2:H:401:1E4:H3	1.68	0.75
1:A:97:ALA:H	1:A:112:ASN:ND2	1.84	0.74
1:F:98:ARG:NH1	1:F:111:ARG:HH21	1.86	0.74
1:A:29:ALA:HB1	1:A:248:THR:CG2	2.17	0.74
1:B:223:LYS:HD2	1:B:223:LYS:H	1.52	0.74
1:G:219:THR:HG23	1:G:221:ALA:N	2.03	0.73
1:H:29:ALA:HB1	1:H:248:THR:CG2	2.19	0.73
1:H:276:LEU:HD21	1:H:288:LEU:HB2	1.69	0.73
1:D:110:GLN:NE2	1:D:330:GLN:H	1.87	0.73
1:H:106:LEU:HG	1:H:107:ASN:H	1.53	0.72
1:H:82:TYR:O	1:H:85:THR:HB	1.90	0.72
1:F:97:ALA:H	1:F:112:ASN:HD21	1.38	0.71
1:F:97:ALA:H	1:F:112:ASN:ND2	1.90	0.69
1:G:216:GLU:O	1:G:219:THR:HG22	1.92	0.69
1:H:291:PRO:HB2	1:H:303:VAL:HB	1.73	0.69
1:F:277:LYS:HD3	1:F:285:ASP:OD2	1.93	0.69
1:F:238:TYR:CZ	1:F:242:LYS:HD2	2.29	0.68
1:D:101:GLU:H	1:D:102:GLY:HA3	1.58	0.68
1:D:223:LYS:H	1:D:223:LYS:HD2	1.60	0.67
1:C:97:ALA:H	1:C:112:ASN:ND2	1.93	0.67
1:D:101:GLU:OE1	1:D:102:GLY:HA3	1.95	0.67
1:C:98:ARG:HH21	1:C:98:ARG:CG	2.06	0.67
1:G:110:GLN:HE22	1:G:330:GLN:H	1.43	0.67
1:B:104:ARG:C	1:B:106:ASN:H	1.99	0.66
1:H:106:LEU:HG	1:H:107:ASN:N	2.10	0.66
1:G:18:PRO:HB3	1:G:46:GLU:OE1	1.95	0.66
1:D:204:ASN:HD22	1:D:207:GLY:H	1.42	0.65
1:G:95:ALA:HA	2:G:401:1E4:H4	1.79	0.65
1:G:29:ALA:HB1	1:G:248:THR:CG2	2.22	0.65
1:B:104:ARG:O	1:B:105:LEU:HB2	1.95	0.65
1:G:291:PRO:HB2	1:G:303:VAL:HB	1.79	0.65
1:A:204:ASN:HA	1:A:210:LEU:HD13	1.78	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:109:VAL:O	1:A:113:VAL:HG23	1.98	0.64
1:D:46:GLU:OE1	1:D:75:LYS:HD3	1.98	0.64
1:D:330:GLN:HG2	1:F:99:GLN:NE2	2.13	0.64
1:E:135:VAL:HG12	2:E:401:1E4:H11	1.80	0.64
1:G:97:ALA:H	1:G:112:ASN:ND2	1.96	0.63
1:E:98:ARG:H	1:E:98:ARG:NE	1.82	0.63
1:A:28:GLY:HA3	2:A:401:1E4:O74	1.99	0.62
1:C:318:SER:O	1:C:322:LEU:HD13	1.98	0.62
1:F:13:LYS:HE2	1:F:14:GLU:HG3	1.81	0.62
1:H:106:LEU:O	1:H:108:LEU:N	2.32	0.62
1:E:25:VAL:HG22	1:E:50:VAL:CG1	2.30	0.61
1:E:163:ASN:HA	1:E:271:PRO:HG2	1.81	0.61
1:C:15:GLU:O	1:C:17:VAL:HG23	2.00	0.61
1:C:110:GLN:NE2	1:C:330:GLN:H	1.98	0.61
1:E:15:GLU:O	1:E:16:HIS:HB2	2.01	0.61
1:B:98:ARG:HG2	1:B:98:ARG:NH1	2.15	0.61
1:C:95:ALA:HA	2:C:401:1E4:H4	1.81	0.61
1:D:273:SER:OG	1:D:287:PHE:HB3	2.00	0.61
1:D:101:GLU:HB2	1:D:102:GLY:CA	2.31	0.61
1:D:28:GLY:HA3	2:D:401:1E4:O74	2.00	0.60
1:G:14:GLU:O	1:G:15:GLU:HG3	2.02	0.60
1:B:223:LYS:H	1:B:223:LYS:CD	2.14	0.60
1:E:204:ASN:HD22	1:E:207:GLY:H	1.49	0.60
1:H:310:GLU:HG3	1:H:311:GLU:N	2.15	0.60
1:D:276:LEU:CD2	1:D:288:LEU:HB2	2.30	0.60
1:D:105:ARG:O	1:D:109:VAL:HG23	2.02	0.59
1:H:95:ALA:HA	2:H:401:1E4:C10	2.31	0.59
1:G:204:ASN:HD22	1:G:207:GLY:H	1.48	0.59
1:B:95:ALA:HA	2:B:401:1E4:C10	2.31	0.59
1:D:29:ALA:HB1	1:D:248:THR:CG2	2.25	0.59
1:F:216:GLU:OE1	1:F:223:LYS:HE2	2.02	0.59
1:A:194:ASP:HA	1:A:234:VAL:HG11	1.85	0.59
1:C:103:GLU:O	1:C:103:GLU:HG2	2.01	0.59
1:D:277:LYS:HE3	1:D:283:LYS:O	2.03	0.59
1:G:304:LYS:HE2	1:H:6:GLN:O	2.03	0.59
1:B:98:ARG:HG2	1:B:98:ARG:HH11	1.67	0.58
1:C:246:TYR:CD2	1:C:248:THR:HG23	2.38	0.58
1:G:300:SER:HA	1:H:12:LEU:HB2	1.84	0.58
1:H:99:GLN:O	1:H:99:GLN:HG2	2.02	0.58
1:F:103:GLU:O	1:F:104:SER:CB	2.50	0.58
1:E:97:ALA:N	1:E:112:ASN:HD21	1.94	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:323:TRP:O	1:E:327:LYS:HG3	2.04	0.58
1:H:110:GLN:HE22	1:H:330:GLN:N	1.92	0.58
1:B:326:GLN:HA	1:B:329:LEU:HD22	1.86	0.58
1:F:13:LYS:O	1:F:13:LYS:HG3	2.03	0.58
1:H:326:GLN:HA	1:H:329:LEU:HD22	1.84	0.58
1:D:110:GLN:HE22	1:D:330:GLN:N	1.97	0.57
1:F:246:TYR:CD2	1:F:248:THR:HG23	2.38	0.57
1:F:325:ILE:O	1:F:329:LEU:HD13	2.04	0.57
1:F:98:ARG:NH1	1:F:111:ARG:NH2	2.52	0.57
1:C:14:GLU:HB2	1:C:16:HIS:ND1	2.20	0.57
1:H:194:ASP:HA	1:H:234:VAL:HG11	1.86	0.57
1:F:111:ARG:O	1:F:115:ILE:HG13	2.05	0.56
1:E:327:LYS:HB2	1:E:327:LYS:NZ	2.20	0.56
1:G:54:GLU:CD	1:G:80:LYS:HD3	2.26	0.56
1:H:25:VAL:HG13	1:H:50:VAL:HG23	1.86	0.56
1:H:279:LEU:HD13	1:H:302:VAL:HG21	1.87	0.56
1:B:109:VAL:O	1:B:113:VAL:HG23	2.05	0.56
1:H:114:ASN:HA	1:H:117:LYS:HD3	1.86	0.56
1:E:304:LYS:HE3	1:F:6:GLN:O	2.06	0.56
1:F:102:GLY:HA2	1:F:103:GLU:O	2.05	0.56
1:F:238:TYR:CE2	1:F:242:LYS:HD2	2.41	0.56
1:B:99:GLN:NE2	1:B:104:ARG:NH2	2.53	0.56
1:A:113:VAL:O	1:A:117:LYS:HG3	2.06	0.55
1:G:95:ALA:HA	2:G:401:1E4:C10	2.36	0.55
1:C:95:ALA:HA	2:C:401:1E4:C10	2.36	0.55
1:G:246:TYR:CD2	1:G:248:THR:HG23	2.41	0.55
1:B:94:THR:O	2:B:401:1E4:H12	2.06	0.55
1:E:9:HIS:CD2	1:F:279:LEU:HD11	2.41	0.55
1:G:189:LEU:HD22	1:G:290:VAL:HA	1.87	0.55
1:H:110:GLN:NE2	1:H:330:GLN:H	1.92	0.55
1:D:29:ALA:CB	1:D:248:THR:HG21	2.28	0.55
1:F:228:GLN:OE1	1:F:231:LYS:HD3	2.07	0.55
1:F:246:TYR:HD2	1:F:248:THR:HG23	1.72	0.55
1:H:106:LEU:O	1:H:109:VAL:N	2.28	0.55
1:H:194:ASP:HA	1:H:234:VAL:CG1	2.36	0.55
1:E:22:ILE:HD12	1:E:44:ALA:HB2	1.87	0.55
1:A:95:ALA:HA	2:A:401:1E4:H4	1.89	0.54
1:D:144:TYR:CD2	1:D:326:GLN:HG2	2.42	0.54
1:G:17:VAL:O	1:G:17:VAL:HG23	2.07	0.54
1:G:302:VAL:HG13	1:H:11:LEU:CD1	2.37	0.54
1:H:96:GLY:H	2:H:401:1E4:H4	1.73	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:246:TYR:CD2	1:D:248:THR:HG23	2.42	0.54
1:B:135:VAL:HG12	2:B:401:1E4:H11	1.89	0.54
1:G:246:TYR:HD2	1:G:248:THR:HG23	1.71	0.54
1:B:96:GLY:H	2:B:401:1E4:H4	1.72	0.54
1:E:15:GLU:O	1:E:16:HIS:CB	2.56	0.54
1:E:246:TYR:CD2	1:E:248:THR:HG23	2.42	0.54
1:G:54:GLU:OE1	1:G:80:LYS:HD3	2.08	0.54
1:A:291:PRO:HB2	1:A:303:VAL:HB	1.89	0.54
1:A:135:VAL:HG12	2:A:401:1E4:H11	1.90	0.54
1:C:94:THR:O	2:C:401:1E4:H12	2.08	0.54
1:D:204:ASN:ND2	1:D:207:GLY:H	2.06	0.54
1:A:36:ILE:O	1:A:40:MET:HG3	2.07	0.53
1:H:106:LEU:CG	1:H:107:ASN:H	2.17	0.53
1:B:14:GLU:HG3	1:B:15:GLU:H	1.73	0.53
1:H:131:LYS:HD3	1:H:131:LYS:N	2.23	0.53
1:A:81:ASP:O	1:A:84:VAL:HG22	2.08	0.53
1:F:292:CYS:HB3	1:F:299:ILE:HG23	1.90	0.53
1:C:236:SER:O	1:C:240:VAL:HG23	2.07	0.53
1:D:170:ARG:HA	1:D:173:MET:HE3	1.89	0.53
1:H:114:ASN:HD22	1:H:117:LYS:HD3	1.73	0.53
1:E:17:VAL:HG23	1:E:17:VAL:O	2.09	0.53
1:D:163:ASN:HA	1:D:271:PRO:HG2	1.91	0.53
1:G:13:LYS:HE2	1:G:14:GLU:OE1	2.09	0.53
1:H:276:LEU:CD2	1:H:288:LEU:HB2	2.38	0.53
1:E:155:ASN:ND2	1:F:12:LEU:HD11	2.24	0.52
1:F:135:VAL:HG12	2:F:401:1E4:H11	1.91	0.52
1:D:97:ALA:N	1:D:112:ASN:HD21	1.99	0.52
1:G:276:LEU:HD21	1:G:288:LEU:HD12	1.91	0.52
1:H:195:SER:O	1:H:314:HIS:HE1	1.93	0.52
1:B:98:ARG:HD3	1:B:98:ARG:O	2.10	0.52
1:D:101:GLU:N	1:D:102:GLY:HA3	2.18	0.52
1:B:98:ARG:HD3	1:B:98:ARG:H	1.73	0.52
1:E:204:ASN:ND2	1:E:207:GLY:H	2.07	0.52
1:H:100:GLN:O	1:H:101:GLU:HB3	2.09	0.52
1:A:187:TRP:CZ3	1:A:271:PRO:HD3	2.45	0.52
1:G:51:ASP:HA	2:G:401:1E4:CL4	2.47	0.52
1:H:104:SER:O	1:H:105:ARG:O	2.27	0.52
1:G:94:THR:O	2:G:401:1E4:H12	2.10	0.51
1:B:114:ASN:HA	1:B:117:LYS:HD3	1.93	0.51
1:B:179:VAL:HG23	1:B:184:CYS:SG	2.50	0.51
1:B:223:LYS:HD2	1:B:223:LYS:N	2.23	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:16:HIS:O	1:H:16:HIS:ND1	2.43	0.51
1:H:100:GLN:O	1:H:101:GLU:CB	2.59	0.51
1:A:106:LEU:O	1:A:107:ASN:HB2	2.10	0.51
1:D:246:TYR:HD2	1:D:248:THR:HG23	1.74	0.51
1:E:206:ALA:HA	1:H:187:TRP:CZ2	2.45	0.51
1:B:97:ALA:N	1:B:112:ASN:HD21	2.04	0.51
1:F:204:ASN:HD22	1:F:207:GLY:H	1.58	0.51
1:H:29:ALA:CB	1:H:248:THR:HG21	2.29	0.51
1:F:189:LEU:HD22	1:F:290:VAL:HA	1.93	0.51
1:H:246:TYR:CD2	1:H:248:THR:HG23	2.46	0.51
1:F:28:GLY:HA3	2:F:401:1E4:H29	1.76	0.50
1:F:276:LEU:HD21	1:F:288:LEU:HB2	1.92	0.50
1:G:109:VAL:O	1:G:113:VAL:HG23	2.11	0.50
1:B:29:ALA:CB	1:B:248:THR:CG2	2.87	0.50
1:F:51:ASP:OD2	2:F:401:1E4:H3	2.11	0.50
1:F:98:ARG:HH11	1:F:111:ARG:HH21	1.57	0.50
1:H:17:VAL:HG23	1:H:17:VAL:O	2.12	0.50
1:H:29:ALA:CB	1:H:248:THR:CG2	2.88	0.50
1:D:275:MET:CE	1:D:277:LYS:HB3	2.41	0.50
1:A:83:SER:HA	1:A:126:TYR:CD2	2.46	0.50
1:B:98:ARG:H	1:B:98:ARG:CD	2.24	0.50
1:B:104:ARG:C	1:B:106:ASN:N	2.63	0.50
1:E:236:SER:O	1:E:240:VAL:HG23	2.11	0.50
1:D:120:ILE:HB	1:D:121:PRO:HD3	1.94	0.50
1:H:244:LYS:HG3	1:H:246:TYR:O	2.11	0.49
1:B:98:ARG:HH11	1:B:98:ARG:CG	2.24	0.49
1:D:276:LEU:HD21	1:D:288:LEU:HD12	1.94	0.49
1:C:259:ALA:O	1:C:263:MET:HG2	2.13	0.49
1:F:276:LEU:CD2	1:F:288:LEU:HB2	2.43	0.49
1:B:14:GLU:HG3	1:B:15:GLU:N	2.26	0.49
1:C:277:LYS:HD3	1:C:285:ASP:OD2	2.12	0.49
1:D:204:ASN:HA	1:D:210:LEU:HD13	1.94	0.49
1:E:266:LEU:O	1:H:180:HIS:HB2	2.13	0.49
1:F:98:ARG:H	1:F:98:ARG:NE	2.10	0.49
1:C:246:TYR:HD2	1:C:248:THR:HG23	1.75	0.49
1:E:246:TYR:HD2	1:E:248:THR:HG23	1.78	0.49
1:D:51:ASP:OD2	2:D:401:1E4:H3	2.12	0.49
1:B:211:LYS:HE3	1:B:217:LEU:HB3	1.95	0.49
1:C:29:ALA:CB	1:C:248:THR:CG2	2.89	0.49
1:E:109:VAL:O	1:E:113:VAL:HG23	2.13	0.49
1:C:104:SER:HB3	1:C:107:ASN:HD22	1.77	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:135:VAL:HG12	2:D:401:1E4:H11	1.95	0.49
1:D:144:TYR:CE2	1:D:326:GLN:HG2	2.48	0.49
1:E:113:VAL:O	1:E:117:LYS:HG3	2.13	0.49
1:C:14:GLU:HG3	1:C:14:GLU:O	2.13	0.48
1:E:95:ALA:HA	2:E:401:1E4:H3	1.95	0.48
1:F:282:ILE:CD1	1:F:288:LEU:HD12	2.43	0.48
1:G:29:ALA:CB	1:G:248:THR:CG2	2.91	0.48
1:A:13:LYS:HD3	1:A:13:LYS:C	2.33	0.48
1:E:188:ILE:CD1	1:E:233:VAL:HG11	2.42	0.48
1:G:52:VAL:HG11	2:G:401:1E4:C48	2.43	0.48
1:H:246:TYR:HD2	1:H:248:THR:HG23	1.77	0.48
1:C:228:GLN:O	1:C:232:GLN:HG3	2.14	0.48
1:H:281:GLY:HA3	1:H:316:LYS:NZ	2.28	0.48
1:A:46:GLU:OE1	1:A:75:LYS:HD3	2.14	0.48
1:G:52:VAL:HG11	2:G:401:1E4:O50	2.14	0.48
1:G:107:ASN:C	1:G:109:VAL:N	2.66	0.48
1:D:25:VAL:HG22	1:D:50:VAL:CG2	2.44	0.48
1:E:95:ALA:HA	2:E:401:1E4:C10	2.44	0.48
1:E:218:GLY:O	1:E:227:LYS:HD2	2.14	0.48
1:H:94:THR:O	2:H:401:1E4:H12	2.14	0.48
1:H:113:VAL:HG21	1:H:329:LEU:HG	1.94	0.48
2:E:401:1E4:H8	3:E:504:HOH:O	2.13	0.48
1:G:173:MET:HE2	1:G:173:MET:HB2	1.71	0.48
1:G:302:VAL:HG13	1:H:11:LEU:HD11	1.94	0.48
1:D:100:GLN:HB3	1:D:101:GLU:CD	2.34	0.48
1:E:96:GLY:H	2:E:401:1E4:H4	1.79	0.48
1:G:106:LEU:O	1:G:107:ASN:ND2	2.47	0.48
1:H:240:VAL:HB	1:H:247:THR:HG22	1.96	0.48
1:A:99:GLN:NE2	1:A:108:LEU:HD13	2.29	0.47
1:G:19:GLN:O	1:G:89:LYS:HE3	2.14	0.47
1:G:29:ALA:CB	1:G:248:THR:HG21	2.30	0.47
1:G:50:VAL:HG11	1:G:82:TYR:CZ	2.48	0.47
1:B:291:PRO:HB2	1:B:303:VAL:HB	1.94	0.47
1:C:25:VAL:HG22	1:C:50:VAL:CG2	2.45	0.47
1:F:7:LEU:HD21	1:H:205:VAL:HB	1.96	0.47
1:F:29:ALA:CB	1:F:248:THR:CG2	2.90	0.47
1:F:282:ILE:HD13	1:F:319:ALA:HB2	1.95	0.47
1:A:3:LEU:HD13	1:C:214:HIS:HB2	1.96	0.47
1:D:48:ALA:HA	1:D:77:VAL:O	2.15	0.47
1:H:277:LYS:HD2	1:H:285:ASP:OD2	2.14	0.47
1:A:179:VAL:HG23	1:A:184:CYS:SG	2.54	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:135:VAL:HG12	2:C:401:1E4:H11	1.95	0.47
1:G:277:LYS:HE3	1:G:283:LYS:O	2.14	0.47
1:E:170:ARG:HA	1:E:173:MET:HE3	1.95	0.47
1:A:277:LYS:HD2	1:A:285:ASP:OD2	2.14	0.47
1:C:46:GLU:CD	1:C:75:LYS:HD3	2.35	0.47
1:A:94:THR:O	2:A:401:1E4:H12	2.15	0.47
1:D:18:PRO:HB2	1:D:21:LYS:HB2	1.97	0.47
1:E:180:HIS:HB2	1:H:266:LEU:O	2.15	0.47
1:E:282:ILE:HD12	1:E:319:ALA:HB2	1.97	0.46
1:G:106:LEU:O	1:G:107:ASN:CB	2.63	0.46
1:D:274:THR:HB	1:D:299:ILE:HD13	1.98	0.46
1:E:276:LEU:H	1:E:276:LEU:HD12	1.80	0.46
1:A:194:ASP:HA	1:A:234:VAL:CG1	2.45	0.46
1:A:95:ALA:HA	2:A:401:1E4:C10	2.46	0.46
1:B:120:ILE:HB	1:B:121:PRO:HD3	1.98	0.46
1:A:54:GLU:CD	1:A:80:LYS:HD3	2.36	0.46
1:G:117:LYS:HE2	1:G:117:LYS:HB3	1.77	0.46
1:H:324:GLY:HA2	1:H:327:LYS:HE2	1.98	0.46
1:D:15:GLU:HG3	1:D:15:GLU:O	2.15	0.46
1:G:110:GLN:NE2	1:G:330:GLN:H	2.09	0.46
1:G:237:ALA:O	1:G:241:ILE:HG13	2.16	0.46
1:G:240:VAL:HB	1:G:247:THR:HG22	1.97	0.46
1:A:241:ILE:HG12	1:A:246:TYR:HA	1.97	0.46
1:E:13:LYS:O	1:E:14:GLU:HB2	2.14	0.46
1:G:179:VAL:CG2	1:G:184:CYS:SG	3.04	0.46
1:A:29:ALA:CB	1:A:248:THR:CG2	2.92	0.46
1:C:291:PRO:HB2	1:C:303:VAL:HB	1.97	0.46
1:E:29:ALA:CB	1:E:248:THR:CG2	2.89	0.46
1:G:170:ARG:HA	1:G:173:MET:HE3	1.98	0.45
1:H:105:ARG:H	1:H:105:ARG:HG2	1.37	0.45
1:A:246:TYR:CD2	1:A:248:THR:HG23	2.51	0.45
1:B:189:LEU:HD22	1:B:290:VAL:HA	1.97	0.45
1:B:236:SER:HB2	1:D:66:HIS:HE1	1.81	0.45
1:D:141:ILE:HG13	1:D:322:LEU:HD22	1.98	0.45
1:F:225:GLN:HA	1:F:225:GLN:NE2	2.31	0.45
1:G:18:PRO:HB2	1:G:21:LYS:HB2	1.97	0.45
1:H:185:HIS:O	1:H:203:MET:HA	2.16	0.45
1:B:3:LEU:HD13	1:D:214:HIS:HB2	1.98	0.45
1:B:117:LYS:HE2	1:B:331:PHE:O	2.16	0.45
1:C:204:ASN:ND2	1:C:207:GLY:H	2.14	0.45
1:G:30:VAL:HG21	2:G:401:1E4:C22	2.46	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:277:LYS:HD2	1:G:285:ASP:OD2	2.17	0.45
1:A:244:LYS:HG3	1:A:246:TYR:O	2.17	0.45
1:B:113:VAL:HG21	1:B:329:LEU:HG	1.99	0.45
1:C:211:LYS:HE2	1:C:217:LEU:O	2.16	0.45
1:E:238:TYR:CE2	1:E:242:LYS:HE2	2.52	0.45
1:F:100:GLN:O	1:F:101:GLU:O	2.35	0.45
1:F:155:ASN:O	1:F:298:GLY:HA3	2.16	0.45
1:B:163:ASN:HA	1:B:271:PRO:HG2	1.99	0.45
1:E:12:LEU:HD22	1:E:13:LYS:O	2.16	0.45
1:E:277:LYS:HD3	1:E:285:ASP:OD2	2.16	0.45
1:F:276:LEU:HD12	1:F:276:LEU:H	1.82	0.45
1:F:83:SER:HA	1:F:126:TYR:CE2	2.52	0.45
1:F:108:LEU:HD13	1:F:108:LEU:C	2.37	0.45
1:A:114:ASN:HA	1:A:117:LYS:HE3	1.98	0.45
1:G:107:ASN:O	1:G:110:GLN:N	2.50	0.45
1:C:228:GLN:OE1	1:C:231:LYS:HD3	2.16	0.45
1:C:229:VAL:O	1:C:233:VAL:HG23	2.16	0.45
1:H:218:GLY:O	1:H:227:LYS:HD2	2.17	0.45
1:B:98:ARG:HD3	1:B:98:ARG:N	2.31	0.45
1:F:82:TYR:CG	1:F:122:ASN:HB3	2.52	0.45
1:F:105:ARG:O	1:F:109:VAL:HG23	2.17	0.45
1:F:108:LEU:HD13	1:F:108:LEU:O	2.16	0.45
1:A:288:LEU:HD13	1:A:315:LEU:HD12	2.00	0.44
1:D:29:ALA:CB	1:D:248:THR:CG2	2.92	0.44
1:E:291:PRO:HB2	1:E:303:VAL:HB	1.98	0.44
1:F:98:ARG:H	1:F:98:ARG:HE	1.63	0.44
1:F:273:SER:OG	1:F:287:PHE:HB3	2.17	0.44
1:H:136:SER:O	1:H:139:VAL:HA	2.18	0.44
1:C:98:ARG:CG	1:C:98:ARG:NH2	2.70	0.44
1:A:98:ARG:HD2	1:A:98:ARG:O	2.17	0.44
1:A:327:LYS:HE2	3:A:549:HOH:O	2.17	0.44
1:F:103:GLU:O	1:F:104:SER:HB2	2.17	0.44
1:G:9:HIS:CG	1:H:279:LEU:HD21	2.51	0.44
1:C:148:LYS:HD3	1:C:331:PHE:CZ	2.53	0.44
1:D:81:ASP:O	1:D:84:VAL:HG22	2.17	0.44
1:H:141:ILE:HD13	1:H:325:ILE:HG21	1.99	0.44
1:A:109:VAL:HG11	1:A:141:ILE:HG21	1.99	0.44
1:A:292:CYS:HB3	1:A:299:ILE:HG23	1.99	0.44
1:C:28:GLY:HA3	2:C:401:1E4:H29	1.82	0.44
1:G:110:GLN:HE22	1:G:330:GLN:N	2.10	0.44
1:C:120:ILE:HB	1:C:121:PRO:HD3	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:51:ASP:OD1	1:G:52:VAL:N	2.51	0.44
1:C:276:LEU:CD2	1:C:288:LEU:HB2	2.39	0.44
1:E:292:CYS:HB3	1:E:299:ILE:HG23	1.98	0.44
1:G:82:TYR:CG	1:G:122:ASN:HB3	2.53	0.44
1:D:101:GLU:HB2	1:D:102:GLY:HA2	2.00	0.44
1:F:274:THR:O	1:F:287:PHE:HA	2.18	0.44
1:A:99:GLN:HG2	1:A:108:LEU:HD21	2.00	0.43
1:C:103:GLU:HA	1:C:104:SER:HA	1.74	0.43
1:F:276:LEU:CD2	1:F:282:ILE:HD12	2.48	0.43
1:H:12:LEU:HD23	1:H:13:LYS:HG2	1.99	0.43
1:E:206:ALA:HA	1:H:187:TRP:CE2	2.53	0.43
1:E:323:TRP:NE1	1:E:327:LYS:HD3	2.32	0.43
1:G:96:GLY:H	2:G:401:1E4:H4	1.82	0.43
1:A:29:ALA:C	1:A:248:THR:HG22	2.38	0.43
1:B:82:TYR:CG	1:B:122:ASN:HB3	2.53	0.43
1:G:75:LYS:HE3	1:G:75:LYS:HB2	1.83	0.43
1:E:276:LEU:CD1	1:E:276:LEU:C	2.87	0.43
1:G:219:THR:HG21	1:G:221:ALA:HB3	2.01	0.43
1:B:38:ILE:HG23	1:B:43:LEU:HB2	2.00	0.43
1:B:315:LEU:HD12	1:B:315:LEU:HA	1.74	0.43
1:C:200:TRP:CH2	1:C:227:LYS:HA	2.53	0.43
1:D:16:HIS:HD2	1:D:17:VAL:N	2.16	0.43
1:D:94:THR:O	2:D:401:1E4:H12	2.18	0.43
1:F:98:ARG:H	1:F:98:ARG:CD	2.32	0.43
1:A:120:ILE:HB	1:A:121:PRO:HD3	2.01	0.43
1:C:51:ASP:HA	2:C:401:1E4:CL4	2.56	0.43
1:G:204:ASN:ND2	1:G:207:GLY:H	2.14	0.43
1:G:280:TYR:O	1:G:282:ILE:HD12	2.19	0.43
1:H:28:GLY:HA3	2:H:401:1E4:O74	2.19	0.43
1:A:41:LYS:HD3	1:A:256:ALA:HB1	2.01	0.43
1:B:204:ASN:HD22	1:B:207:GLY:H	1.66	0.43
1:G:236:SER:O	1:G:240:VAL:HG23	2.19	0.43
1:H:242:LYS:HE2	1:H:242:LYS:HB3	1.66	0.43
1:A:179:VAL:CG2	1:A:184:CYS:SG	3.06	0.43
1:C:30:VAL:HG21	2:C:401:1E4:C21	2.49	0.43
1:H:315:LEU:HD12	1:H:315:LEU:HA	1.82	0.43
1:B:180:HIS:HB2	1:C:266:LEU:O	2.18	0.43
1:H:241:ILE:HG12	1:H:246:TYR:HA	2.01	0.43
1:A:18:PRO:HB2	1:A:21:LYS:HB2	2.01	0.42
1:A:106:LEU:HD12	1:A:106:LEU:N	2.33	0.42
1:C:136:SER:O	1:C:139:VAL:HA	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:51:ASP:OD1	1:E:52:VAL:N	2.50	0.42
1:H:98:ARG:O	1:H:111:ARG:NH2	2.46	0.42
1:C:104:SER:HB3	1:C:107:ASN:ND2	2.34	0.42
1:E:327:LYS:NZ	1:E:327:LYS:CB	2.82	0.42
1:H:12:LEU:C	1:H:13:LYS:HG2	2.39	0.42
1:B:236:SER:HB2	1:D:66:HIS:CE1	2.54	0.42
1:B:246:TYR:CD2	1:B:248:THR:HG23	2.54	0.42
1:D:100:GLN:NE2	1:D:100:GLN:HA	2.33	0.42
1:D:251:ILE:O	1:D:255:VAL:HG23	2.19	0.42
1:E:80:LYS:NZ	1:E:80:LYS:HB3	2.34	0.42
1:E:99:GLN:OE1	1:E:103:GLU:HG3	2.19	0.42
1:C:204:ASN:HD22	1:C:207:GLY:H	1.67	0.42
1:E:3:LEU:HD13	1:G:214:HIS:HB2	2.01	0.42
1:F:206:ALA:HA	1:G:187:TRP:CZ2	2.54	0.42
1:F:164:LEU:HD11	1:F:250:ALA:HB1	2.00	0.42
1:A:204:ASN:HD22	1:A:207:GLY:H	1.66	0.42
1:B:17:VAL:O	1:B:17:VAL:HG13	2.20	0.42
1:F:225:GLN:HA	1:F:225:GLN:HE21	1.84	0.42
1:F:279:LEU:N	1:F:279:LEU:HD22	2.34	0.42
1:G:279:LEU:HD13	1:G:302:VAL:HG21	2.01	0.42
1:H:236:SER:O	1:H:240:VAL:HG23	2.19	0.42
1:A:236:SER:O	1:A:240:VAL:HG23	2.20	0.42
1:D:244:LYS:HG3	1:D:246:TYR:O	2.19	0.42
1:G:106:LEU:C	1:G:106:LEU:HD13	2.39	0.42
1:G:276:LEU:HD12	1:G:276:LEU:H	1.84	0.42
1:B:145:VAL:HG13	1:B:331:PHE:HE2	1.85	0.42
1:E:276:LEU:HD11	1:E:286:VAL:HG23	2.02	0.42
1:F:196:SER:OG	1:F:230:HIS:HE1	2.02	0.42
1:A:196:SER:OG	1:A:230:HIS:HE1	2.03	0.41
1:C:82:TYR:CG	1:C:122:ASN:HB3	2.55	0.41
1:D:54:GLU:OE1	1:D:80:LYS:HE2	2.20	0.41
1:D:101:GLU:CB	1:D:102:GLY:CA	2.97	0.41
1:D:196:SER:OG	1:D:230:HIS:HE1	2.02	0.41
1:F:100:GLN:O	1:F:101:GLU:C	2.58	0.41
1:F:103:GLU:O	1:F:104:SER:OG	2.37	0.41
1:A:272:ILE:O	1:A:289:SER:HA	2.21	0.41
1:C:105:ARG:O	1:C:108:LEU:HB3	2.21	0.41
1:C:173:MET:HE2	1:C:173:MET:HB2	1.86	0.41
1:E:243:LEU:HB3	1:G:55:ASP:O	2.20	0.41
1:A:6:GLN:O	1:B:304:LYS:HE3	2.21	0.41
1:A:190:GLY:HA2	1:A:315:LEU:HD11	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:237:ALA:O	1:B:241:ILE:HG13	2.21	0.41
1:G:12:LEU:HD23	1:G:13:LYS:H	1.85	0.41
1:G:272:ILE:O	1:G:289:SER:HA	2.21	0.41
1:H:97:ALA:N	1:H:112:ASN:ND2	2.55	0.41
1:H:225:GLN:NE2	1:H:225:GLN:HA	2.36	0.41
1:B:75:LYS:HE3	1:B:75:LYS:HB2	1.73	0.41
1:B:103:SER:O	1:B:104:ARG:HB2	2.20	0.41
1:B:194:ASP:HA	1:B:234:VAL:HG11	2.02	0.41
1:C:127:SER:HB3	1:C:130:CYS:HB3	2.02	0.41
1:D:105:ARG:CZ	1:D:105:ARG:HB3	2.50	0.41
1:E:25:VAL:HG22	1:E:50:VAL:HG13	2.02	0.41
1:E:194:ASP:HA	1:E:234:VAL:HG11	2.02	0.41
1:G:120:ILE:HB	1:G:121:PRO:HD3	2.02	0.41
1:B:14:GLU:CG	1:B:15:GLU:H	2.34	0.41
1:H:26:GLY:O	1:H:31:GLY:HA3	2.20	0.41
1:B:307:LEU:HB3	1:B:311:GLU:HB2	2.03	0.41
1:D:179:VAL:CG1	1:D:183:SER:HB2	2.51	0.41
1:E:301:ASP:OD2	1:F:10:ASN:HA	2.20	0.41
1:F:277:LYS:HB2	1:F:284:GLU:O	2.21	0.41
1:G:155:ASN:ND2	1:G:156:ARG:HG3	2.35	0.41
1:C:292:CYS:HB3	1:C:299:ILE:HG23	2.03	0.41
1:D:272:ILE:O	1:D:289:SER:HA	2.20	0.41
1:F:103:GLU:HB3	1:F:104:SER:H	1.57	0.41
1:A:185:HIS:O	1:A:203:MET:HA	2.21	0.40
1:A:317:LYS:HE3	1:A:317:LYS:HB2	1.72	0.40
1:C:170:ARG:HA	1:C:173:MET:HE3	2.03	0.40
1:G:141:ILE:O	1:G:144:TYR:HB3	2.21	0.40
1:A:51:ASP:OD1	1:A:52:VAL:N	2.54	0.40
1:D:25:VAL:HG11	1:D:119:ILE:HD13	2.04	0.40
1:H:25:VAL:HG22	1:H:50:VAL:CG2	2.51	0.40
1:H:30:VAL:HG21	2:H:401:1E4:C21	2.51	0.40
1:E:324:GLY:HA2	1:E:327:LYS:HE3	2.03	0.40
1:B:17:VAL:O	1:B:19:GLN:NE2	2.47	0.40
1:C:131:LYS:HE2	1:C:131:LYS:HB2	1.90	0.40
1:E:74:PRO:O	1:E:75:LYS:HD2	2.22	0.40
1:E:94:THR:O	2:E:401:1E4:H12	2.22	0.40
1:E:117:LYS:HE2	1:E:117:LYS:HB3	1.91	0.40
1:F:265:ASN:HB2	1:F:296:GLN:HB3	2.02	0.40
1:G:302:VAL:HG13	1:H:11:LEU:HD12	2.01	0.40
1:D:189:LEU:HD22	1:D:290:VAL:HA	2.04	0.40
1:F:18:PRO:HB3	1:F:46:GLU:OE1	2.22	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	321/331 (97%)	313 (98%)	7 (2%)	1 (0%)	41	43
1	B	323/331 (98%)	313 (97%)	9 (3%)	1 (0%)	41	43
1	C	324/331 (98%)	316 (98%)	7 (2%)	1 (0%)	41	43
1	D	329/331 (99%)	318 (97%)	11 (3%)	0	100	100
1	E	329/331 (99%)	319 (97%)	9 (3%)	1 (0%)	41	43
1	F	325/331 (98%)	312 (96%)	9 (3%)	4 (1%)	13	9
1	G	320/331 (97%)	308 (96%)	10 (3%)	2 (1%)	25	24
1	H	325/331 (98%)	311 (96%)	11 (3%)	3 (1%)	17	15
All	All	2596/2648 (98%)	2510 (97%)	73 (3%)	13 (0%)	29	28

All (13) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	E	16	HIS
1	F	101	GLU
1	F	104	SER
1	G	107	ASN
1	H	13	LYS
1	H	105	ARG
1	H	107	ASN
1	A	329	LEU
1	B	16	HIS
1	G	108	LEU
1	C	16	HIS
1	F	103	GLU
1	F	105	ARG

5.3.2 Protein sidechains (i)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	279/284 (98%)	272 (98%)	7 (2%)	47	57
1	B	281/284 (99%)	272 (97%)	9 (3%)	39	47
1	C	281/284 (99%)	274 (98%)	7 (2%)	47	57
1	D	284/284 (100%)	280 (99%)	4 (1%)	67	78
1	E	284/284 (100%)	275 (97%)	9 (3%)	39	47
1	F	282/284 (99%)	272 (96%)	10 (4%)	36	43
1	G	278/284 (98%)	272 (98%)	6 (2%)	52	62
1	H	283/284 (100%)	270 (95%)	13 (5%)	27	31
All	All	2252/2272 (99%)	2187 (97%)	65 (3%)	42	51

All (65) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	98	ARG
1	A	99	GLN
1	A	133	LEU
1	A	211	LYS
1	A	276	LEU
1	A	330	GLN
1	A	331	PHE
1	B	98	ARG
1	B	103	SER
1	B	106	ASN
1	B	108	LEU
1	B	194	ASP
1	B	211	LYS
1	B	276	LEU
1	B	329	LEU
1	B	330	GLN
1	C	14	GLU
1	C	15	GLU
1	C	98	ARG

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Mol	Chain	Res	Type
1	C	103	GLU
1	C	104	SER
1	C	238	TYR
1	C	276	LEU
1	D	12	LEU
1	D	223	LYS
1	D	276	LEU
1	D	310	GLU
1	E	12	LEU
1	E	72	ARG
1	E	98	ARG
1	E	100	GLN
1	E	254	SER
1	E	276	LEU
1	E	314	HIS
1	E	317	LYS
1	E	330	GLN
1	F	13	LYS
1	F	19	GLN
1	F	75	LYS
1	F	98	ARG
1	F	110	GLN
1	F	223	LYS
1	F	276	LEU
1	F	283	LYS
1	F	316	LYS
1	F	330	GLN
1	G	12	LEU
1	G	14	GLU
1	G	276	LEU
1	G	314	HIS
1	G	322	LEU
1	G	330	GLN
1	H	12	LEU
1	H	15	GLU
1	H	85	THR
1	H	98	ARG
1	H	99	GLN
1	H	101	GLU
1	H	105	ARG
1	H	148	LYS
1	H	238	TYR

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Mol	Chain	Res	Type
1	H	242	LYS
1	H	276	LEU
1	H	310	GLU
1	H	329	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (62) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	6	GLN
1	A	99	GLN
1	A	112	ASN
1	A	122	ASN
1	A	204	ASN
1	A	230	HIS
1	A	330	GLN
1	B	16	HIS
1	B	99	GLN
1	B	112	ASN
1	B	204	ASN
1	B	230	HIS
1	B	297	ASN
1	C	6	GLN
1	C	107	ASN
1	C	110	GLN
1	C	112	ASN
1	C	122	ASN
1	C	163	ASN
1	C	204	ASN
1	C	230	HIS
1	C	297	ASN
1	C	326	GLN
1	D	16	HIS
1	D	107	ASN
1	D	110	GLN
1	D	112	ASN
1	D	137	ASN
1	D	204	ASN
1	D	228	GLN
1	D	230	HIS
1	D	297	ASN
1	E	9	HIS
1	E	16	HIS

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Mol	Chain	Res	Type
1	E	107	ASN
1	E	112	ASN
1	E	204	ASN
1	E	230	HIS
1	E	326	GLN
1	F	19	GLN
1	F	99	GLN
1	F	100	GLN
1	F	112	ASN
1	F	204	ASN
1	F	225	GLN
1	F	230	HIS
1	F	326	GLN
1	G	20	ASN
1	G	107	ASN
1	G	112	ASN
1	G	204	ASN
1	G	230	HIS
1	G	297	ASN
1	H	20	ASN
1	H	99	GLN
1	H	110	GLN
1	H	112	ASN
1	H	114	ASN
1	H	204	ASN
1	H	225	GLN
1	H	230	HIS
1	H	314	HIS

5.3.3 RNA (i)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains (i)

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

8 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
2	1E4	E	401	-	54,54,54	1.63	10 (18%)	74,75,75	2.30	16 (21%)
2	1E4	C	401	-	54,54,54	1.64	10 (18%)	74,75,75	2.14	15 (20%)
2	1E4	B	401	-	54,54,54	1.67	11 (20%)	74,75,75	2.20	15 (20%)
2	1E4	F	401	-	54,54,54	1.83	14 (25%)	74,75,75	2.55	15 (20%)
2	1E4	D	401	-	54,54,54	1.80	14 (25%)	74,75,75	2.60	15 (20%)
2	1E4	H	401	-	54,54,54	1.70	13 (24%)	74,75,75	2.32	16 (21%)
2	1E4	A	401	-	54,54,54	1.58	10 (18%)	74,75,75	2.20	12 (16%)
2	1E4	G	401	-	54,54,54	1.72	13 (24%)	74,75,75	2.48	16 (21%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	1E4	E	401	-	-	17/45/45/45	0/4/4/4
2	1E4	C	401	-	-	16/45/45/45	0/4/4/4
2	1E4	B	401	-	-	19/45/45/45	0/4/4/4
2	1E4	F	401	-	-	20/45/45/45	0/4/4/4
2	1E4	D	401	-	-	15/45/45/45	0/4/4/4
2	1E4	H	401	-	-	17/45/45/45	0/4/4/4
2	1E4	A	401	-	-	16/45/45/45	0/4/4/4
2	1E4	G	401	-	-	18/45/45/45	0/4/4/4

All (95) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	F	401	1E4	C4-C5	4.45	1.47	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	401	1E4	O67-C39	4.05	1.34	1.22
2	B	401	1E4	O67-C39	3.97	1.34	1.22
2	G	401	1E4	O67-C39	3.97	1.34	1.22
2	D	401	1E4	O65-C39	-3.94	1.18	1.30
2	H	401	1E4	O67-C39	3.92	1.34	1.22
2	C	401	1E4	O65-C39	-3.87	1.18	1.30
2	D	401	1E4	O67-C39	3.86	1.34	1.22
2	F	401	1E4	O65-C39	-3.85	1.18	1.30
2	F	401	1E4	O67-C39	3.82	1.34	1.22
2	E	401	1E4	O67-C39	3.80	1.33	1.22
2	D	401	1E4	C4-C5	3.80	1.46	1.39
2	D	401	1E4	C16-C15	3.74	1.57	1.51
2	A	401	1E4	O67-C39	3.73	1.33	1.22
2	G	401	1E4	O65-C39	-3.69	1.19	1.30
2	H	401	1E4	O65-C39	-3.68	1.19	1.30
2	E	401	1E4	O65-C39	-3.65	1.19	1.30
2	B	401	1E4	O65-C39	-3.62	1.19	1.30
2	C	401	1E4	O42-C2	3.58	1.42	1.37
2	A	401	1E4	O65-C39	-3.56	1.19	1.30
2	H	401	1E4	C4-C5	3.38	1.45	1.39
2	F	401	1E4	C16-C15	3.33	1.56	1.51
2	G	401	1E4	O42-C2	3.28	1.42	1.37
2	A	401	1E4	O42-C2	3.25	1.42	1.37
2	D	401	1E4	C21-C20	3.22	1.44	1.38
2	G	401	1E4	C4-C5	3.22	1.45	1.39
2	E	401	1E4	C21-C20	3.14	1.44	1.38
2	B	401	1E4	O42-C2	3.08	1.42	1.37
2	F	401	1E4	C6-C5	2.99	1.43	1.38
2	D	401	1E4	O42-C2	2.98	1.41	1.37
2	D	401	1E4	C21-C22	2.94	1.44	1.39
2	E	401	1E4	C4-C5	2.92	1.44	1.39
2	F	401	1E4	C21-C20	2.83	1.43	1.38
2	F	401	1E4	O9-C4	2.79	1.43	1.37
2	C	401	1E4	C4-C5	2.76	1.44	1.39
2	B	401	1E4	C21-C20	2.76	1.43	1.38
2	F	401	1E4	C11-C14	2.75	1.58	1.53
2	C	401	1E4	C16-C15	2.75	1.55	1.51
2	H	401	1E4	C21-C20	2.74	1.43	1.38
2	E	401	1E4	C16-C15	2.71	1.55	1.51
2	A	401	1E4	C21-C20	2.68	1.43	1.38
2	H	401	1E4	O9-C4	2.67	1.42	1.37
2	G	401	1E4	C16-C15	2.63	1.55	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	G	401	1E4	C21-C20	2.62	1.43	1.38
2	D	401	1E4	C11-C14	2.60	1.58	1.53
2	B	401	1E4	C16-C15	2.57	1.55	1.51
2	H	401	1E4	C6-C5	2.55	1.42	1.38
2	E	401	1E4	C21-C22	2.54	1.44	1.39
2	D	401	1E4	C6-C5	2.53	1.42	1.38
2	G	401	1E4	C49-C48	2.53	1.54	1.51
2	F	401	1E4	C21-C22	2.53	1.44	1.39
2	A	401	1E4	C4-C5	2.53	1.44	1.39
2	E	401	1E4	O42-C2	2.50	1.41	1.37
2	F	401	1E4	C49-C48	2.46	1.54	1.51
2	E	401	1E4	C6-C5	2.45	1.42	1.38
2	H	401	1E4	C10-C11	2.45	1.55	1.51
2	H	401	1E4	C40-C14	2.43	1.58	1.53
2	A	401	1E4	C6-C5	2.43	1.42	1.38
2	B	401	1E4	C6-C5	2.40	1.42	1.38
2	B	401	1E4	C21-C22	2.39	1.43	1.39
2	H	401	1E4	C21-C22	2.36	1.43	1.39
2	F	401	1E4	C10-C11	2.34	1.55	1.51
2	F	401	1E4	C6-C1	2.32	1.43	1.39
2	G	401	1E4	C21-C22	2.32	1.43	1.39
2	A	401	1E4	C40-C14	2.31	1.57	1.53
2	D	401	1E4	C15-C40	2.31	1.57	1.53
2	B	401	1E4	C4-C5	2.30	1.43	1.39
2	A	401	1E4	C21-C22	2.27	1.43	1.39
2	C	401	1E4	C3-C2	2.27	1.42	1.38
2	C	401	1E4	C21-C20	2.27	1.42	1.38
2	B	401	1E4	C10-C11	2.25	1.55	1.51
2	G	401	1E4	C15-C40	2.24	1.57	1.53
2	D	401	1E4	C49-C48	2.24	1.54	1.51
2	H	401	1E4	O42-C2	2.22	1.40	1.37
2	F	401	1E4	C40-C14	2.22	1.57	1.53
2	A	401	1E4	O9-C4	2.21	1.41	1.37
2	C	401	1E4	C21-C22	2.21	1.43	1.39
2	H	401	1E4	C15-C40	2.19	1.57	1.53
2	B	401	1E4	C6-C1	2.17	1.42	1.39
2	F	401	1E4	O42-C2	2.17	1.40	1.37
2	G	401	1E4	C6-C5	2.13	1.42	1.38
2	D	401	1E4	O17-C20	2.12	1.42	1.37
2	E	401	1E4	C10-C11	2.12	1.54	1.51
2	C	401	1E4	C40-C14	2.12	1.57	1.53
2	H	401	1E4	C6-C1	2.11	1.42	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	401	1E4	O9-C4	2.10	1.41	1.37
2	G	401	1E4	C32-C31	2.10	1.42	1.38
2	G	401	1E4	C10-C11	2.09	1.54	1.51
2	E	401	1E4	C15-C40	2.08	1.57	1.53
2	A	401	1E4	C3-C2	2.08	1.42	1.38
2	D	401	1E4	C6-C1	2.08	1.42	1.39
2	B	401	1E4	C3-C2	2.07	1.42	1.38
2	H	401	1E4	C11-C14	2.07	1.57	1.53
2	G	401	1E4	C25-C24	2.05	1.41	1.37
2	C	401	1E4	C15-C40	2.02	1.57	1.53

All (120) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	D	401	1E4	O9-C4-C5	15.35	135.35	116.40
2	F	401	1E4	O9-C4-C5	14.94	134.84	116.40
2	G	401	1E4	O9-C4-C5	13.17	132.66	116.40
2	H	401	1E4	O9-C4-C5	12.68	132.06	116.40
2	E	401	1E4	O9-C4-C5	12.43	131.75	116.40
2	A	401	1E4	O9-C4-C5	12.39	131.70	116.40
2	B	401	1E4	O9-C4-C5	11.90	131.09	116.40
2	C	401	1E4	O9-C4-C5	11.80	130.97	116.40
2	D	401	1E4	C4-C5-CL4	7.36	128.07	119.43
2	F	401	1E4	C4-C5-CL4	7.32	128.03	119.43
2	D	401	1E4	O9-C4-C3	-7.18	107.06	123.58
2	F	401	1E4	O9-C4-C3	-6.80	107.95	123.58
2	G	401	1E4	C4-C5-CL4	6.56	127.13	119.43
2	G	401	1E4	O9-C4-C3	-6.11	109.52	123.58
2	H	401	1E4	C4-C5-CL4	5.97	126.44	119.43
2	E	401	1E4	C4-C5-CL4	5.89	126.34	119.43
2	C	401	1E4	C4-C5-CL4	5.82	126.26	119.43
2	A	401	1E4	C4-C5-CL4	5.79	126.23	119.43
2	A	401	1E4	O9-C4-C3	-5.72	110.42	123.58
2	E	401	1E4	O9-C4-C3	-5.71	110.45	123.58
2	H	401	1E4	O9-C4-C3	-5.62	110.66	123.58
2	B	401	1E4	C4-C5-CL4	5.45	125.82	119.43
2	B	401	1E4	O9-C4-C3	-5.42	111.13	123.58
2	C	401	1E4	O9-C4-C3	-5.34	111.29	123.58
2	G	401	1E4	C16-C15-C40	4.17	120.26	112.20
2	G	401	1E4	C34-N35-C29	4.03	123.21	117.90
2	F	401	1E4	C6-C5-CL4	-3.99	112.06	118.49
2	E	401	1E4	C16-C15-C40	3.94	119.81	112.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	D	401	1E4	C6-C5-CL4	-3.84	112.29	118.49
2	G	401	1E4	C6-C5-CL4	-3.80	112.36	118.49
2	H	401	1E4	C34-N35-C29	3.80	122.90	117.90
2	F	401	1E4	C34-N35-C29	3.79	122.90	117.90
2	C	401	1E4	C34-N35-C29	3.77	122.86	117.90
2	B	401	1E4	C34-N35-C29	3.75	122.83	117.90
2	D	401	1E4	C34-N35-C29	3.74	122.82	117.90
2	G	401	1E4	O74-C40-C15	3.68	117.70	108.81
2	H	401	1E4	C16-C15-C40	3.68	119.31	112.20
2	A	401	1E4	C34-N35-C29	3.62	122.67	117.90
2	E	401	1E4	C21-C22-C29	3.60	125.79	120.59
2	E	401	1E4	C34-N35-C29	3.59	122.63	117.90
2	H	401	1E4	C6-C5-CL4	-3.58	112.71	118.49
2	G	401	1E4	C15-C40-C14	3.54	118.01	112.47
2	D	401	1E4	C16-C15-C40	3.54	119.05	112.20
2	A	401	1E4	C6-C5-CL4	-3.51	112.83	118.49
2	E	401	1E4	C6-C5-CL4	-3.47	112.90	118.49
2	B	401	1E4	C11-C14-C40	3.46	117.87	112.47
2	C	401	1E4	C6-C5-CL4	-3.44	112.94	118.49
2	B	401	1E4	C16-C15-C40	3.42	118.81	112.20
2	H	401	1E4	C11-C14-C40	3.42	117.81	112.47
2	B	401	1E4	C15-C40-C14	3.38	117.75	112.47
2	H	401	1E4	O74-C40-C15	3.35	116.91	108.81
2	G	401	1E4	C11-C14-C40	3.30	117.62	112.47
2	A	401	1E4	C16-C15-C40	3.29	118.56	112.20
2	C	401	1E4	C16-C15-C40	3.24	118.46	112.20
2	E	401	1E4	C15-C40-C14	3.23	117.52	112.47
2	D	401	1E4	O74-C40-C15	3.22	116.60	108.81
2	A	401	1E4	O74-C40-C15	3.21	116.57	108.81
2	F	401	1E4	C31-C29-N35	-3.17	117.54	122.26
2	D	401	1E4	C31-C29-N35	-3.13	117.61	122.26
2	B	401	1E4	O74-C40-C15	3.11	116.33	108.81
2	A	401	1E4	C31-C29-N35	-3.11	117.63	122.26
2	G	401	1E4	C31-C29-N35	-3.10	117.64	122.26
2	B	401	1E4	C6-C5-CL4	-3.09	113.50	118.49
2	E	401	1E4	O74-C40-C15	3.07	116.23	108.81
2	B	401	1E4	C21-C22-C29	3.07	125.03	120.59
2	G	401	1E4	C21-C22-C29	3.06	125.02	120.59
2	D	401	1E4	C21-C22-C29	3.05	125.00	120.59
2	F	401	1E4	C21-C22-C29	3.04	124.99	120.59
2	H	401	1E4	C31-C29-N35	-3.00	117.80	122.26
2	B	401	1E4	C31-C29-N35	-2.99	117.81	122.26

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	E	401	1E4	C31-C29-N35	-2.99	117.81	122.26
2	F	401	1E4	O42-C2-C1	2.99	118.47	114.80
2	D	401	1E4	C10-O9-C4	2.98	124.89	118.27
2	C	401	1E4	O74-C40-C15	2.97	116.00	108.81
2	F	401	1E4	C43-O42-C2	-2.93	113.10	117.53
2	C	401	1E4	C31-C29-N35	-2.90	117.94	122.26
2	E	401	1E4	O42-C2-C1	2.90	118.36	114.80
2	E	401	1E4	C11-C14-C40	2.89	116.98	112.47
2	H	401	1E4	C43-O42-C2	-2.89	113.17	117.53
2	G	401	1E4	O65-C39-C33	2.86	122.26	114.85
2	H	401	1E4	C15-C40-C14	2.85	116.92	112.47
2	H	401	1E4	O65-C39-C33	2.80	122.11	114.85
2	G	401	1E4	O42-C2-C1	2.74	118.16	114.80
2	G	401	1E4	C2-C1-N47	2.72	121.54	116.66
2	H	401	1E4	O42-C2-C1	2.72	118.14	114.80
2	D	401	1E4	C11-C14-C40	2.68	116.66	112.47
2	A	401	1E4	O65-C39-C33	2.66	121.75	114.85
2	A	401	1E4	C21-C22-C29	2.66	124.44	120.59
2	H	401	1E4	C21-C22-C29	2.62	124.38	120.59
2	A	401	1E4	C11-C14-C40	2.59	116.51	112.47
2	C	401	1E4	C21-C22-C29	2.57	124.31	120.59
2	D	401	1E4	O42-C2-C1	2.50	117.87	114.80
2	E	401	1E4	O77-C15-C40	-2.41	103.23	109.10
2	C	401	1E4	C11-C14-C40	2.41	116.23	112.47
2	A	401	1E4	C15-C40-C14	2.39	116.21	112.47
2	E	401	1E4	C23-C22-C29	-2.38	117.14	120.59
2	B	401	1E4	O77-C15-C40	-2.37	103.33	109.10
2	F	401	1E4	O9-C10-C11	2.37	114.04	107.36
2	D	401	1E4	O65-C39-C33	2.34	120.91	114.85
2	C	401	1E4	O65-C39-C33	2.31	120.83	114.85
2	H	401	1E4	O67-C39-C33	-2.29	115.34	121.45
2	F	401	1E4	O74-C40-C15	2.26	114.28	108.81
2	B	401	1E4	O42-C2-C1	2.25	117.56	114.80
2	G	401	1E4	C23-C22-C29	-2.23	117.35	120.59
2	F	401	1E4	O77-C15-C40	-2.23	103.67	109.10
2	E	401	1E4	O67-C39-C33	-2.22	115.54	121.45
2	B	401	1E4	O65-C39-C33	2.19	120.53	114.85
2	H	401	1E4	O9-C10-C11	2.17	113.49	107.36
2	E	401	1E4	O65-C39-C33	2.17	120.48	114.85
2	G	401	1E4	O67-C39-C33	-2.14	115.74	121.45
2	C	401	1E4	C15-C40-C14	2.12	115.78	112.47
2	D	401	1E4	C4-C3-C2	2.11	123.15	118.97

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	F	401	1E4	O65-C39-C33	2.09	120.28	114.85
2	F	401	1E4	C10-O9-C4	2.09	122.92	118.27
2	C	401	1E4	O42-C2-C1	2.08	117.35	114.80
2	C	401	1E4	O9-C10-C11	2.08	113.22	107.36
2	B	401	1E4	C23-C22-C29	-2.07	117.59	120.59
2	D	401	1E4	C23-C22-C29	-2.04	117.64	120.59
2	F	401	1E4	C4-C3-C2	2.03	123.00	118.97
2	C	401	1E4	C58-N59-C54	2.03	119.34	117.06

There are no chirality outliers.

All (138) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	401	1E4	O9-C10-C11-C14
2	A	401	1E4	O9-C10-C11-O71
2	A	401	1E4	C11-C14-C40-C15
2	A	401	1E4	C11-C14-C40-O74
2	A	401	1E4	O75-C14-C40-C15
2	A	401	1E4	O75-C14-C40-O74
2	A	401	1E4	C49-C48-N47-C1
2	B	401	1E4	O9-C10-C11-C14
2	B	401	1E4	O9-C10-C11-O71
2	B	401	1E4	C11-C14-C40-C15
2	B	401	1E4	C11-C14-C40-O74
2	B	401	1E4	O75-C14-C40-C15
2	B	401	1E4	C40-C15-C16-O17
2	B	401	1E4	O77-C15-C16-O17
2	C	401	1E4	O9-C10-C11-C14
2	C	401	1E4	O9-C10-C11-O71
2	C	401	1E4	C11-C14-C40-C15
2	C	401	1E4	C11-C14-C40-O74
2	C	401	1E4	O75-C14-C40-C15
2	C	401	1E4	O75-C14-C40-O74
2	C	401	1E4	C49-C48-N47-C1
2	D	401	1E4	C5-C4-O9-C10
2	D	401	1E4	C11-C14-C40-O74
2	D	401	1E4	O75-C14-C40-C15
2	D	401	1E4	O75-C14-C40-O74
2	E	401	1E4	O9-C10-C11-C14
2	E	401	1E4	O9-C10-C11-O71
2	E	401	1E4	C11-C14-C40-C15
2	E	401	1E4	C11-C14-C40-O74

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Mol	Chain	Res	Type	Atoms
2	E	401	1E4	O75-C14-C40-C15
2	E	401	1E4	O75-C14-C40-O74
2	F	401	1E4	C5-C4-O9-C10
2	F	401	1E4	O9-C10-C11-C14
2	F	401	1E4	O9-C10-C11-O71
2	F	401	1E4	C11-C14-C40-O74
2	F	401	1E4	O75-C14-C40-O74
2	F	401	1E4	C16-C15-C40-C14
2	F	401	1E4	C16-C15-C40-O74
2	F	401	1E4	O77-C15-C40-C14
2	G	401	1E4	C5-C4-O9-C10
2	G	401	1E4	C11-C14-C40-C15
2	G	401	1E4	O75-C14-C40-C15
2	G	401	1E4	N47-C48-C49-S51
2	G	401	1E4	C48-C49-S51-C54
2	H	401	1E4	O9-C10-C11-C14
2	H	401	1E4	O9-C10-C11-O71
2	H	401	1E4	C11-C14-C40-C15
2	H	401	1E4	C11-C14-C40-O74
2	H	401	1E4	O75-C14-C40-C15
2	H	401	1E4	C49-C48-N47-C1
2	D	401	1E4	C3-C4-O9-C10
2	F	401	1E4	C3-C4-O9-C10
2	H	401	1E4	C1-C2-O42-C43
2	A	401	1E4	O50-C48-N47-C1
2	C	401	1E4	O50-C48-N47-C1
2	H	401	1E4	O50-C48-N47-C1
2	B	401	1E4	O50-C48-N47-C1
2	F	401	1E4	C1-C2-O42-C43
2	E	401	1E4	C34-C33-C39-O65
2	F	401	1E4	O77-C15-C40-O74
2	E	401	1E4	O50-C48-N47-C1
2	F	401	1E4	C3-C2-O42-C43
2	H	401	1E4	C3-C2-O42-C43
2	B	401	1E4	O75-C14-C40-O74
2	H	401	1E4	O75-C14-C40-O74
2	A	401	1E4	C5-C4-O9-C10
2	E	401	1E4	C32-C33-C39-O65
2	E	401	1E4	C1-C2-O42-C43
2	F	401	1E4	O75-C14-C40-C15
2	D	401	1E4	O50-C48-N47-C1
2	D	401	1E4	C11-C14-C40-C15

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Mol	Chain	Res	Type	Atoms
2	H	401	1E4	C32-C33-C39-O67
2	H	401	1E4	C34-C33-C39-O67
2	F	401	1E4	C21-C20-O17-C16
2	F	401	1E4	C25-C20-O17-C16
2	G	401	1E4	C11-C14-C40-O74
2	C	401	1E4	C5-C4-O9-C10
2	A	401	1E4	C21-C20-O17-C16
2	B	401	1E4	C21-C20-O17-C16
2	D	401	1E4	C21-C20-O17-C16
2	B	401	1E4	C16-C15-C40-O74
2	E	401	1E4	C3-C2-O42-C43
2	G	401	1E4	C21-C20-O17-C16
2	D	401	1E4	C34-C33-C39-O65
2	A	401	1E4	C25-C20-O17-C16
2	B	401	1E4	C25-C20-O17-C16
2	C	401	1E4	C21-C20-O17-C16
2	D	401	1E4	C25-C20-O17-C16
2	B	401	1E4	O77-C15-C40-O74
2	D	401	1E4	C32-C33-C39-O65
2	G	401	1E4	C25-C20-O17-C16
2	E	401	1E4	C21-C20-O17-C16
2	F	401	1E4	O50-C48-N47-C1
2	C	401	1E4	C25-C20-O17-C16
2	H	401	1E4	C21-C20-O17-C16
2	E	401	1E4	C25-C20-O17-C16
2	H	401	1E4	C25-C20-O17-C16
2	G	401	1E4	O77-C15-C16-O17
2	H	401	1E4	C5-C4-O9-C10
2	D	401	1E4	O77-C15-C40-C14
2	B	401	1E4	C3-C4-O9-C10
2	B	401	1E4	C5-C4-O9-C10
2	E	401	1E4	C5-C4-O9-C10
2	H	401	1E4	C3-C4-O9-C10
2	E	401	1E4	C49-C48-N47-C1
2	E	401	1E4	C3-C4-O9-C10
2	D	401	1E4	O9-C10-C11-C14
2	G	401	1E4	C40-C15-C16-O17
2	G	401	1E4	C16-C15-C40-O74
2	D	401	1E4	C16-C15-C40-C14
2	G	401	1E4	O75-C14-C40-O74
2	G	401	1E4	O77-C15-C40-O74
2	F	401	1E4	C32-C33-C39-O65

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Mol	Chain	Res	Type	Atoms
2	C	401	1E4	C32-C33-C39-O65
2	A	401	1E4	C16-C15-C40-C14
2	C	401	1E4	C3-C4-O9-C10
2	G	401	1E4	C2-C1-N47-C48
2	G	401	1E4	C3-C4-O9-C10
2	B	401	1E4	C16-C15-C40-C14
2	C	401	1E4	C16-C15-C40-C14
2	C	401	1E4	C34-C33-C39-O65
2	C	401	1E4	O77-C15-C40-C14
2	A	401	1E4	C3-C4-O9-C10
2	F	401	1E4	C34-C33-C39-O65
2	A	401	1E4	O77-C15-C40-C14
2	G	401	1E4	O50-C48-C49-S51
2	B	401	1E4	C49-C48-N47-C1
2	B	401	1E4	C32-C33-C39-O65
2	F	401	1E4	O77-C15-C16-O17
2	G	401	1E4	C6-C1-N47-C48
2	B	401	1E4	C34-C33-C39-O65
2	A	401	1E4	C32-C33-C39-O65
2	H	401	1E4	C48-C49-S51-C54
2	F	401	1E4	C11-C14-C40-C15
2	G	401	1E4	C16-C15-C40-C14
2	A	401	1E4	C34-C33-C39-O65
2	D	401	1E4	O9-C10-C11-O71
2	E	401	1E4	O77-C15-C16-O17

There are no ring outliers.

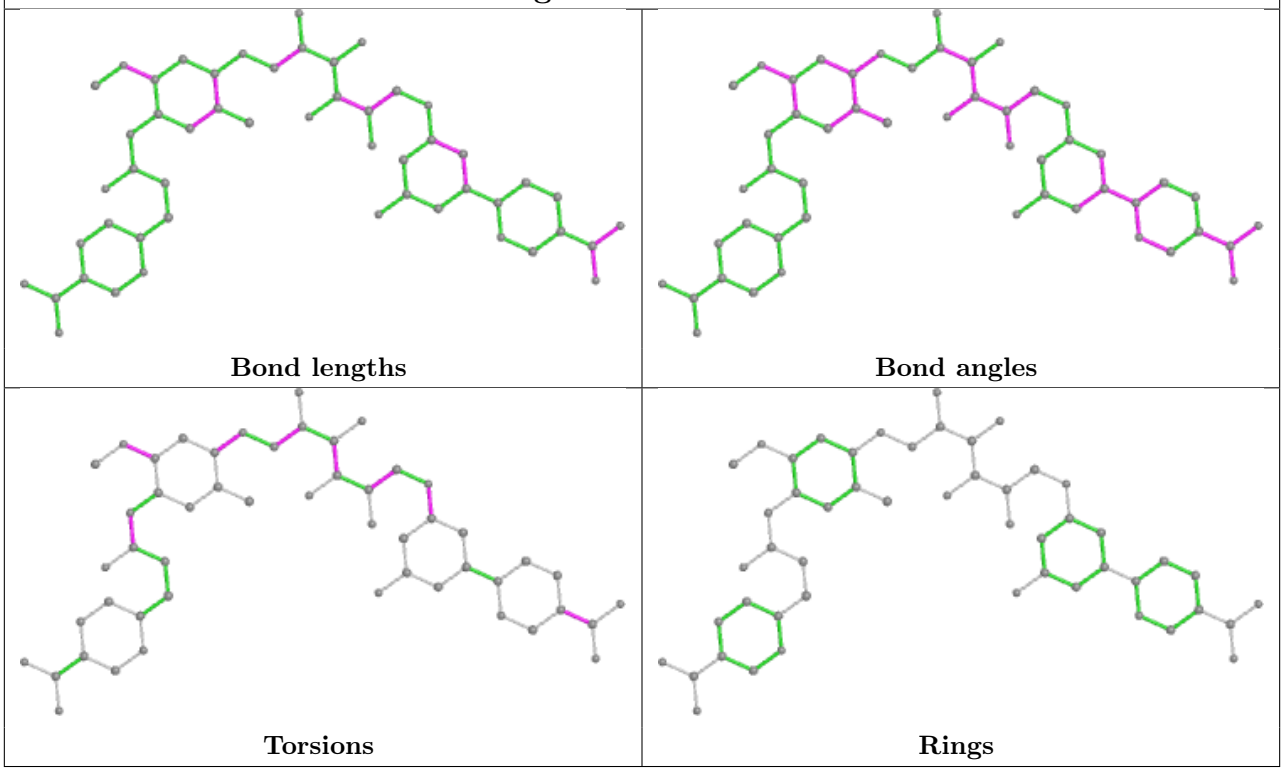
8 monomers are involved in 47 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	E	401	1E4	6	0
2	C	401	1E4	8	0
2	B	401	1E4	6	0
2	F	401	1E4	4	0
2	D	401	1E4	4	0
2	H	401	1E4	6	0
2	A	401	1E4	5	0
2	G	401	1E4	8	0

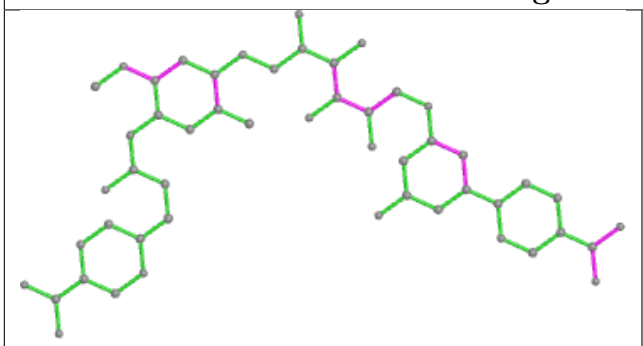
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will

also be included. For torsion angles, if less then 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

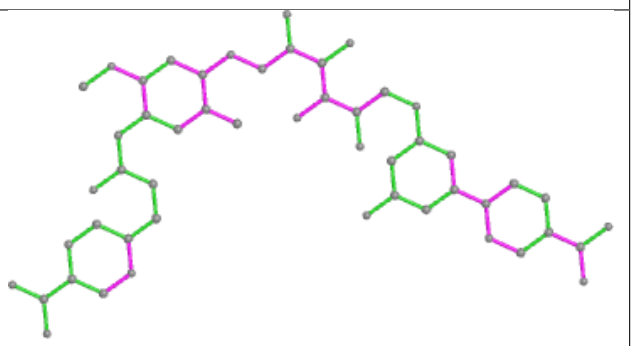
Ligand 1E4 E 401



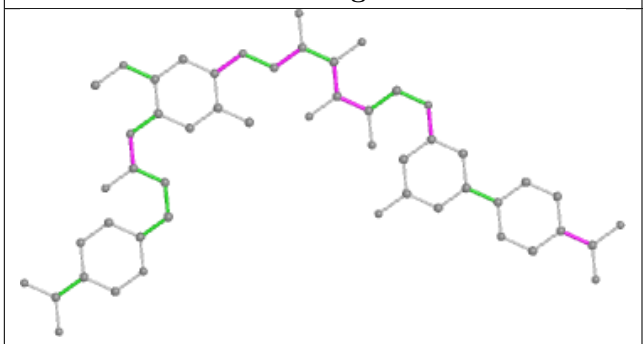
Ligand 1E4 C 401



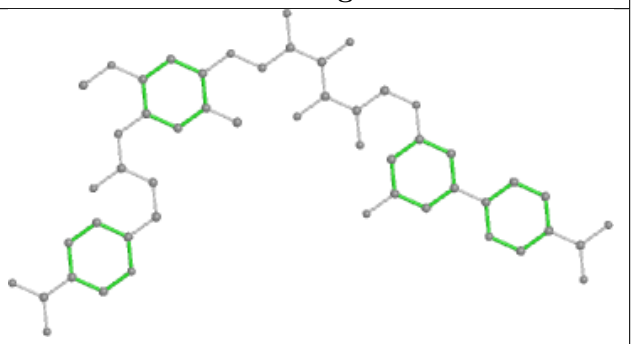
Bond lengths



Bond angles

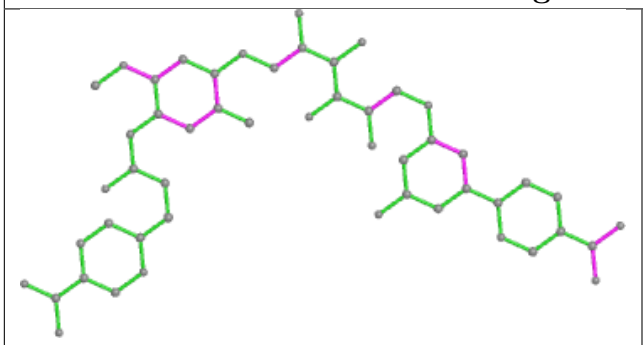


Torsions

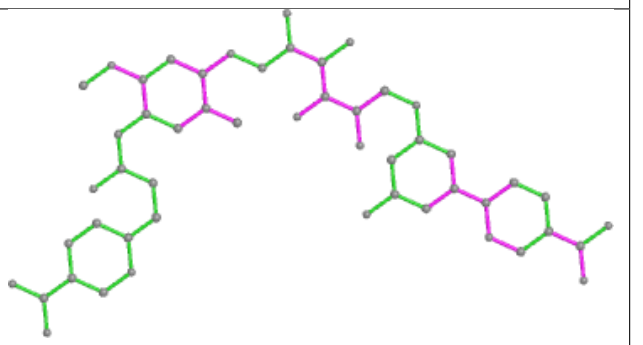


Rings

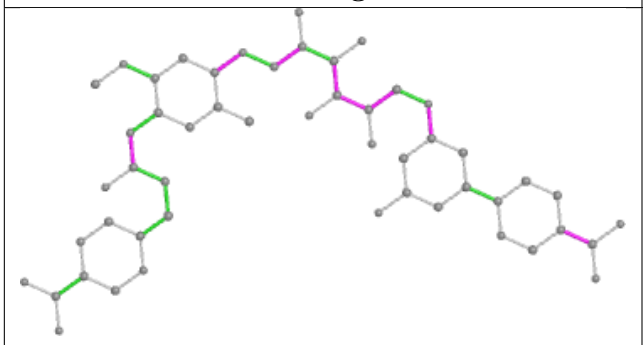
Ligand 1E4 B 401



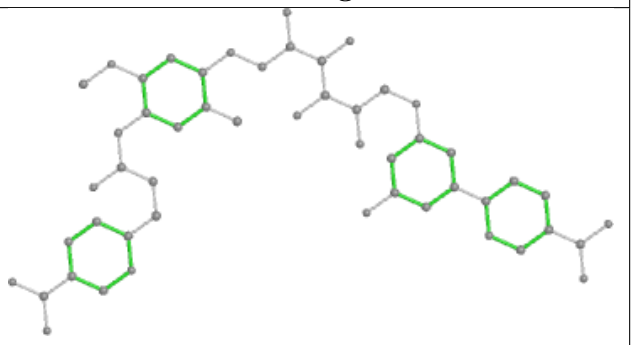
Bond lengths



Bond angles

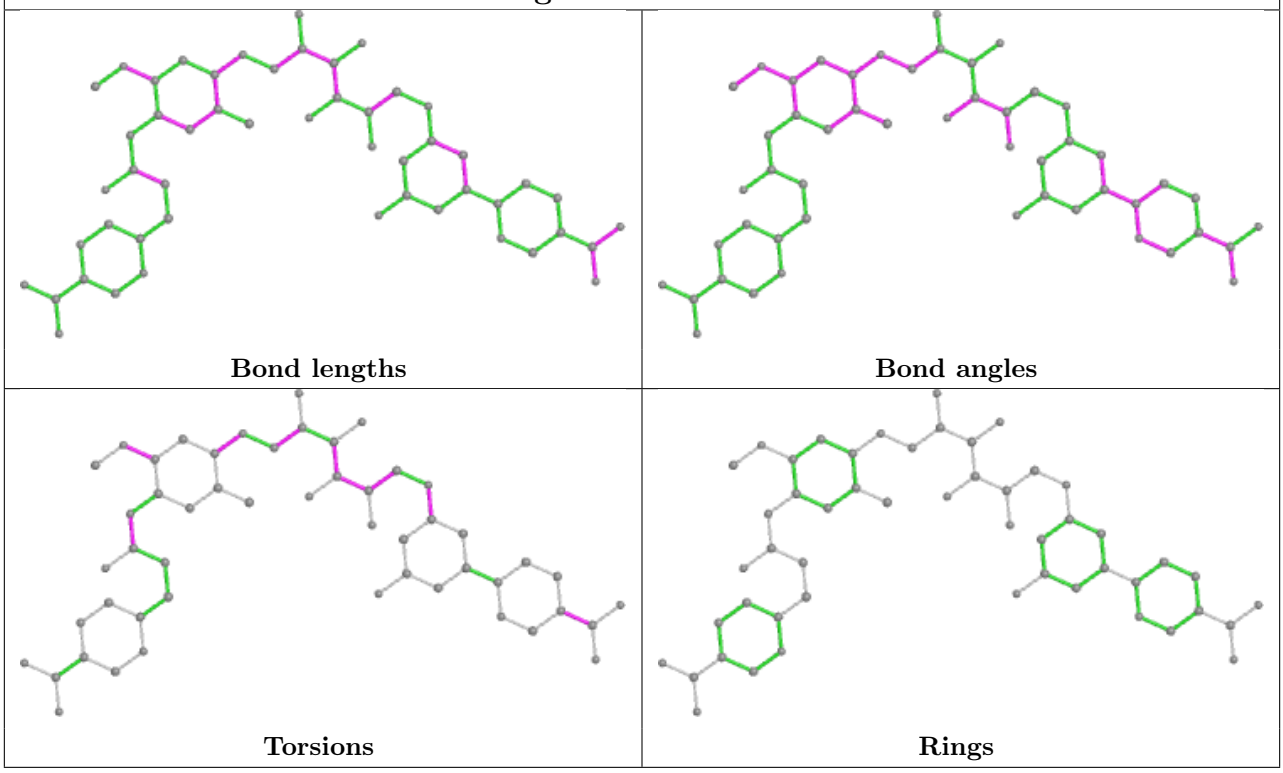


Torsions

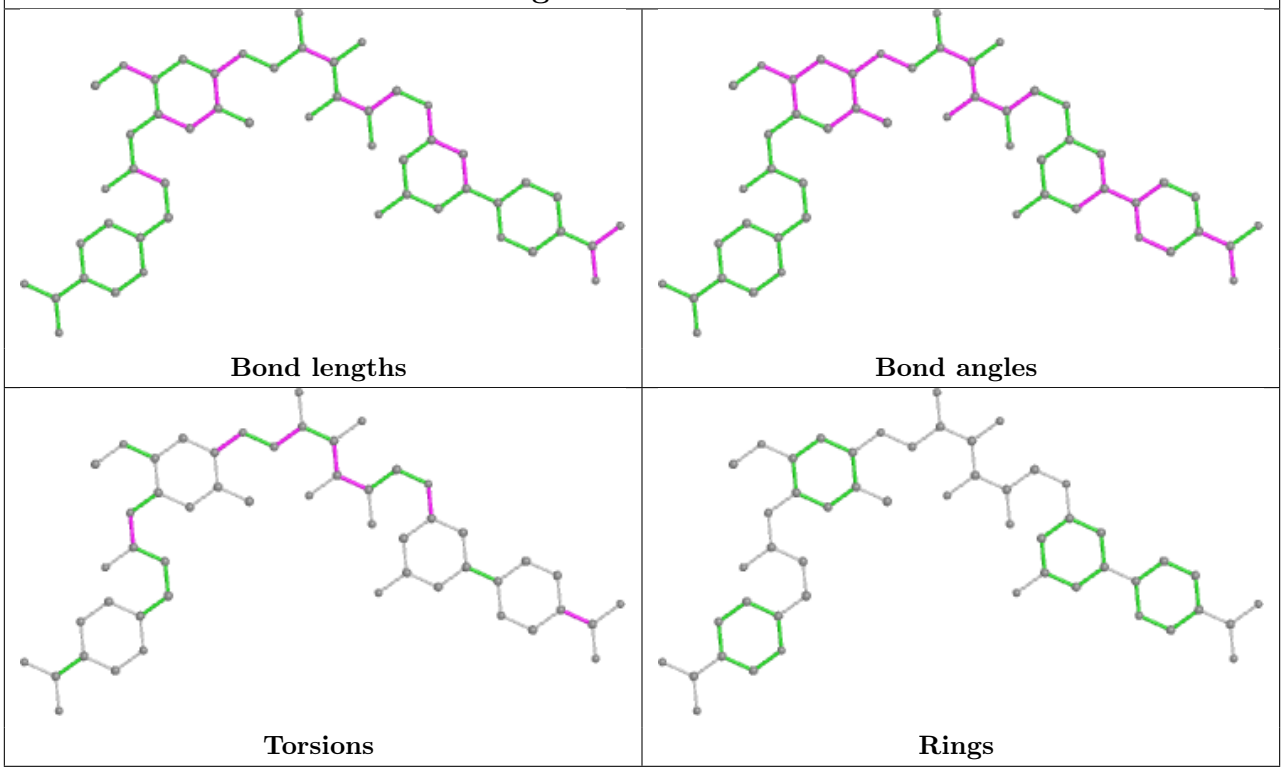


Rings

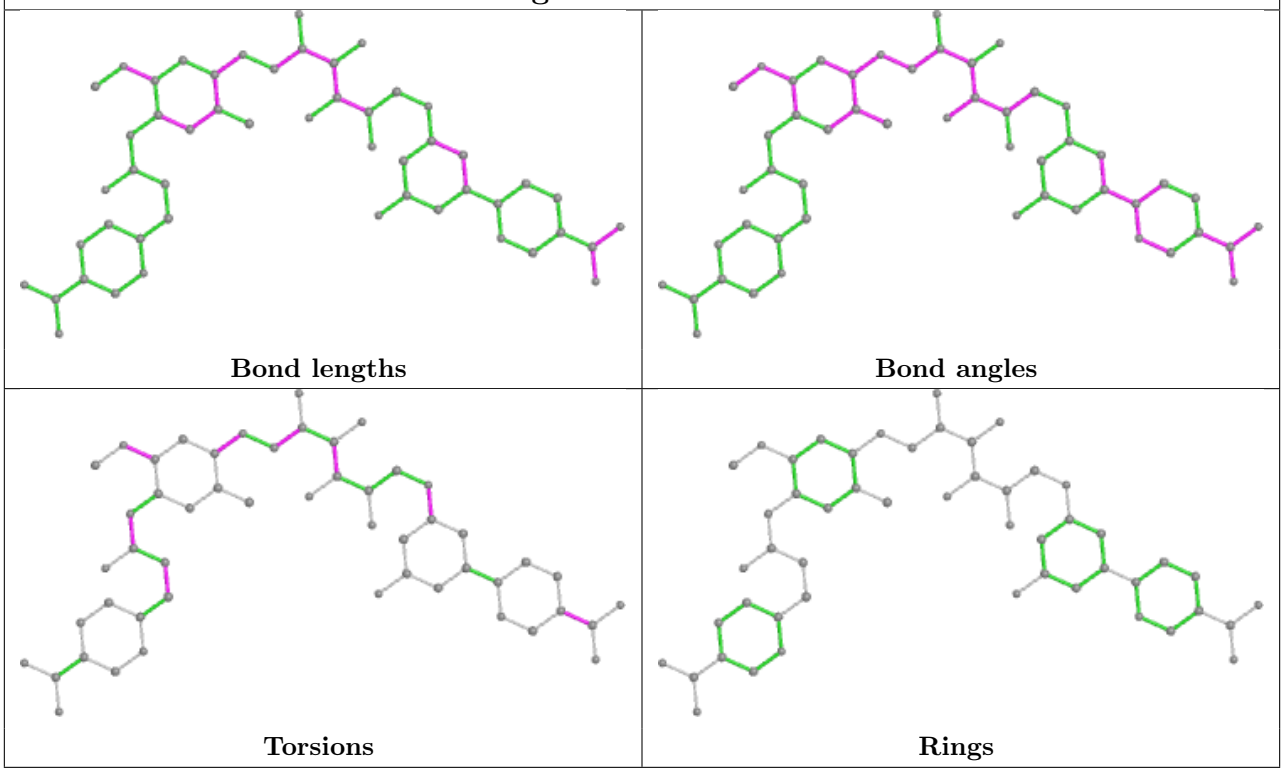
Ligand 1E4 F 401



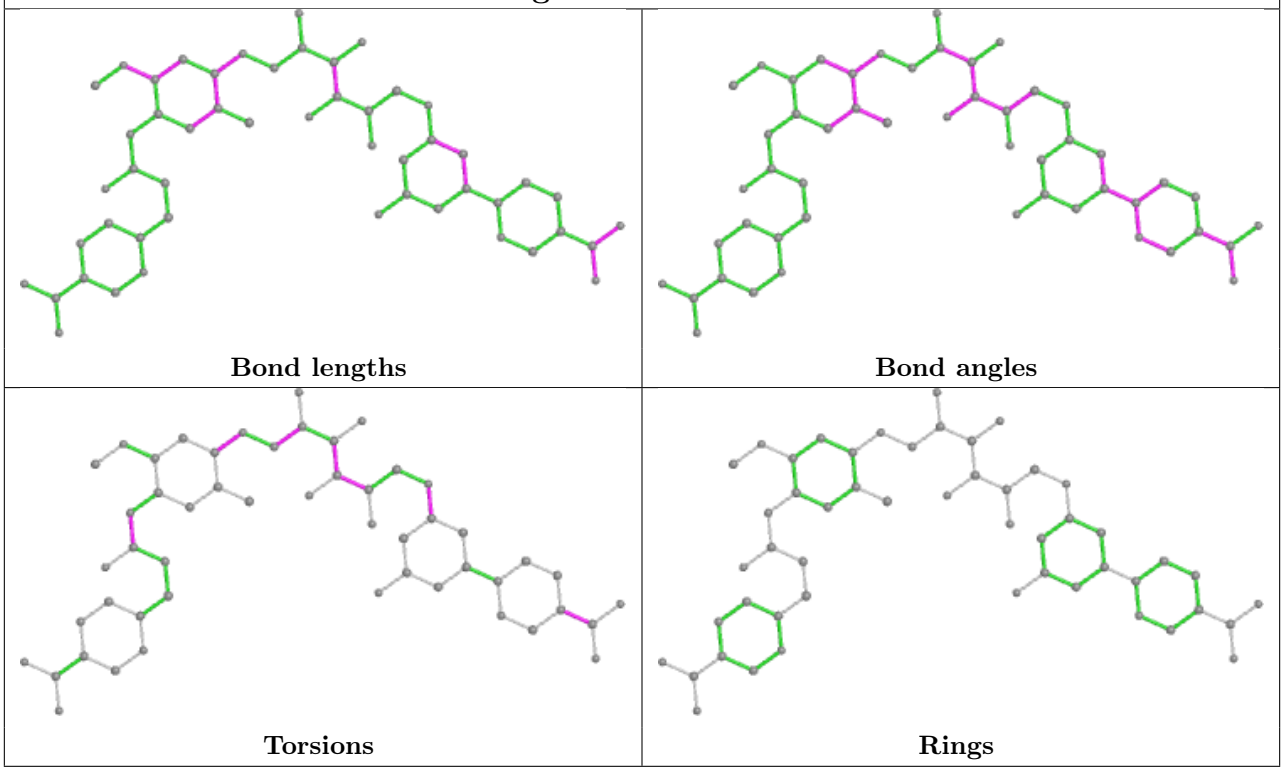
Ligand 1E4 D 401



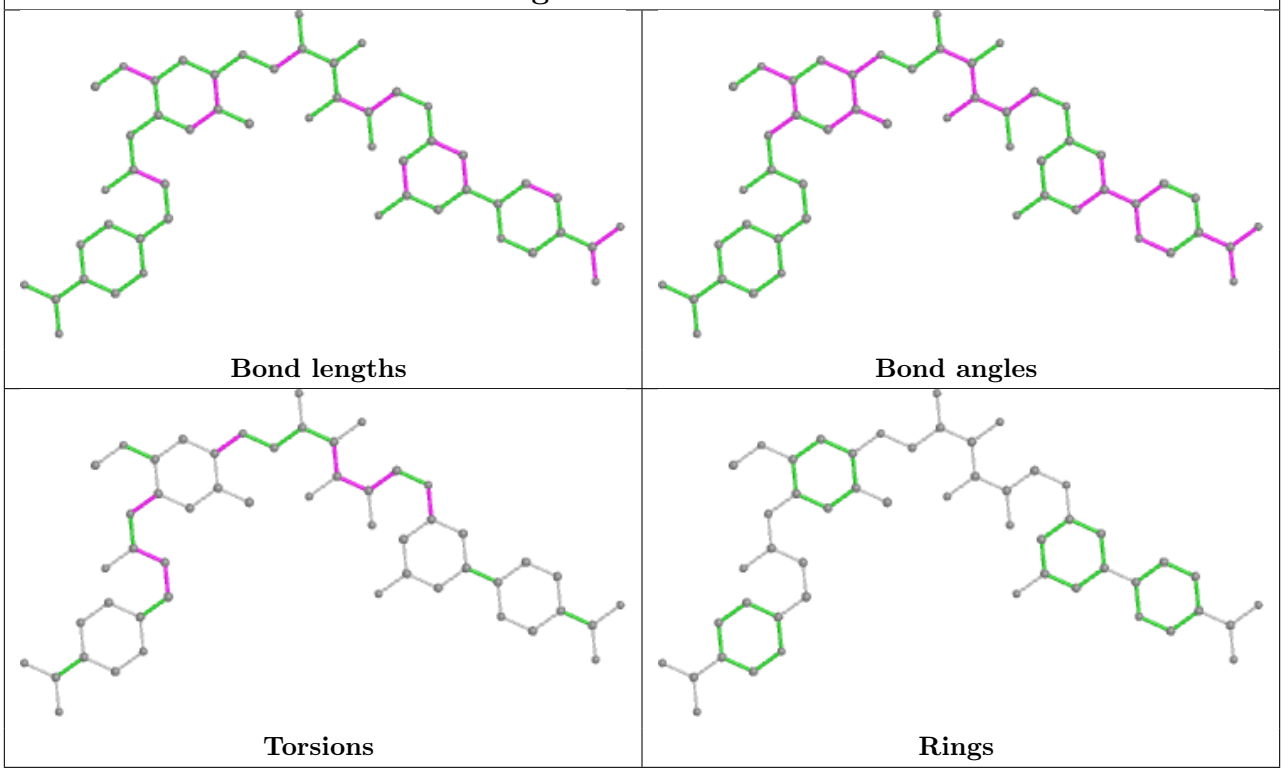
Ligand 1E4 H 401



Ligand 1E4 A 401



Ligand 1E4 G 401



5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data (i)

6.1 Protein, DNA and RNA chains (i)

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled 'Q< 0.9' lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
1	A	325/331 (98%)	-0.11	8 (2%)	57	58	22, 31, 48, 77	1 (0%)
1	B	327/331 (98%)	-0.13	12 (3%)	41	42	22, 30, 52, 74	1 (0%)
1	C	328/331 (99%)	0.06	11 (3%)	45	46	24, 35, 57, 82	1 (0%)
1	D	331/331 (100%)	-0.06	8 (2%)	59	59	23, 33, 52, 80	1 (0%)
1	E	331/331 (100%)	0.17	13 (3%)	39	40	26, 38, 63, 81	1 (0%)
1	F	329/331 (99%)	0.08	14 (4%)	35	36	24, 36, 60, 87	1 (0%)
1	G	324/331 (97%)	-0.10	10 (3%)	49	50	23, 32, 50, 80	1 (0%)
1	H	329/331 (99%)	-0.00	14 (4%)	35	36	23, 32, 54, 85	1 (0%)
All	All	2624/2648 (99%)	-0.01	90 (3%)	45	46	22, 33, 57, 87	8 (0%)

All (90) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	H	12	LEU	7.6
1	F	103	GLU	6.6
1	H	105	ARG	6.1
1	E	15	GLU	5.8
1	C	102	GLY	5.7
1	B	16	HIS	5.6
1	A	106	LEU	5.4
1	A	98	ARG	5.2
1	H	16	HIS	5.0
1	B	12	LEU	4.9
1	C	14	GLU	4.8
1	D	12	LEU	4.7
1	G	14	GLU	4.7
1	F	2	ALA	4.6
1	C	15	GLU	4.6
1	E	100	GLN	4.4

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Mol	Chain	Res	Type	RSRZ
1	G	12	LEU	4.4
1	C	238	TYR	4.4
1	E	12	LEU	4.4
1	C	12	LEU	4.4
1	D	100	GLN	4.4
1	H	238	TYR	4.4
1	D	101	GLU	4.3
1	D	221	ALA	4.3
1	F	102	GLY	4.3
1	E	98	ARG	4.2
1	E	99	GLN	4.2
1	F	12	LEU	4.2
1	C	16	HIS	4.1
1	F	98	ARG	4.1
1	H	100	GLN	4.1
1	H	221	ALA	3.9
1	H	99	GLN	3.9
1	F	13	LYS	3.9
1	F	17	VAL	3.8
1	H	104	SER	3.7
1	D	15	GLU	3.7
1	C	98	ARG	3.5
1	G	107	ASN	3.5
1	A	16	HIS	3.5
1	F	323	TRP	3.5
1	H	106	LEU	3.4
1	B	98	ARG	3.3
1	G	105	ARG	3.3
1	A	15	GLU	3.2
1	C	103	GLU	3.2
1	H	101	GLU	3.2
1	C	107	ASN	3.1
1	B	99	GLN	3.1
1	H	107	ASN	3.0
1	F	14	GLU	3.0
1	H	98	ARG	3.0
1	A	12	LEU	2.8
1	F	221	ALA	2.7
1	B	223	LYS	2.7
1	B	104	ARG	2.6
1	E	218	GLY	2.6
1	F	104	SER	2.6

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Mol	Chain	Res	Type	RSRZ
1	E	223	LYS	2.6
1	E	1	ALA	2.6
1	A	99	GLN	2.5
1	D	98	ARG	2.5
1	F	100	GLN	2.5
1	F	223	LYS	2.5
1	A	107	ASN	2.5
1	E	14	GLU	2.5
1	E	216	GLU	2.5
1	B	238	TYR	2.4
1	C	1	ALA	2.4
1	G	106	LEU	2.4
1	B	221	ALA	2.4
1	B	13	LYS	2.3
1	H	97	ALA	2.3
1	A	331	PHE	2.3
1	G	238	TYR	2.3
1	E	16	HIS	2.3
1	B	1	ALA	2.2
1	E	13	LYS	2.2
1	G	331	PHE	2.2
1	D	1	ALA	2.2
1	G	15	GLU	2.2
1	H	1	ALA	2.2
1	E	217	LEU	2.1
1	F	80	LYS	2.1
1	G	16	HIS	2.1
1	B	105	LEU	2.0
1	C	97	ALA	2.0
1	D	40	MET	2.0
1	B	216	GLU	2.0
1	G	223	LYS	2.0

6.2 Non-standard residues in protein, DNA, RNA chains (i)

There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates (i)

There are no monosaccharides in this entry.

6.4 Ligands (i)

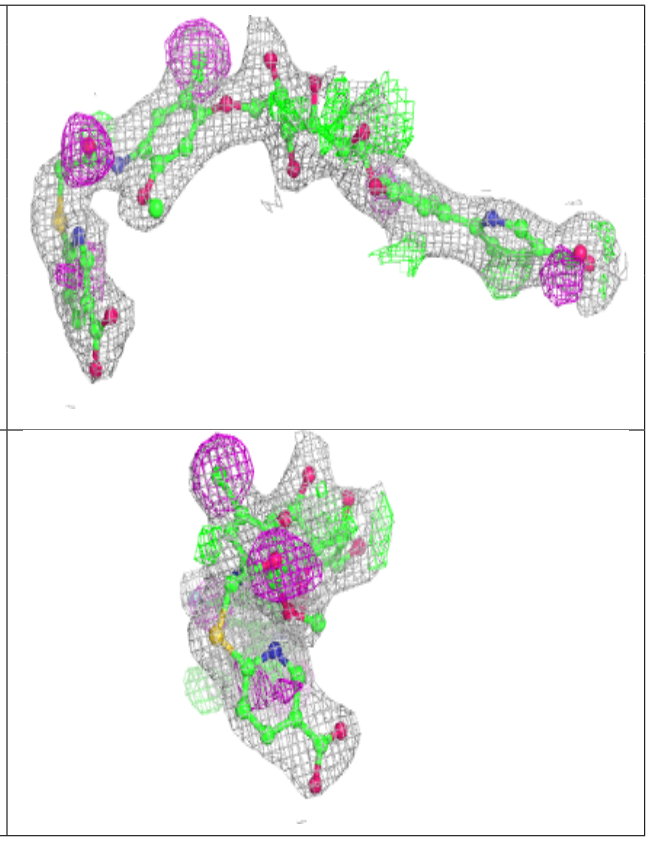
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

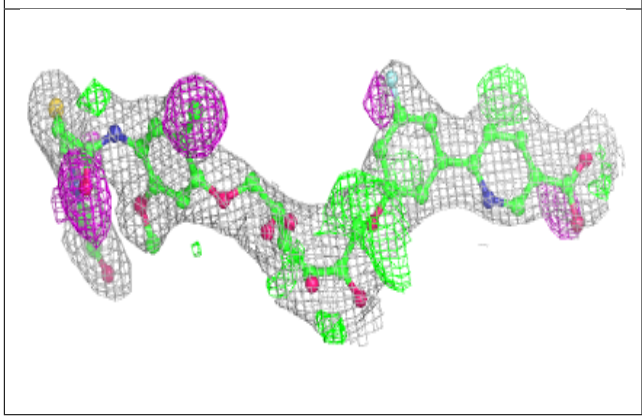
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	1E4	G	401	51/51	0.73	0.24	23,48,53,60	0
2	1E4	A	401	51/51	0.75	0.23	22,45,52,56	0
2	1E4	H	401	51/51	0.77	0.23	22,45,55,58	0
2	1E4	B	401	51/51	0.78	0.22	14,43,53,57	0
2	1E4	C	401	51/51	0.78	0.20	27,47,52,55	0
2	1E4	F	401	51/51	0.80	0.20	30,47,57,63	0
2	1E4	E	401	51/51	0.81	0.21	28,48,53,58	0
2	1E4	D	401	51/51	0.83	0.19	25,47,52,53	0

The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

Electron density around 1E4 G 401:

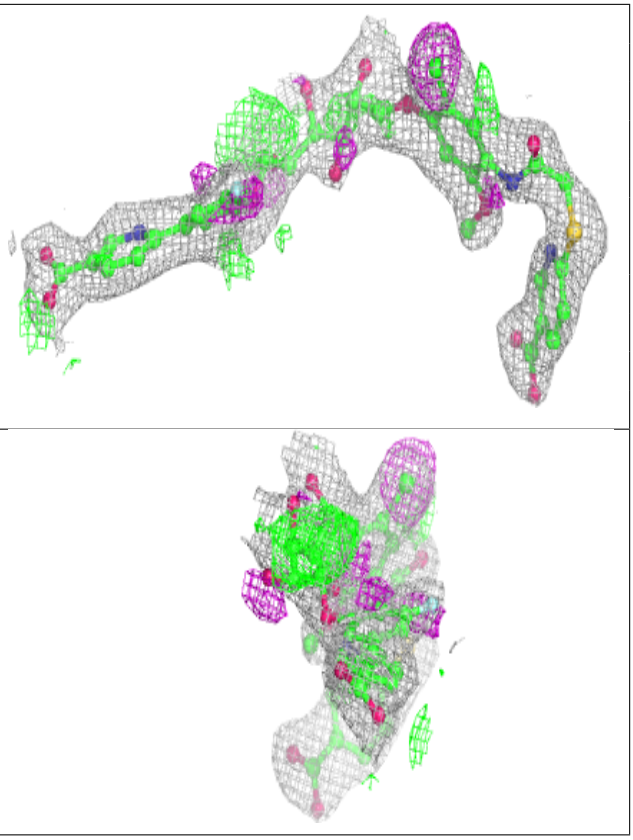
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)





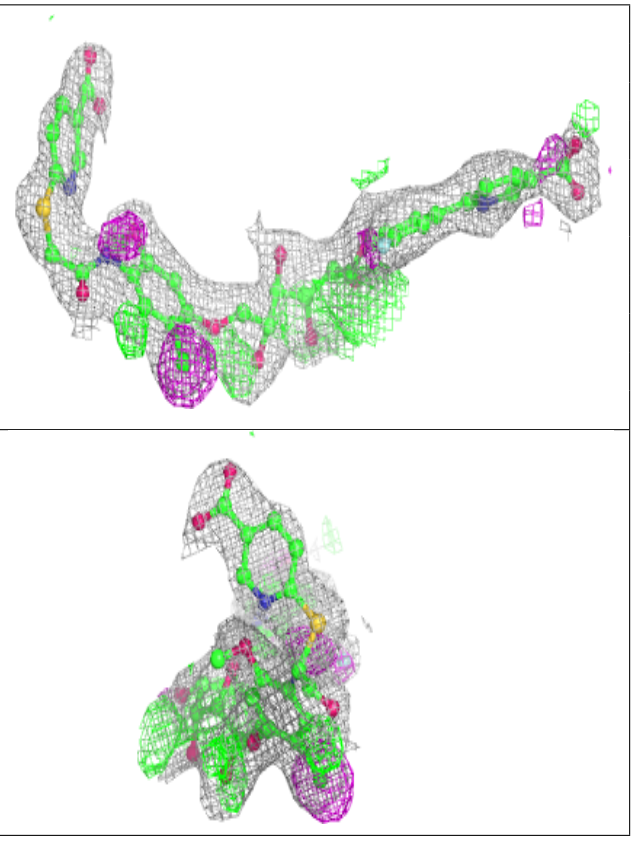
Electron density around 1E4 A 401:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



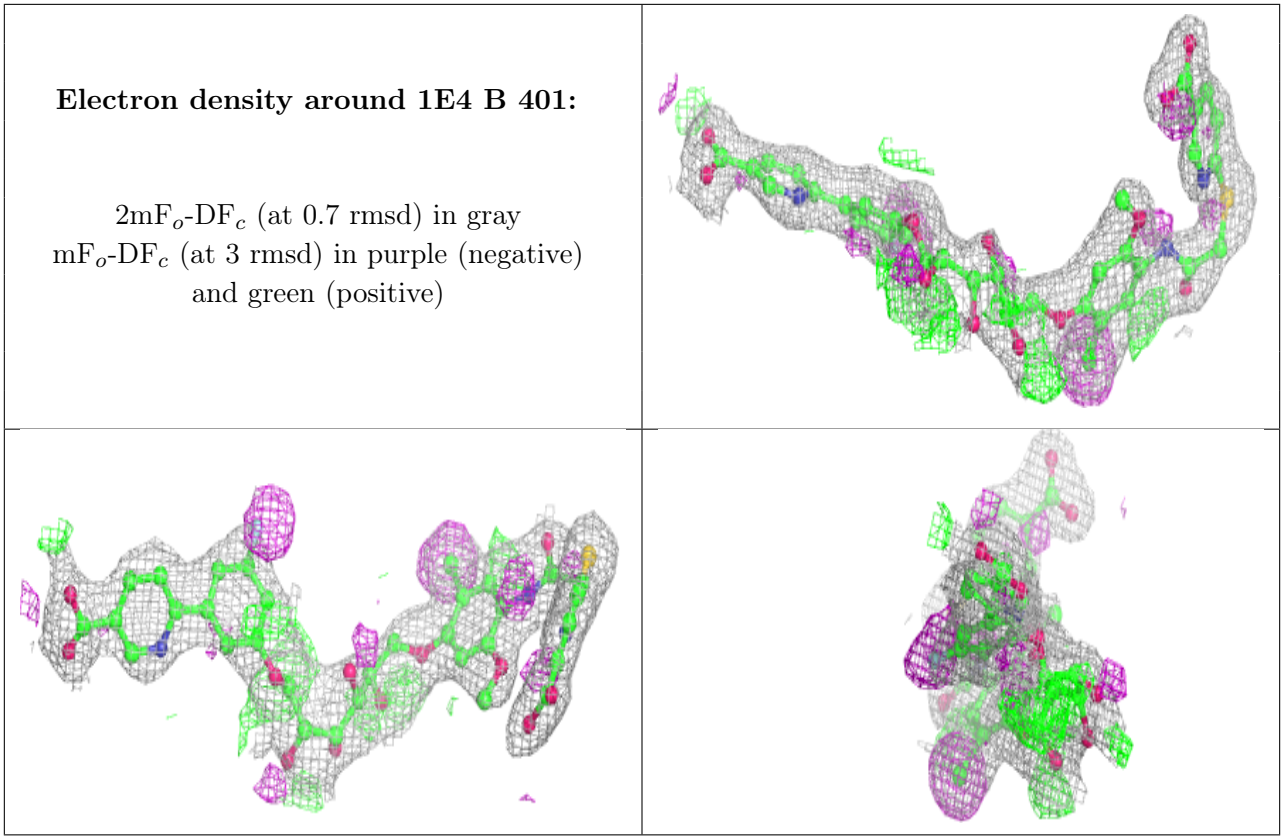
Electron density around 1E4 H 401:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



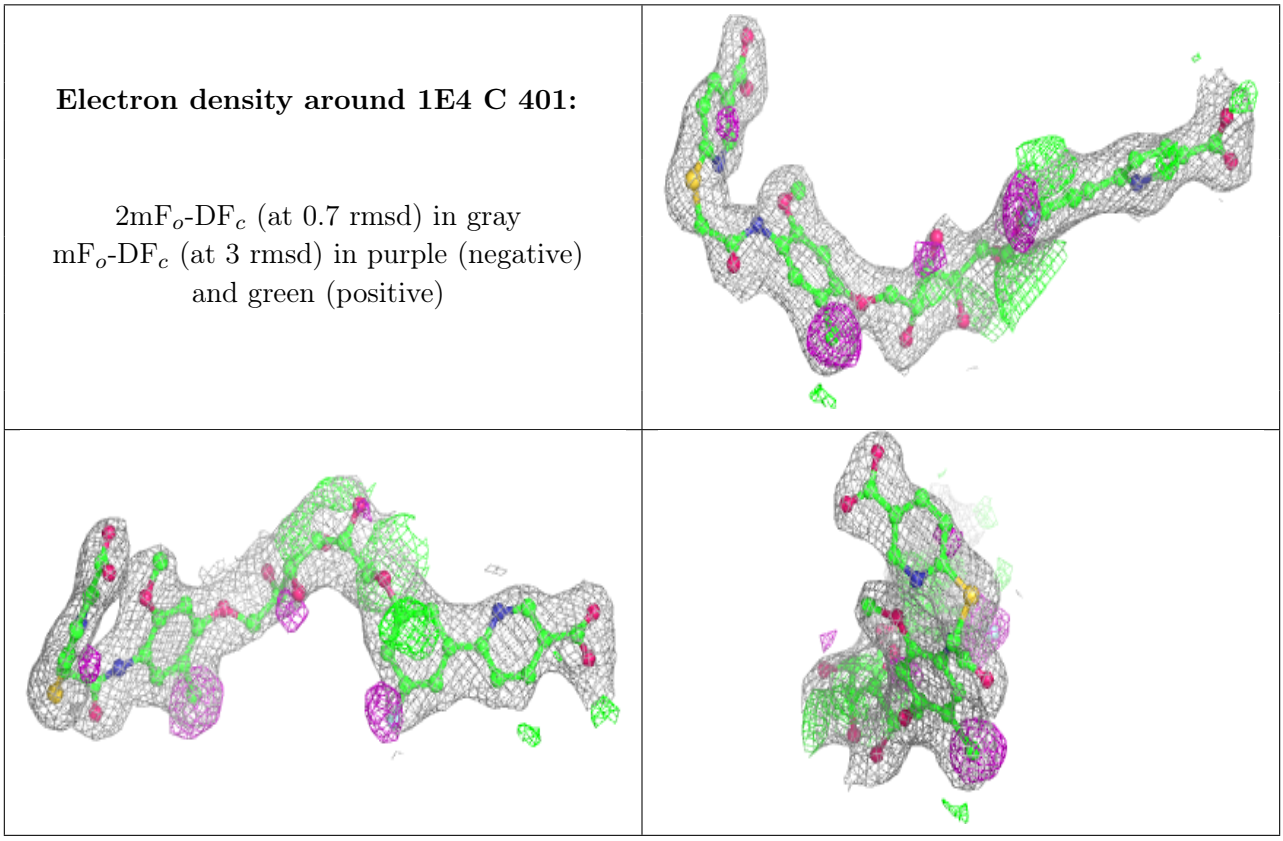
Electron density around 1E4 B 401:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



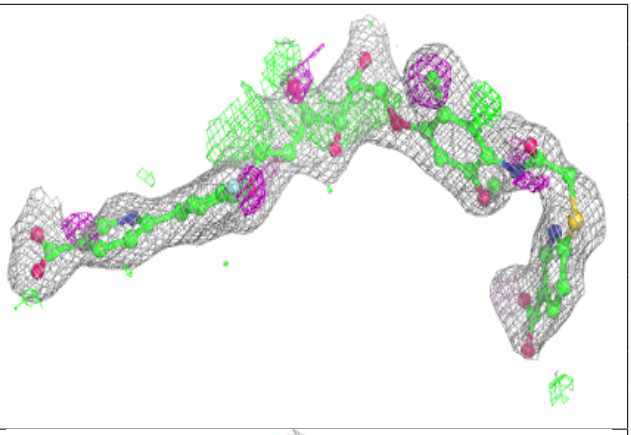
Electron density around 1E4 C 401:

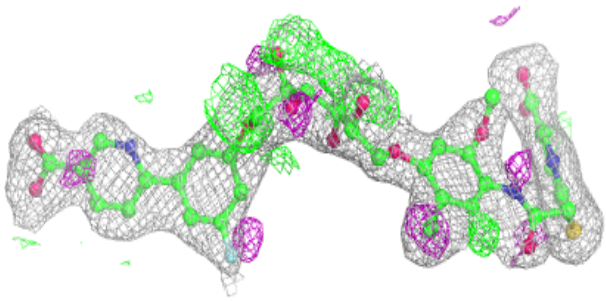
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

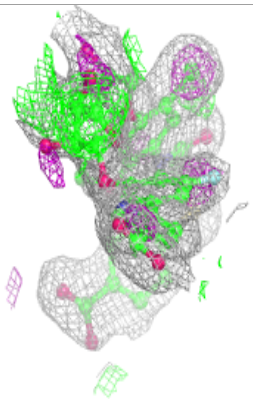


Electron density around 1E4 F 401:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

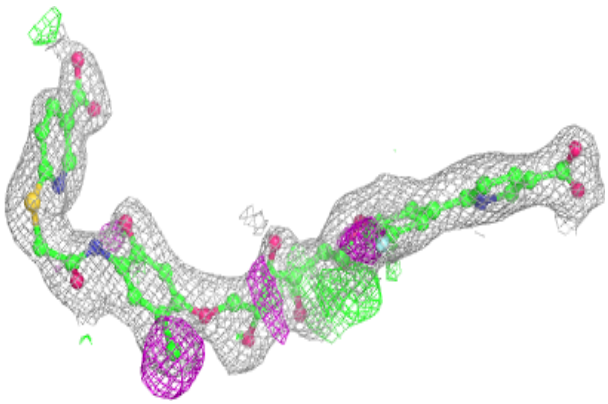


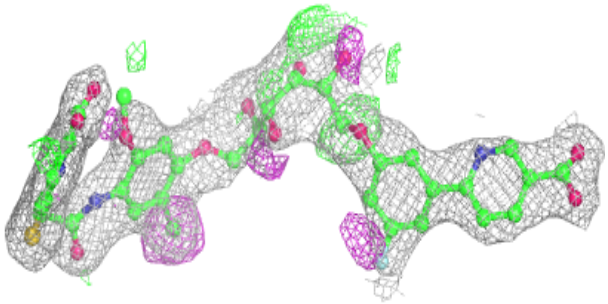


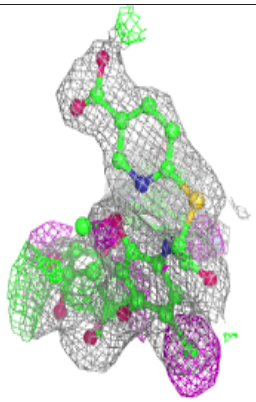


Electron density around 1E4 E 401:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

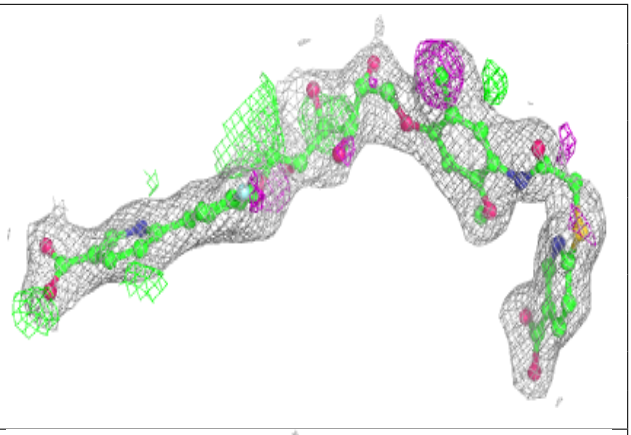


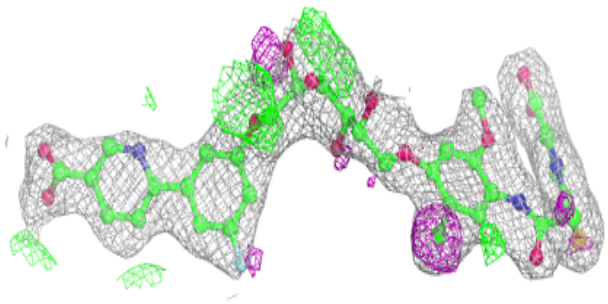


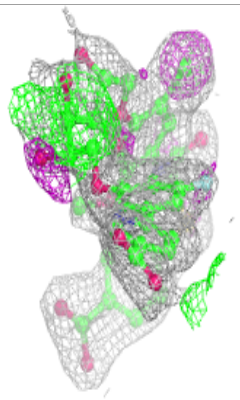


Electron density around 1E4 D 401:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)







6.5 Other polymers (i)

There are no such residues in this entry.