Full wwPDB X-ray Structure Validation Report ⓘ

Apr 30, 2024 – 07:25 pm BST

PDB ID	:	4UR3
Title	:	Crystal structure of the PCE reductive dehalogenase from S. multivorans P2(1) crystal form
Authors	:	Bommer, M.; Kunze, C.; Fesseler, J.; Schubert, T.; Diekert, G.; Dobbek, H.
Deposited on	:	2014-06-25
Resolution	:	2.23 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 ⓘ 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 ⓘ) were used in the production of this report:

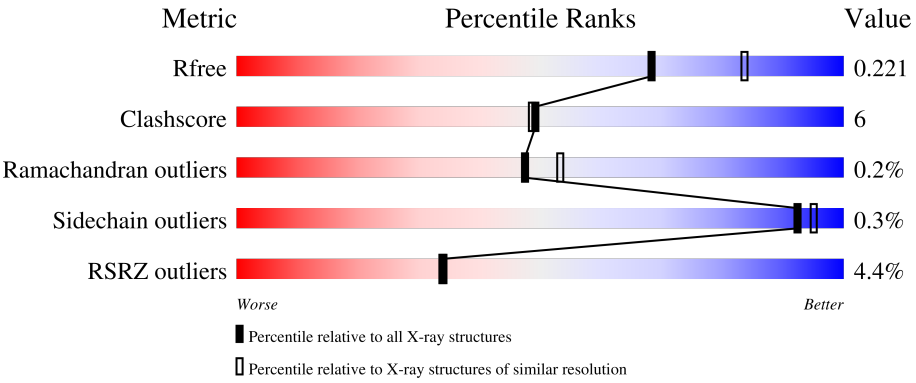
MolProbity	:	4.02b-467
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36.2
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36.2

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 2.23 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	2391 (2.26-2.22)
Clashscore	141614	2539 (2.26-2.22)
Ramachandran outliers	138981	2489 (2.26-2.22)
Sidechain outliers	138945	2490 (2.26-2.22)
RSRZ outliers	127900	2353 (2.26-2.22)

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	464	3% 87% 11%
1	B	464	7% 84% 9% 6%
1	C	464	% 85% 11% 5%
1	D	464	4% 83% 11% 6%
1	E	464	7% 76% 17% 6%

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Mol	Chain	Length	Quality of chain
1	F	464	3% 80% 12% 8%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	BVQ	A	503	X	-	-	-
3	BVQ	B	503	X	-	-	-
3	BVQ	C	503	X	-	-	-
3	BVQ	D	503	X	-	-	-
3	BVQ	E	503	X	-	-	-
3	BVQ	F	503	X	-	-	-

2 Entry composition

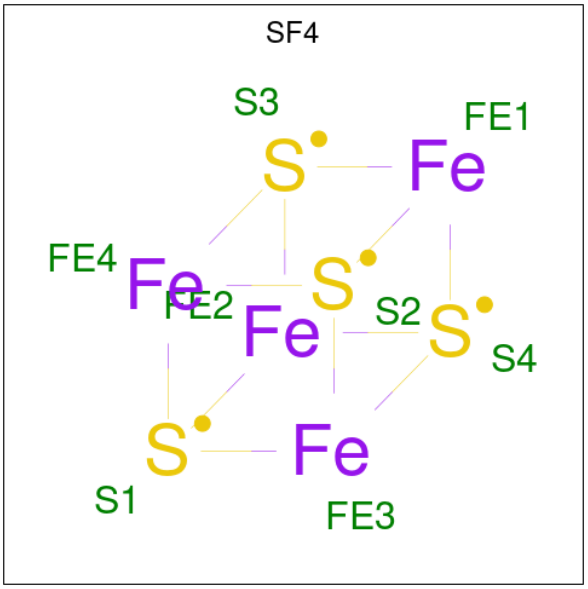
There are 4 unique types of molecules in this entry. The entry contains 22528 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 TETRACHLOROETHENE REDUCTIVE DEHALOGENASE CATALYTIC SUBUNIT.

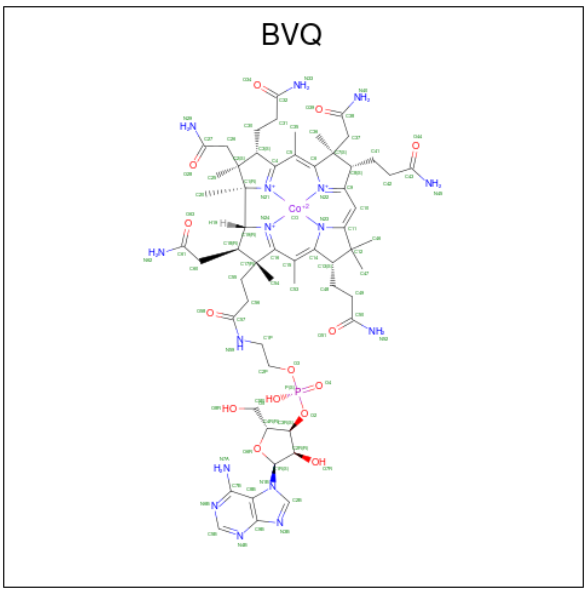
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	458	Total	C	N	O	S	0	0	0
			3608	2291	618	667	32			
1	B	436	Total	C	N	O	S	0	1	0
			3443	2185	588	639	31			
1	C	442	Total	C	N	O	S	0	1	0
			3497	2221	598	647	31			
1	D	437	Total	C	N	O	S	0	0	0
			3444	2186	589	639	30			
1	E	435	Total	C	N	O	S	0	1	0
			3436	2181	587	637	31			
1	F	429	Total	C	N	O	S	0	0	0
			3385	2153	578	624	30			

- Molecule 2 is IRON/SULFUR CLUSTER (three-letter code: SF4) (formula: Fe_4S_4).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total Fe S 8 4 4	0	0
2	A	1	Total Fe S 8 4 4	0	0
2	B	1	Total Fe S 8 4 4	0	0
2	B	1	Total Fe S 8 4 4	0	0
2	C	1	Total Fe S 8 4 4	0	0
2	C	1	Total Fe S 8 4 4	0	0
2	D	1	Total Fe S 8 4 4	0	0
2	D	1	Total Fe S 8 4 4	0	0
2	E	1	Total Fe S 8 4 4	0	0
2	E	1	Total Fe S 8 4 4	0	0
2	F	1	Total Fe S 8 4 4	0	0
2	F	1	Total Fe S 8 4 4	0	0

- Molecule 3 is NORPSEUDO-B12 (three-letter code: BVQ) (formula: $C_{57}H_{82}CoN_{16}O_{14}P$).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
3	A	1	Total	C	Co	N	O	P	0	0
			89	57	1	16	14	1		
3	B	1	Total	C	Co	N	O	P	0	0
			89	57	1	16	14	1		
3	C	1	Total	C	Co	N	O	P	0	0
			89	57	1	16	14	1		
3	D	1	Total	C	Co	N	O	P	0	0
			89	57	1	16	14	1		
3	E	1	Total	C	Co	N	O	P	0	0
			89	57	1	16	14	1		
3	F	1	Total	C	Co	N	O	P	0	0
			89	57	1	16	14	1		

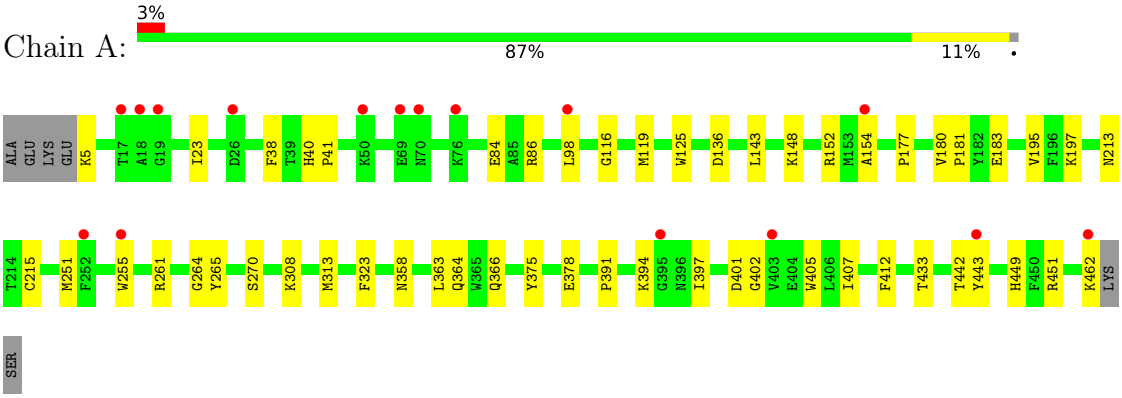
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	193	Total	O	0	0
			193	193		
4	B	204	Total	O	0	0
			204	204		
4	C	254	Total	O	0	0
			254	254		
4	D	199	Total	O	0	0
			199	199		
4	E	103	Total	O	0	0
			103	103		
4	F	132	Total	O	0	0
			132	132		

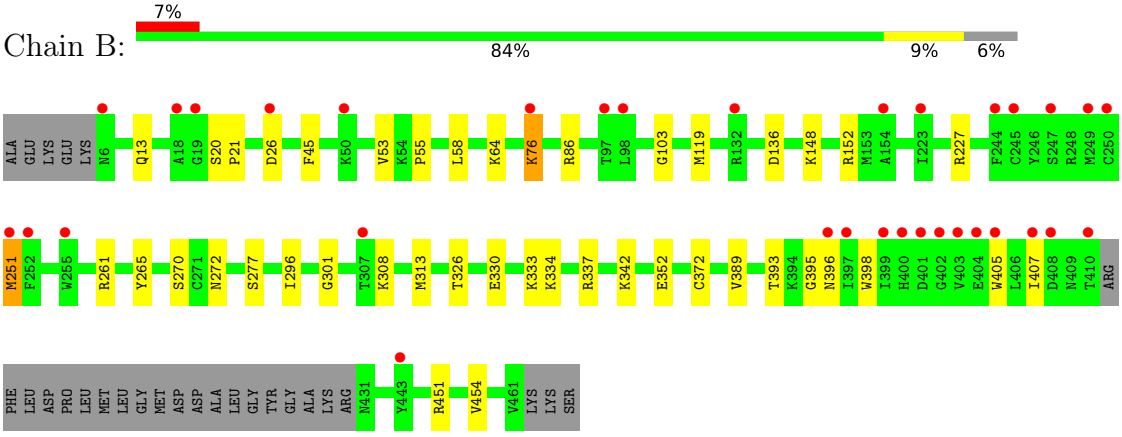
3 Residue-property plots (i)

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.

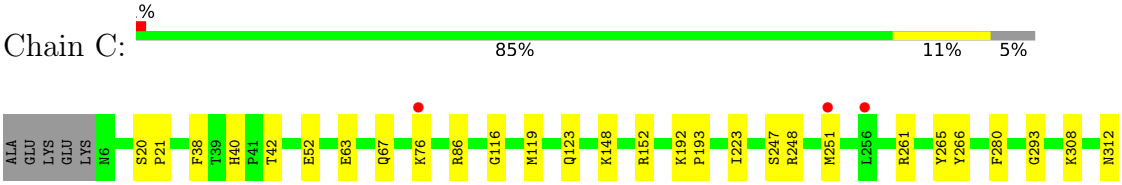
• Molecule 1: TETRACHLOROETHENE REDUCTIVE DEHALOGENASE CATALYTIC SUBUNIT

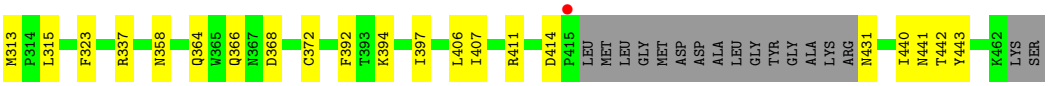


• Molecule 1: TETRACHLOROETHENE REDUCTIVE DEHALOGENASE CATALYTIC SUBUNIT



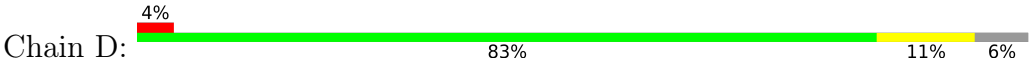
• Molecule 1: TETRACHLOROETHENE REDUCTIVE DEHALOGENASE CATALYTIC SUBUNIT

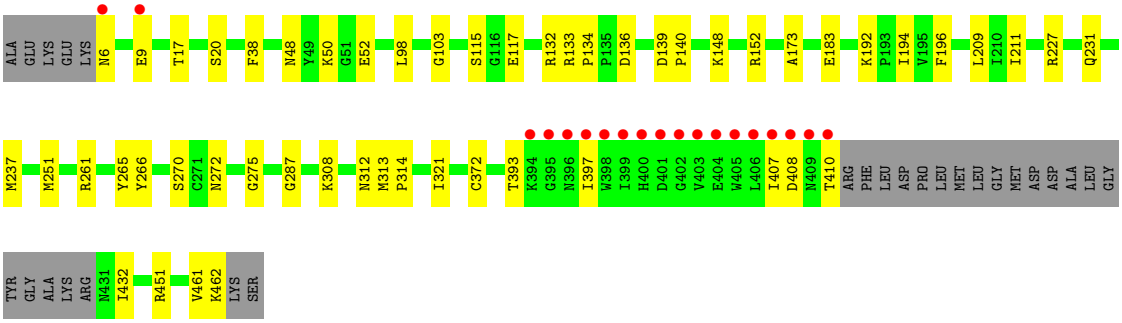




• Molecule 1: TETRACHLOROETHENE REDUCTIVE DEHALOGENASE CATALYTIC SUBUNIT

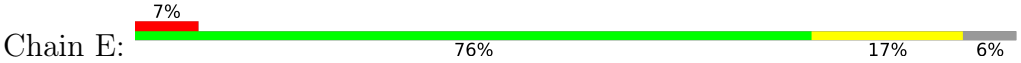
Chain D:

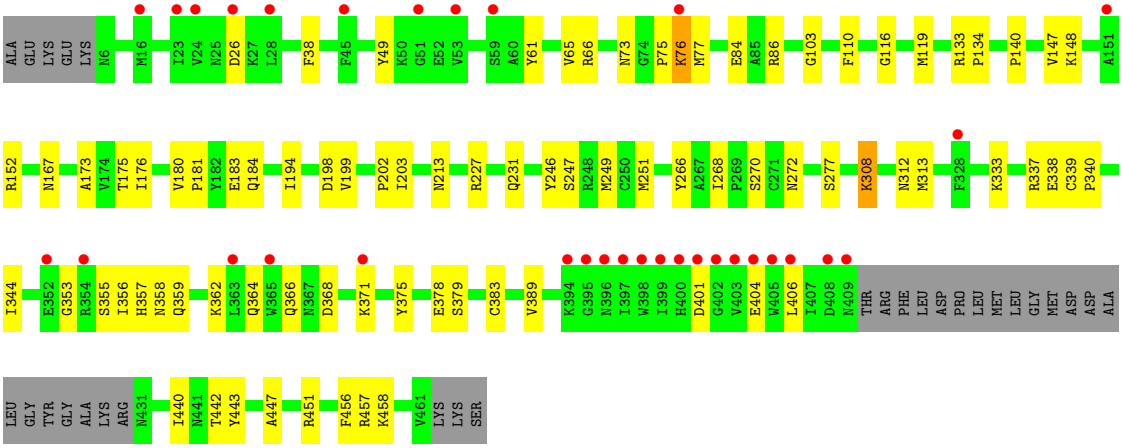




• Molecule 1: TETRACHLOROETHENE REDUCTIVE DEHALOGENASE CATALYTIC SUBUNIT

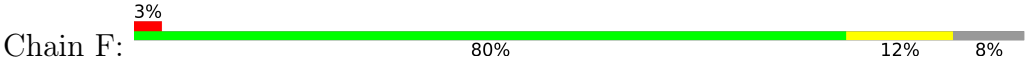
Chain E:

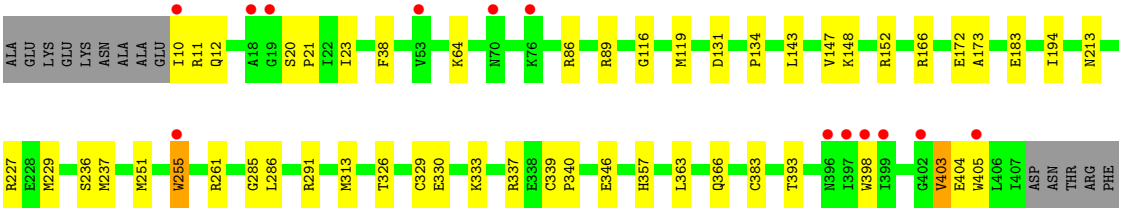


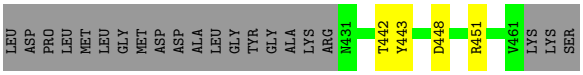


• Molecule 1: TETRACHLOROETHENE REDUCTIVE DEHALOGENASE CATALYTIC SUBUNIT

Chain F:






LEU
ASP
PRO
LEU
MET
LEU
GLY
MET
ASP
ASP
ALA
LEU
GLY
TYR
GLY
ALA
LYS
ARG
N431
T442
Y443
D448
R451
V461
LYS
LYS
SER

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	74.31Å 110.60Å 178.79Å 90.00° 95.91° 90.00°	Depositor
Resolution (Å)	48.76 – 2.23 48.76 – 2.24	Depositor EDS
% Data completeness (in resolution range)	98.4 (48.76-2.23) 98.5 (48.76-2.24)	Depositor EDS
R_{merge}	0.17	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	5.27 (at 2.24Å)	Xtriage
Refinement program	PHENIX (PHENIX.REFINE)	Depositor
R, R_{free}	0.179 , 0.218 0.186 , 0.221	Depositor DCC
R_{free} test set	6850 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å^2)	27.7	Xtriage
Anisotropy	0.219	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.37 , 51.0	EDS
L-test for twinning[2]	$< \|L\| > = 0.46$, $< L^2 > = 0.28$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	22528	wwPDB-VP
Average B, all atoms (Å^2)	35.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.47% 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

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: BVQ, SF4

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	0.24	0/3701	0.44	0/5024
1	B	0.28	1/3532 (0.0%)	0.45	0/4798
1	C	0.25	0/3588	0.46	0/4873
1	D	0.27	0/3533	0.47	0/4799
1	E	0.28	0/3525	0.52	2/4788 (0.0%)
1	F	0.24	0/3474	0.46	0/4719
All	All	0.26	1/21353 (0.0%)	0.47	2/29001 (0.0%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	76	LYS	CE-NZ	6.88	1.66	1.49

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	E	26	ASP	CB-CG-OD1	6.53	124.17	118.30
1	E	76	LYS	CA-CB-CG	5.32	125.10	113.40

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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	3608	0	3505	37	0
1	B	3443	0	3329	31	0
1	C	3497	0	3386	37	0
1	D	3444	0	3334	35	0
1	E	3436	0	3322	63	0
1	F	3385	0	3282	44	0
2	A	16	0	0	0	0
2	B	16	0	0	0	0
2	C	16	0	0	0	0
2	D	16	0	0	0	0
2	E	16	0	0	1	0
2	F	16	0	0	1	0
3	A	89	0	82	4	0
3	B	89	0	82	4	0
3	C	89	0	82	9	0
3	D	89	0	82	6	0
3	E	89	0	82	9	0
3	F	89	0	82	8	0
4	A	193	0	0	4	0
4	B	204	0	0	4	0
4	C	254	0	0	3	0
4	D	199	0	0	5	0
4	E	103	0	0	2	0
4	F	132	0	0	4	0
All	All	22528	0	20650	247	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 6.

All (247) 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:D:50:LYS:NZ	4:D:2034:HOH:O	1.94	0.99
1:F:227:ARG:NH1	1:F:393:THR:O	2.02	0.92
1:D:227:ARG:NH1	1:D:393:THR:O	2.10	0.84
1:F:11:ARG:NH2	1:F:285:GLY:O	2.14	0.80
1:E:338:GLU:HG2	1:E:389:VAL:HG11	1.64	0.79
1:E:247:SER:HB2	1:F:255:TRP:CZ2	2.21	0.76
1:D:275:GLY:O	1:D:308:LYS:NZ	2.19	0.75
1:A:364:GLN:HE21	1:A:366:GLN:HE22	1.33	0.73
1:F:64:LYS:HG2	1:F:89:ARG:HE	1.54	0.73
1:F:89:ARG:HH11	1:F:236:SER:HB3	1.53	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:119:MET:SD	4:A:2068:HOH:O	2.47	0.73
1:E:247:SER:HB2	1:F:255:TRP:HZ2	1.52	0.72
1:E:359:GLN:OE1	1:E:362:LYS:NZ	2.21	0.71
1:F:89:ARG:NH1	1:F:236:SER:HB3	2.06	0.71
1:B:119:MET:SD	4:B:2075:HOH:O	2.49	0.70
1:E:358:ASN:HB3	1:E:366:GLN:HE21	1.57	0.69
1:B:313:MET:SD	4:B:2147:HOH:O	2.50	0.68
1:F:64:LYS:NZ	4:F:2027:HOH:O	2.27	0.68
1:D:227:ARG:NH1	4:D:2130:HOH:O	2.26	0.66
1:C:86:ARG:NH1	1:D:134:PRO:O	2.19	0.66
1:E:451:ARG:HD2	1:F:451:ARG:HH21	1.61	0.65
1:E:456:PHE:HB3	1:E:458:LYS:HE2	1.77	0.65
1:F:172:GLU:OE2	4:F:2079:HOH:O	2.14	0.64
3:D:503:BVQ:H35	3:D:503:BVQ:H36A	1.80	0.64
1:D:20:SER:O	4:D:2008:HOH:O	2.15	0.64
1:F:143:LEU:HB3	1:F:313:MET:HE3	1.80	0.63
1:F:403:VAL:HG12	1:F:404:GLU:HG3	1.80	0.63
3:F:503:BVQ:H35	3:F:503:BVQ:H36A	1.80	0.63
1:E:333:LYS:HB2	1:E:337:ARG:HE	1.64	0.62
1:D:270:SER:OG	1:D:308:LYS:HG3	2.00	0.61
1:E:451:ARG:NH2	1:F:448:ASP:OD1	2.34	0.61
3:E:503:BVQ:H36A	3:E:503:BVQ:H35	1.83	0.61
3:A:503:BVQ:H35	3:A:503:BVQ:H36A	1.81	0.60
1:B:334:LYS:HD3	1:B:389:VAL:HB	1.83	0.60
1:C:358:ASN:HB3	1:C:366:GLN:HE21	1.65	0.60
1:E:355:SER:OG	1:E:356:ILE:N	2.33	0.60
3:B:503:BVQ:H35	3:B:503:BVQ:H36A	1.82	0.60
3:C:503:BVQ:H36A	3:C:503:BVQ:H35	1.84	0.60
1:E:38:PHE:CD2	3:E:503:BVQ:H53A	2.37	0.60
1:A:364:GLN:HE21	1:A:366:GLN:NE2	1.98	0.59
1:E:173:ALA:HB2	1:E:194:ILE:HD11	1.84	0.59
1:C:364:GLN:HE21	1:C:366:GLN:NE2	2.00	0.59
1:B:227:ARG:NH1	1:B:393:THR:O	2.35	0.59
1:E:86:ARG:NH1	1:F:134:PRO:O	2.34	0.59
1:E:458:LYS:H	1:E:458:LYS:HD3	1.68	0.59
1:A:270:SER:OG	1:A:308:LYS:HG3	2.03	0.58
1:E:198:ASP:OD1	1:E:213:ASN:ND2	2.36	0.58
3:C:503:BVQ:H55A	3:C:503:BVQ:H53	1.86	0.58
1:C:251[A]:MET:SD	1:D:251:MET:HG3	2.44	0.58
1:E:451:ARG:HD2	1:F:451:ARG:NH2	2.18	0.57
1:D:132:ARG:NH2	4:D:2082:HOH:O	2.37	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:431:ASN:N	4:C:2234:HOH:O	2.37	0.57
3:A:503:BVQ:H55A	3:A:503:BVQ:H53	1.87	0.57
1:C:392:PHE:HA	1:C:397:ILE:HD12	1.87	0.56
1:E:458:LYS:HD3	1:E:458:LYS:N	2.19	0.56
1:E:75:PRO:O	1:E:76:LYS:HB2	2.05	0.56
1:F:291:ARG:NH1	1:F:329:CYS:O	2.39	0.56
1:F:346:GLU:O	4:F:2117:HOH:O	2.18	0.55
1:D:17:THR:HG23	1:E:140:PRO:HG3	1.89	0.54
1:E:75:PRO:HG3	1:E:379:SER:HA	1.89	0.54
1:D:397:ILE:HG12	1:D:407:ILE:HG23	1.87	0.54
3:D:503:BVQ:H55A	3:D:503:BVQ:H53	1.89	0.54
1:A:375:TYR:HA	1:A:378:GLU:HG3	1.90	0.54
1:E:76:LYS:HB3	1:E:77:MET:HG2	1.90	0.54
1:E:401:ASP:OD2	1:E:404:GLU:HG2	2.08	0.53
1:A:264:GLY:HA2	4:A:2077:HOH:O	2.09	0.53
1:C:86:ARG:HD2	1:D:136:ASP:OD2	2.09	0.53
1:A:98:LEU:CD2	1:A:251:MET:HG2	2.39	0.53
1:E:251[A]:MET:SD	1:F:251:MET:HG3	2.49	0.53
1:F:366:GLN:NE2	4:F:2120:HOH:O	2.31	0.53
3:B:503:BVQ:H55A	3:B:503:BVQ:H53	1.91	0.53
1:C:313:MET:HE2	1:C:315:LEU:HD21	1.91	0.53
1:C:364:GLN:HE21	1:C:366:GLN:HE22	1.57	0.53
1:B:333:LYS:HB2	1:B:337:ARG:HH11	1.73	0.53
1:C:76:LYS:O	1:C:76:LYS:HG3	2.07	0.53
3:E:503:BVQ:H55A	3:E:503:BVQ:H53	1.89	0.53
1:A:116:GLY:HA2	1:A:119:MET:HE3	1.90	0.52
1:E:202:PRO:HB3	1:E:268:ILE:HD11	1.91	0.52
1:E:375:TYR:HA	1:E:378:GLU:HG3	1.91	0.52
1:F:23:ILE:HD11	1:F:363:LEU:HD22	1.92	0.51
1:B:26:ASP:OD1	4:B:2016:HOH:O	2.19	0.51
1:D:287:GLY:HA2	1:D:321:ILE:HD11	1.92	0.51
1:A:213:ASN:ND2	4:A:2105:HOH:O	2.33	0.51
1:B:333:LYS:HB2	1:B:337:ARG:NH1	2.26	0.51
1:E:457:ARG:HB3	4:E:2096:HOH:O	2.10	0.51
1:F:38:PHE:CD2	3:F:503:BVQ:H53A	2.45	0.51
1:E:75:PRO:HD3	1:E:379:SER:O	2.11	0.51
1:E:357:HIS:O	3:E:503:BVQ:H2PA	2.10	0.51
1:C:63:GLU:O	1:C:67:GLN:HG3	2.11	0.51
1:E:61:TYR:O	1:E:65:VAL:HG23	2.10	0.50
1:A:397:ILE:HD11	1:A:412:PHE:CZ	2.46	0.50
1:F:147:VAL:HB	1:F:313:MET:HE2	1.92	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:173:ALA:HB2	1:D:194:ILE:HD11	1.93	0.50
1:D:38:PHE:CD2	3:D:503:BVQ:H53A	2.46	0.50
1:C:86:ARG:NH2	1:D:133:ARG:O	2.36	0.50
1:E:277:SER:OG	1:E:308:LYS:NZ	2.44	0.50
1:C:52:GLU:OE1	4:C:2040:HOH:O	2.20	0.49
1:B:270:SER:OG	1:B:308:LYS:HG3	2.11	0.49
1:D:6:ASN:HB3	1:D:9:GLU:OE1	2.13	0.49
1:D:231:GLN:NE2	4:D:2131:HOH:O	2.45	0.49
1:A:401:ASP:OD1	1:A:402:GLY:N	2.45	0.49
1:E:227:ARG:O	1:E:231:GLN:HG2	2.12	0.49
1:E:266:TYR:CZ	1:E:312:ASN:HB3	2.48	0.49
1:B:13:GLN:OE1	1:B:405:TRP:HB2	2.12	0.49
1:C:368:ASP:OD2	4:C:2222:HOH:O	2.20	0.49
1:A:391:PRO:HA	1:A:394:LYS:HG2	1.94	0.49
1:E:368:ASP:OD1	1:E:371:LYS:HG2	2.14	0.48
1:E:199:VAL:HG21	1:E:203:ILE:HD13	1.94	0.48
1:F:38:PHE:CZ	3:F:503:BVQ:H46A	2.48	0.48
1:A:323:PHE:HD2	1:A:407:ILE:HD11	1.78	0.48
1:E:451:ARG:NH2	1:F:448:ASP:HA	2.29	0.48
1:E:246:TYR:O	1:E:249:MET:HB2	2.14	0.48
1:A:154:ALA:HA	1:A:255:TRP:CE3	2.49	0.47
1:F:166:ARG:NH2	1:F:213:ASN:OD1	2.44	0.47
1:C:261:ARG:HA	1:C:265:TYR:O	2.14	0.47
1:C:337:ARG:NH2	1:C:414:ASP:OD2	2.48	0.47
1:E:353:GLY:HA2	1:E:366:GLN:HG2	1.97	0.47
1:A:358:ASN:HB3	1:A:366:GLN:HE21	1.79	0.47
1:E:333:LYS:HG3	1:E:337:ARG:HH21	1.79	0.47
1:E:383:CYS:HB3	2:E:502:SF4:S1	2.53	0.47
1:A:38:PHE:CD2	3:A:503:BVQ:H53A	2.50	0.47
1:A:451:ARG:HH22	1:B:451:ARG:HH12	1.61	0.47
1:B:148:LYS:O	1:B:152:ARG:HG2	2.14	0.47
1:A:5:LYS:HA	1:A:405:TRP:CH2	2.50	0.46
1:E:364:GLN:HE22	3:E:503:BVQ:P	2.38	0.46
1:F:333:LYS:HB2	1:F:337:ARG:NH1	2.30	0.46
1:E:442:THR:HG22	1:E:443:TYR:CD2	2.50	0.46
3:F:503:BVQ:H25B	3:F:503:BVQ:H30	1.78	0.46
1:A:23:ILE:HD11	1:A:363:LEU:HD23	1.97	0.46
1:B:277:SER:OG	1:B:308:LYS:HE3	2.15	0.46
1:F:119:MET:HE1	1:F:261:ARG:NH1	2.31	0.46
1:E:451:ARG:NH1	1:F:451:ARG:HH22	2.13	0.46
1:B:261:ARG:HA	1:B:265:TYR:O	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:270:SER:OG	1:E:308:LYS:HG3	2.16	0.46
1:F:229:MET:HB3	1:F:237:MET:O	2.16	0.46
1:A:397:ILE:HD11	1:A:412:PHE:CE1	2.50	0.46
1:C:38:PHE:CD2	3:C:503:BVQ:H53A	2.50	0.46
1:E:180:VAL:HA	1:E:181:PRO:HD3	1.62	0.46
1:F:383:CYS:HB3	2:F:502:SF4:S1	2.56	0.46
1:E:406:LEU:HA	1:E:406:LEU:HD23	1.57	0.46
1:E:183:GLU:H	1:E:183:GLU:CD	2.18	0.45
1:F:357:HIS:O	3:F:503:BVQ:H2P	2.16	0.45
1:F:11:ARG:HH22	1:F:286:LEU:HA	1.82	0.45
3:F:503:BVQ:H60	3:F:503:BVQ:H25A	1.98	0.45
1:D:115:SER:OG	1:D:117:GLU:HG3	2.16	0.45
1:E:447:ALA:HB1	1:F:451:ARG:HG3	1.99	0.45
1:A:261:ARG:HA	1:A:265:TYR:O	2.16	0.45
1:B:45:PHE:HD2	1:B:53:VAL:HG12	1.81	0.45
1:E:38:PHE:HD2	3:E:503:BVQ:H53A	1.80	0.45
1:A:86:ARG:NH1	1:B:136:ASP:OD2	2.46	0.45
1:A:181:PRO:HB2	1:A:183:GLU:OE2	2.16	0.45
1:A:449:HIS:ND1	4:A:2188:HOH:O	2.36	0.45
1:C:116:GLY:HA2	1:C:119:MET:HE3	1.98	0.45
1:C:148:LYS:O	1:C:152:ARG:HG2	2.16	0.45
1:A:251:MET:HE2	1:B:251[B]:MET:SD	2.56	0.44
1:A:136:ASP:OD2	1:B:86:ARG:HD2	2.18	0.44
1:A:195:VAL:HG21	1:A:197:LYS:HE3	1.99	0.44
1:D:261:ARG:HA	1:D:265:TYR:O	2.18	0.44
3:F:503:BVQ:H47	3:F:503:BVQ:H48A	1.92	0.44
1:C:119:MET:HE3	1:C:261:ARG:NH1	2.32	0.44
1:C:247:SER:HB3	1:D:251:MET:HE1	1.99	0.44
1:F:326:THR:O	1:F:330:GLU:HG3	2.17	0.44
1:D:139:ASP:HA	1:D:140:PRO:HD2	1.83	0.44
1:E:344:ILE:O	4:E:2083:HOH:O	2.21	0.44
1:F:116:GLY:HA2	1:F:119:MET:CE	2.48	0.44
1:C:20:SER:HA	1:C:21:PRO:HD3	1.73	0.44
1:B:55:PRO:HD2	1:B:58:LEU:HD12	2.00	0.44
1:B:352:GLU:OE2	4:B:2018:HOH:O	2.21	0.44
1:B:398:TRP:CZ3	1:B:407:ILE:HG13	2.53	0.44
1:C:323:PHE:HD2	1:C:407:ILE:HD11	1.82	0.44
3:D:503:BVQ:H26A	3:D:503:BVQ:H19	1.81	0.44
3:E:503:BVQ:H25B	3:E:503:BVQ:H30	1.68	0.44
1:C:38:PHE:CZ	3:C:503:BVQ:H46A	2.53	0.43
1:C:280:PHE:CD2	1:C:308:LYS:HD2	2.53	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:147:VAL:HG21	1:E:313:MET:HE3	2.00	0.43
1:C:440:ILE:HG13	1:C:441:ASN:N	2.33	0.43
1:E:133:ARG:HA	1:E:134:PRO:HD3	1.90	0.43
1:F:339:CYS:HA	1:F:340:PRO:HD3	1.78	0.43
1:F:398:TRP:HB3	1:F:405:TRP:CE3	2.53	0.43
1:B:342:LYS:HA	1:B:342:LYS:HD3	1.72	0.43
1:C:116:GLY:HA2	1:C:119:MET:CE	2.48	0.43
1:A:462:LYS:HB2	1:A:462:LYS:HE2	1.57	0.43
1:D:372:CYS:SG	3:D:503:BVQ:H47A	2.58	0.43
1:A:451:ARG:HH22	1:B:451:ARG:NH1	2.16	0.43
1:B:326:THR:O	1:B:330:GLU:HG3	2.18	0.43
1:C:266:TYR:CZ	1:C:312:ASN:HB3	2.54	0.43
1:D:237:MET:HG2	1:D:432:ILE:HD13	2.01	0.43
1:B:372:CYS:SG	3:B:503:BVQ:H47A	2.59	0.43
1:B:103:GLY:O	1:B:272:ASN:HB2	2.19	0.43
1:C:223:ILE:HG23	1:C:248:ARG:CZ	2.49	0.43
1:D:313:MET:HA	1:D:314:PRO:HD3	1.91	0.43
1:E:181:PRO:HD2	1:E:184:GLN:OE1	2.19	0.43
1:C:123:GLN:OE1	1:D:183:GLU:HG3	2.19	0.43
1:D:148:LYS:O	1:D:152:ARG:HG2	2.19	0.43
1:F:131:ASP:N	1:F:131:ASP:OD1	2.52	0.43
1:F:173:ALA:HB2	1:F:194:ILE:HD11	2.01	0.43
1:B:451:ARG:O	1:B:454:VAL:HG12	2.18	0.42
1:C:372:CYS:SG	3:C:503:BVQ:H47A	2.59	0.42
3:C:503:BVQ:H47	3:C:503:BVQ:H48A	1.94	0.42
1:A:125:TRP:CH2	1:B:64:LYS:HE2	2.54	0.42
3:C:503:BVQ:H25B	3:C:503:BVQ:H30	1.86	0.42
1:F:442:THR:HG22	1:F:443:TYR:CD2	2.54	0.42
1:D:48:ASN:OD1	1:D:52:GLU:HG3	2.19	0.42
1:E:75:PRO:O	1:E:76:LYS:CB	2.67	0.42
1:C:442:THR:HG22	1:C:443:TYR:CD2	2.55	0.42
3:E:503:BVQ:H60	3:E:503:BVQ:H26A	2.02	0.42
1:D:266:TYR:CZ	1:D:312:ASN:HB3	2.54	0.42
1:A:442:THR:HG22	1:A:443:TYR:CD2	2.55	0.42
1:E:73:ASN:ND2	1:E:84:GLU:OE2	2.43	0.42
3:D:503:BVQ:H25A	3:D:503:BVQ:H60	2.02	0.42
1:D:103:GLY:O	1:D:272:ASN:HB2	2.19	0.42
1:E:49:TYR:CE2	1:E:66:ARG:HD3	2.55	0.42
1:E:175:THR:OG1	1:E:176:ILE:N	2.53	0.42
1:D:98:LEU:CD2	1:D:251:MET:HG2	2.50	0.41
1:B:227:ARG:NH2	1:B:395:GLY:HA3	2.35	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:293:GLY:O	3:C:503:BVQ:H1R	2.21	0.41
1:E:339:CYS:HA	1:E:340:PRO:HD3	1.78	0.41
1:E:103:GLY:O	1:E:272:ASN:HB2	2.20	0.41
1:D:196:PHE:HA	1:D:211:ILE:O	2.21	0.41
1:E:148:LYS:O	1:E:152:ARG:HG2	2.21	0.41
1:F:148:LYS:O	1:F:152:ARG:HG2	2.20	0.41
1:A:148:LYS:O	1:A:152:ARG:HG2	2.20	0.41
1:D:408:ASP:CG	1:D:410:THR:HB	2.41	0.41
1:F:10:ILE:HG23	1:F:12:GLN:H	1.84	0.41
1:C:394:LYS:NZ	1:C:411:ARG:O	2.51	0.41
1:E:133:ARG:HG2	1:F:86:ARG:HH12	1.85	0.41
1:A:451:ARG:NH2	1:B:451:ARG:HH12	2.19	0.41
1:C:76:LYS:O	1:C:76:LYS:CG	2.69	0.41
1:D:192:LYS:HD2	1:D:209:LEU:HG	2.03	0.41
1:A:143:LEU:HD13	1:A:313:MET:HG3	2.02	0.41
3:C:503:BVQ:H56A	3:C:503:BVQ:H18	1.93	0.41
1:A:177:PRO:HG2	1:A:180:VAL:CG2	2.51	0.40
3:A:503:BVQ:H56A	3:A:503:BVQ:H18	1.94	0.40
1:B:296:ILE:HG23	1:B:301:GLY:HA2	2.03	0.40
3:B:503:BVQ:H25A	3:B:503:BVQ:H60	2.03	0.40
3:F:503:BVQ:H26A	3:F:503:BVQ:H19	1.85	0.40
1:E:199:VAL:HG21	1:E:203:ILE:CD1	2.51	0.40
3:E:503:BVQ:H56A	3:E:503:BVQ:H18	1.80	0.40
1:C:40:HIS:CE1	1:C:42:THR:HG1	2.38	0.40
1:D:461:VAL:C	1:D:462:LYS:HD2	2.41	0.40
1:E:440:ILE:HD12	1:E:440:ILE:HA	1.88	0.40
1:F:20:SER:HA	1:F:21:PRO:HD2	1.93	0.40
1:A:40:HIS:CD2	1:A:41:PRO:HD2	2.56	0.40
1:A:84:GLU:OE1	1:A:433:THR:OG1	2.21	0.40
1:C:192:LYS:HA	1:C:193:PRO:HD3	1.92	0.40
1:B:20:SER:HA	1:B:21:PRO:HD3	1.75	0.40
1:E:116:GLY:HA2	1:E:119:MET:CE	2.52	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	456/464 (98%)	443 (97%)	12 (3%)	1 (0%)	47 53
1	B	433/464 (93%)	415 (96%)	16 (4%)	2 (0%)	29 28
1	C	439/464 (95%)	426 (97%)	13 (3%)	0	100 100
1	D	433/464 (93%)	421 (97%)	12 (3%)	0	100 100
1	E	432/464 (93%)	411 (95%)	20 (5%)	1 (0%)	47 53
1	F	425/464 (92%)	412 (97%)	12 (3%)	1 (0%)	47 53
All	All	2618/2784 (94%)	2528 (97%)	85 (3%)	5 (0%)	47 53

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	76	LYS
1	B	396	ASN
1	F	403	VAL
1	A	215	CYS
1	E	110	PHE

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	384/389 (99%)	384 (100%)	0	100 100
1	B	368/389 (95%)	366 (100%)	2 (0%)	88 92
1	C	374/389 (96%)	373 (100%)	1 (0%)	92 95
1	D	368/389 (95%)	367 (100%)	1 (0%)	92 95
1	E	367/389 (94%)	365 (100%)	2 (0%)	88 92
1	F	362/389 (93%)	360 (99%)	2 (1%)	86 90
All	All	2223/2334 (95%)	2215 (100%)	8 (0%)	92 93

All (8) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	251[A]	MET
1	B	251[B]	MET
1	C	406	LEU
1	D	451	ARG
1	E	167	ASN
1	E	308	LYS
1	F	183	GLU
1	F	255	TRP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (8) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	366	GLN
1	C	366	GLN
1	D	231	GLN
1	E	167	ASN
1	E	366	GLN
1	E	370	ASN
1	E	409	ASN
1	E	449	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)

18 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	SF4	E	501	1	0,12,12	-	-	-		
3	BVQ	C	503	-	87,99,99	0.99	3 (3%)	129,162,162	1.24	14 (10%)
2	SF4	B	502	1	0,12,12	-	-	-		
3	BVQ	D	503	4	87,99,99	0.96	3 (3%)	129,162,162	1.21	14 (10%)
2	SF4	F	502	1	0,12,12	-	-	-		
2	SF4	B	501	1	0,12,12	-	-	-		
3	BVQ	A	503	4	87,99,99	0.96	3 (3%)	129,162,162	1.15	14 (10%)
3	BVQ	F	503	-	87,99,99	0.99	3 (3%)	129,162,162	1.16	16 (12%)
3	BVQ	B	503	4	87,99,99	0.95	4 (4%)	129,162,162	1.28	16 (12%)
2	SF4	C	501	1	0,12,12	-	-	-		
2	SF4	D	502	1	0,12,12	-	-	-		
2	SF4	C	502	1	0,12,12	-	-	-		
2	SF4	F	501	1	0,12,12	-	-	-		
3	BVQ	E	503	4	87,99,99	1.00	3 (3%)	129,162,162	1.25	18 (13%)
2	SF4	E	502	1	0,12,12	-	-	-		
2	SF4	D	501	1	0,12,12	-	-	-		
2	SF4	A	502	1	0,12,12	-	-	-		
2	SF4	A	501	1	0,12,12	-	-	-		

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	SF4	F	501	1	-	-	0/6/5/5
3	BVQ	C	503	-	3/3/35/37	5/50/221/221	0/3/11/11
2	SF4	E	501	1	-	-	0/6/5/5
2	SF4	D	501	1	-	-	0/6/5/5
2	SF4	B	502	1	-	-	0/6/5/5
3	BVQ	D	503	4	3/3/35/37	2/50/221/221	0/3/11/11
2	SF4	F	502	1	-	-	0/6/5/5
2	SF4	B	501	1	-	-	0/6/5/5
3	BVQ	A	503	4	3/3/35/37	3/50/221/221	0/3/11/11
2	SF4	C	501	1	-	-	0/6/5/5

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	BVQ	E	503	4	3/3/35/37	11/50/221/221	0/3/11/11
2	SF4	C	502	1	-	-	0/6/5/5
3	BVQ	B	503	4	3/3/35/37	6/50/221/221	0/3/11/11
2	SF4	D	502	1	-	-	0/6/5/5
2	SF4	E	502	1	-	-	0/6/5/5
3	BVQ	F	503	-	3/3/35/37	8/50/221/221	0/3/11/11
2	SF4	A	502	1	-	-	0/6/5/5
2	SF4	A	501	1	-	-	0/6/5/5

All (19) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	F	503	BVQ	C14-N23	6.75	1.43	1.35
3	C	503	BVQ	C14-N23	6.69	1.43	1.35
3	E	503	BVQ	C14-N23	6.65	1.43	1.35
3	D	503	BVQ	C14-N23	6.55	1.43	1.35
3	A	503	BVQ	C14-N23	6.40	1.43	1.35
3	B	503	BVQ	C14-N23	6.12	1.42	1.35
3	A	503	BVQ	C13-C14	3.36	1.59	1.52
3	E	503	BVQ	C13-C14	3.26	1.58	1.52
3	D	503	BVQ	C13-C14	3.15	1.58	1.52
3	B	503	BVQ	C13-C14	3.11	1.58	1.52
3	F	503	BVQ	C13-C14	3.00	1.58	1.52
3	C	503	BVQ	C13-C14	2.96	1.58	1.52
3	C	503	BVQ	C16-C15	2.80	1.52	1.44
3	F	503	BVQ	C16-C15	2.77	1.52	1.44
3	B	503	BVQ	C16-C15	2.71	1.52	1.44
3	E	503	BVQ	C16-C15	2.67	1.52	1.44
3	A	503	BVQ	C16-C15	2.56	1.51	1.44
3	D	503	BVQ	C16-C15	2.21	1.50	1.44
3	B	503	BVQ	C9B-N4B	-2.04	1.34	1.37

All (92) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	B	503	BVQ	C1R-N1B-C8B	7.16	138.00	125.57
3	C	503	BVQ	C1R-N1B-C8B	6.64	137.10	125.57
3	D	503	BVQ	C1R-N1B-C8B	5.50	135.11	125.57
3	E	503	BVQ	C48-C13-C14	4.10	118.70	108.49
3	E	503	BVQ	C1R-N1B-C8B	3.86	132.27	125.57
3	A	503	BVQ	C48-C13-C14	3.81	117.99	108.49

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	E	503	BVQ	C30-C3-C2	-3.70	111.25	119.09
3	D	503	BVQ	C48-C13-C14	3.69	117.69	108.49
3	A	503	BVQ	C1R-N1B-C8B	3.55	131.72	125.57
3	C	503	BVQ	C48-C13-C14	3.53	117.27	108.49
3	B	503	BVQ	C48-C13-C14	3.52	117.25	108.49
3	E	503	BVQ	C55-C17-C18	-3.46	104.46	111.15
3	F	503	BVQ	C48-C13-C14	3.39	116.94	108.49
3	F	503	BVQ	C10-C9-N22	3.37	129.59	125.73
3	C	503	BVQ	C10-C9-N22	3.35	129.57	125.73
3	B	503	BVQ	C10-C9-N22	3.28	129.50	125.73
3	D	503	BVQ	C10-C9-N22	3.19	129.38	125.73
3	F	503	BVQ	C30-C3-C2	-3.13	112.46	119.09
3	E	503	BVQ	C10-C9-N22	3.12	129.31	125.73
3	E	503	BVQ	C56-C55-C17	-3.07	109.61	115.52
3	A	503	BVQ	C35-C5-C6	2.97	127.16	122.43
3	C	503	BVQ	C30-C3-C2	-2.94	112.87	119.09
3	E	503	BVQ	C12-C11-C10	-2.88	119.62	123.37
3	B	503	BVQ	C20-C1-C19	-2.79	106.67	109.36
3	F	503	BVQ	C55-C17-C18	-2.79	105.76	111.15
3	A	503	BVQ	C30-C3-C2	-2.77	113.23	119.09
3	D	503	BVQ	C35-C5-C6	2.74	126.79	122.43
3	D	503	BVQ	C55-C17-C18	-2.74	105.86	111.15
3	A	503	BVQ	C10-C9-N22	2.72	128.85	125.73
3	B	503	BVQ	C35-C5-C6	2.65	126.66	122.43
3	A	503	BVQ	C12-C11-C10	-2.63	119.95	123.37
3	B	503	BVQ	C30-C3-C2	-2.62	113.55	119.09
3	F	503	BVQ	C35-C5-C6	2.59	126.56	122.43
3	A	503	BVQ	C35-C5-C4	-2.58	111.53	116.79
3	D	503	BVQ	C30-C3-C2	-2.55	113.69	119.09
3	C	503	BVQ	C35-C5-C6	2.53	126.45	122.43
3	C	503	BVQ	P-O2-C3R	2.51	128.53	119.41
3	C	503	BVQ	C35-C5-C4	-2.49	111.71	116.79
3	F	503	BVQ	C15-C16-N24	-2.49	118.83	122.42
3	B	503	BVQ	C12-C11-N23	2.48	115.29	111.83
3	F	503	BVQ	C35-C5-C4	-2.48	111.74	116.79
3	D	503	BVQ	C12-C11-N23	2.45	115.25	111.83
3	F	503	BVQ	C1R-N1B-C8B	2.45	129.82	125.57
3	A	503	BVQ	C12-C11-N23	2.45	115.24	111.83
3	E	503	BVQ	C35-C5-C6	2.44	126.31	122.43
3	D	503	BVQ	C35-C5-C4	-2.43	111.83	116.79
3	D	503	BVQ	C36-C7-C8	-2.43	107.58	112.08
3	C	503	BVQ	C12-C11-N23	2.43	115.22	111.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	C	503	BVQ	C12-C11-C10	-2.39	120.25	123.37
3	E	503	BVQ	C8-C9-C10	-2.37	118.20	123.32
3	A	503	BVQ	C55-C17-C18	-2.37	106.57	111.15
3	B	503	BVQ	C12-C11-C10	-2.36	120.29	123.37
3	E	503	BVQ	C5-C6-N22	-2.36	120.26	123.88
3	A	503	BVQ	P-O2-C3R	2.34	127.91	119.41
3	F	503	BVQ	C12-C11-C10	-2.33	120.33	123.37
3	E	503	BVQ	C12-C11-N23	2.33	115.07	111.83
3	E	503	BVQ	C35-C5-C4	-2.32	112.06	116.79
3	B	503	BVQ	C35-C5-C4	-2.32	112.07	116.79
3	F	503	BVQ	C12-C11-N23	2.30	115.04	111.83
3	D	503	BVQ	P-O2-C3R	2.30	127.78	119.41
3	E	503	BVQ	C48-C13-C12	-2.26	110.28	116.63
3	E	503	BVQ	P-O2-C3R	2.26	127.63	119.41
3	A	503	BVQ	C20-C1-C19	-2.25	107.18	109.36
3	D	503	BVQ	C1-C19-C18	-2.25	118.18	121.88
3	E	503	BVQ	C13-C12-C11	2.25	103.51	100.97
3	C	503	BVQ	C13-C12-C11	2.25	103.50	100.97
3	F	503	BVQ	C8-C9-C10	-2.24	118.48	123.32
3	F	503	BVQ	C13-C12-C11	2.24	103.49	100.97
3	B	503	BVQ	C55-C17-C18	-2.23	106.83	111.15
3	E	503	BVQ	C2-C1-N21	2.22	104.86	101.77
3	D	503	BVQ	C5-C6-N22	-2.21	120.50	123.88
3	C	503	BVQ	C5-C6-N22	-2.20	120.51	123.88
3	F	503	BVQ	C2-C1-N21	2.19	104.82	101.77
3	F	503	BVQ	C20-C1-C19	-2.19	107.25	109.36
3	C	503	BVQ	C55-C17-C18	-2.18	106.94	111.15
3	A	503	BVQ	C5-C6-N22	-2.16	120.58	123.88
3	F	503	BVQ	P-O2-C3R	2.16	127.26	119.41
3	C	503	BVQ	C2-C1-N21	2.15	104.77	101.77
3	B	503	BVQ	P-O2-C3R	2.15	127.22	119.41
3	C	503	BVQ	C8-C9-C10	-2.14	118.70	123.32
3	A	503	BVQ	C13-C12-C11	2.13	103.38	100.97
3	A	503	BVQ	C15-C16-N24	-2.10	119.40	122.42
3	D	503	BVQ	C20-C1-C19	-2.09	107.34	109.36
3	B	503	BVQ	C8-C9-C10	-2.08	118.82	123.32
3	D	503	BVQ	C13-C12-C11	2.08	103.32	100.97
3	E	503	BVQ	C41-C8-C7	2.08	119.87	114.14
3	F	503	BVQ	C5-C6-N22	-2.06	120.72	123.88
3	B	503	BVQ	C30-C3-C4	2.04	114.37	109.63
3	B	503	BVQ	C19-C1-N21	2.04	104.25	102.16
3	B	503	BVQ	C13-C12-C11	2.02	103.25	100.97

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	B	503	BVQ	C15-C16-N24	-2.02	119.51	122.42
3	E	503	BVQ	C15-C16-N24	-2.01	119.52	122.42

All (18) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
3	A	503	BVQ	N24
3	A	503	BVQ	N23
3	A	503	BVQ	N21
3	B	503	BVQ	N24
3	B	503	BVQ	N23
3	B	503	BVQ	N21
3	C	503	BVQ	N24
3	C	503	BVQ	N23
3	C	503	BVQ	N21
3	D	503	BVQ	N24
3	D	503	BVQ	N23
3	D	503	BVQ	N21
3	E	503	BVQ	N24
3	E	503	BVQ	N23
3	E	503	BVQ	N21
3	F	503	BVQ	N24
3	F	503	BVQ	N23
3	F	503	BVQ	N21

All (35) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	503	BVQ	C14-C13-C48-C49
3	B	503	BVQ	C14-C13-C48-C49
3	C	503	BVQ	C14-C13-C48-C49
3	D	503	BVQ	C14-C13-C48-C49
3	E	503	BVQ	C2P-O3-P-O4
3	E	503	BVQ	C2P-O3-P-O5
3	E	503	BVQ	C14-C13-C48-C49
3	F	503	BVQ	C2P-O3-P-O2
3	F	503	BVQ	C2P-O3-P-O4
3	F	503	BVQ	C2P-O3-P-O5
3	F	503	BVQ	C38-C37-C7-C6
3	F	503	BVQ	C14-C13-C48-C49
3	D	503	BVQ	C38-C37-C7-C6
3	E	503	BVQ	C2P-O3-P-O2

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Mol	Chain	Res	Type	Atoms
3	F	503	BVQ	C8-C41-C42-C43
3	E	503	BVQ	C2-C3-C30-C31
3	B	503	BVQ	C38-C37-C7-C6
3	E	503	BVQ	C38-C37-C7-C6
3	C	503	BVQ	C41-C42-C43-O44
3	C	503	BVQ	C41-C42-C43-N45
3	B	503	BVQ	C41-C42-C43-O44
3	E	503	BVQ	C4-C3-C30-C31
3	E	503	BVQ	C8-C41-C42-C43
3	E	503	BVQ	N59-C1P-C2P-O3
3	B	503	BVQ	C41-C42-C43-N45
3	A	503	BVQ	C38-C37-C7-C6
3	C	503	BVQ	C38-C37-C7-C6
3	E	503	BVQ	C3R-O2-P-O4
3	E	503	BVQ	C3R-O2-P-O5
3	C	503	BVQ	C2P-O3-P-O2
3	B	503	BVQ	C8-C41-C42-C43
3	F	503	BVQ	C2-C3-C30-C31
3	A	503	BVQ	C2-C3-C30-C31
3	F	503	BVQ	C1P-C2P-O3-P
3	B	503	BVQ	C42-C41-C8-C9

There are no ring outliers.

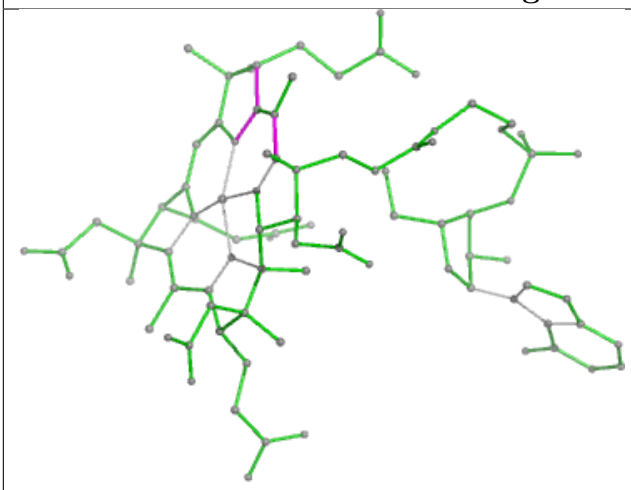
8 monomers are involved in 42 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	C	503	BVQ	9	0
3	D	503	BVQ	6	0
2	F	502	SF4	1	0
3	A	503	BVQ	4	0
3	F	503	BVQ	8	0
3	B	503	BVQ	4	0
3	E	503	BVQ	9	0
2	E	502	SF4	1	0

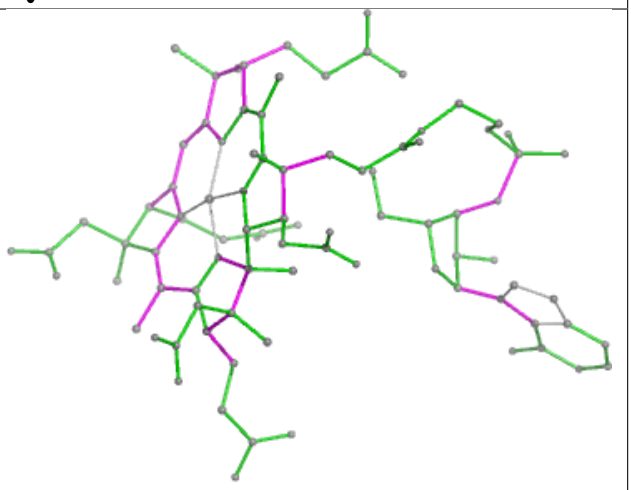
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

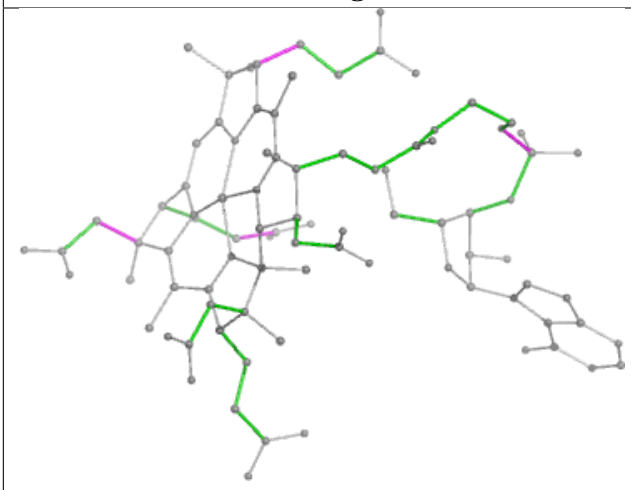
Ligand BVQ C 503



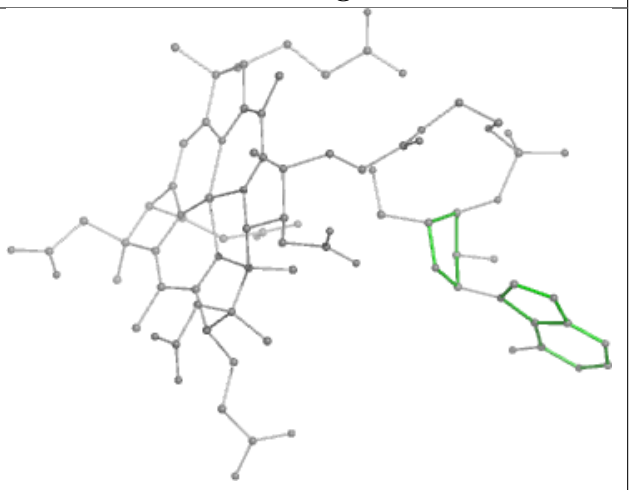
Bond lengths



Bond angles

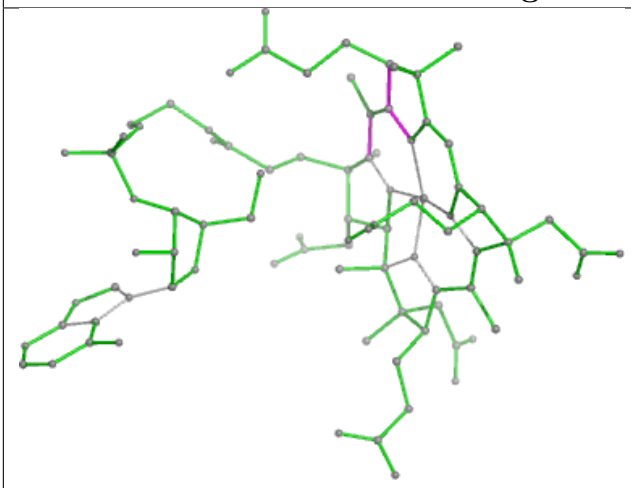


Torsions

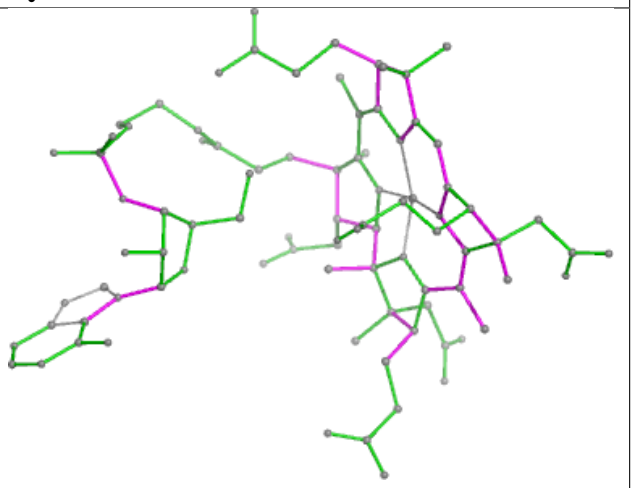


Rings

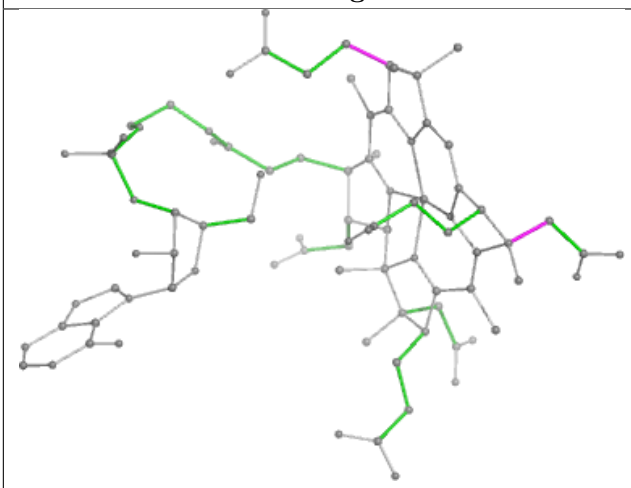
Ligand BVQ D 503



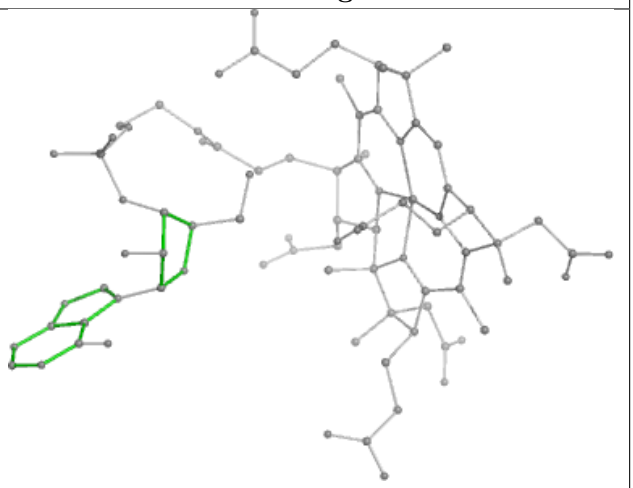
Bond lengths



Bond angles

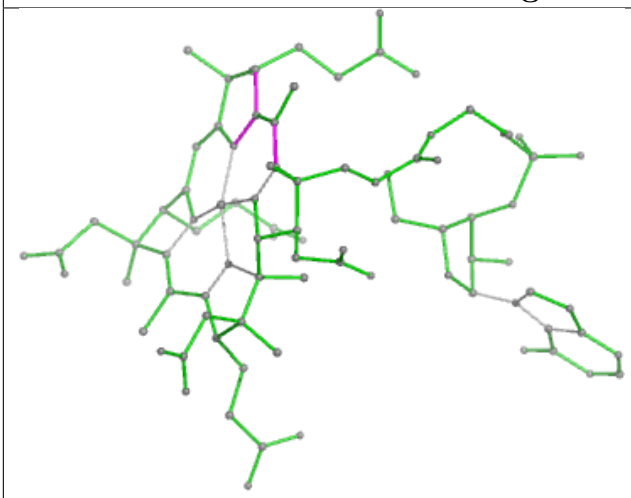


Torsions

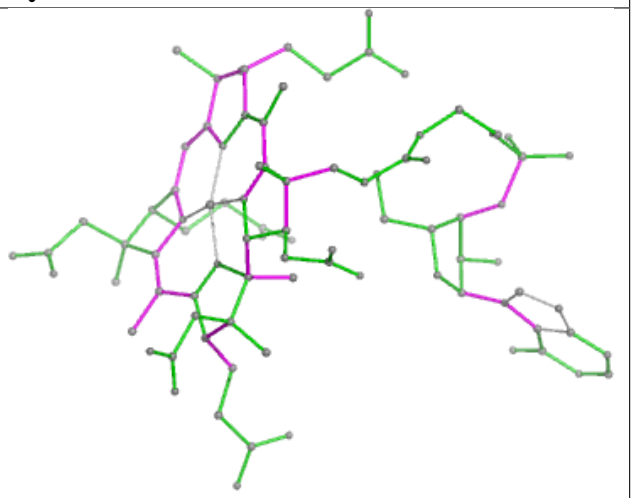


Rings

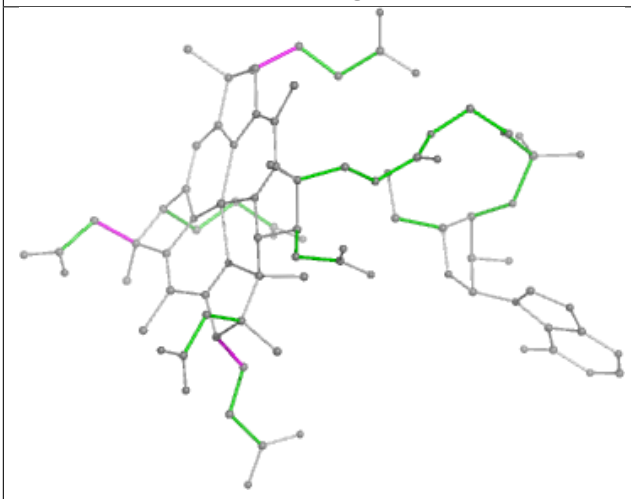
Ligand BVQ A 503



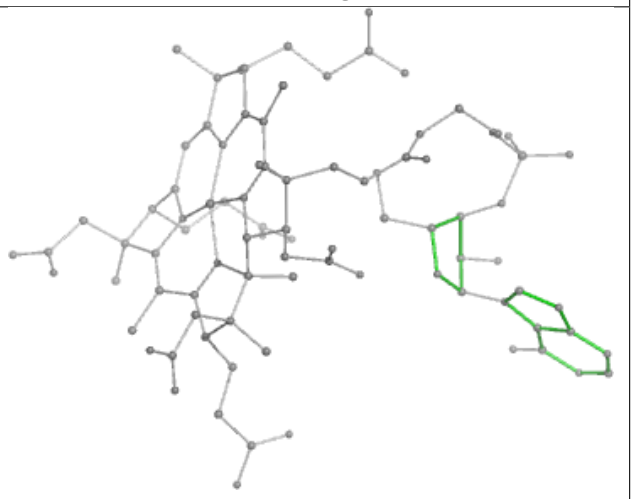
Bond lengths



Bond angles

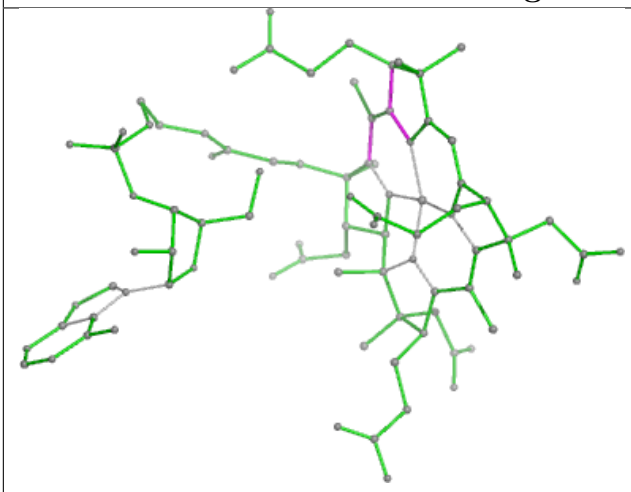


Torsions

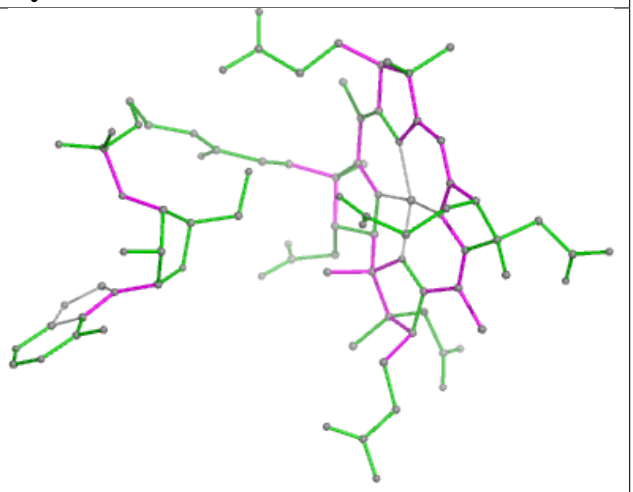


Rings

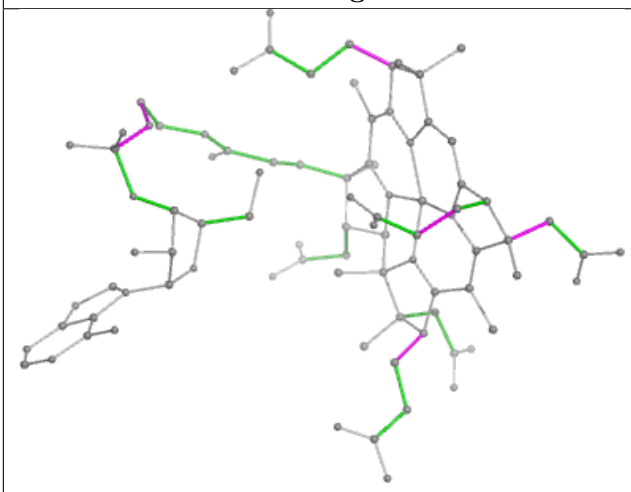
Ligand BVQ F 503



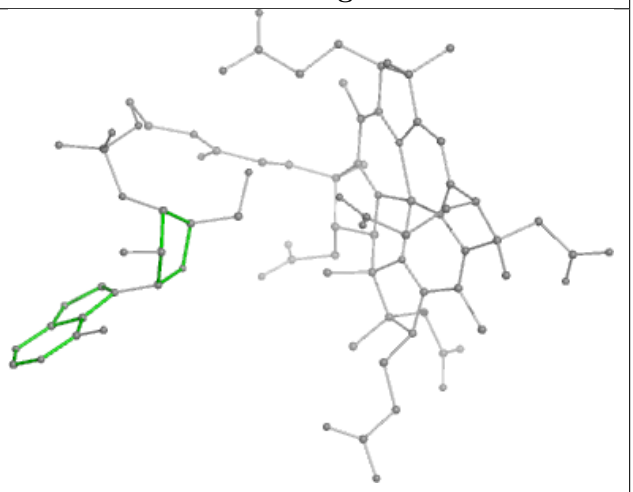
Bond lengths



Bond angles

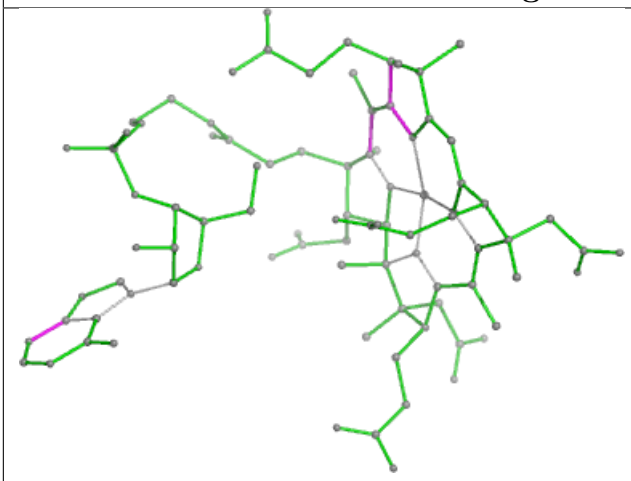


Torsions

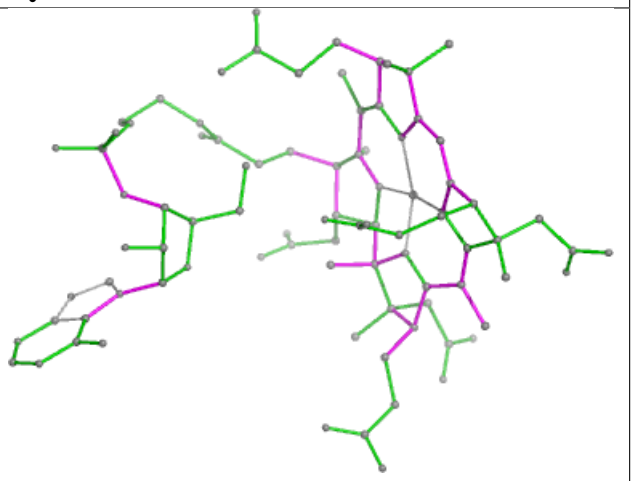


Rings

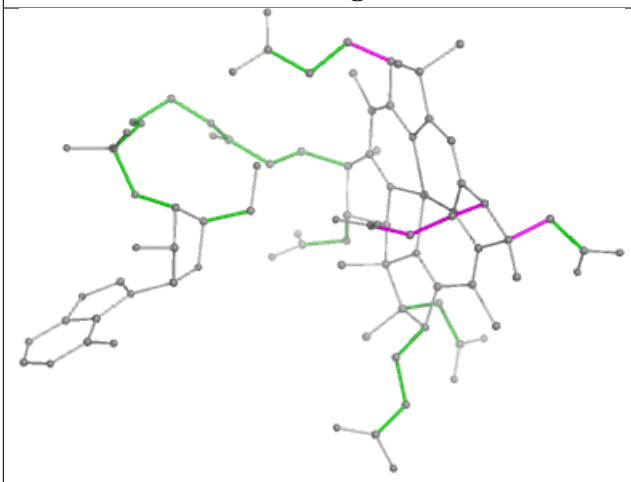
Ligand BVQ B 503



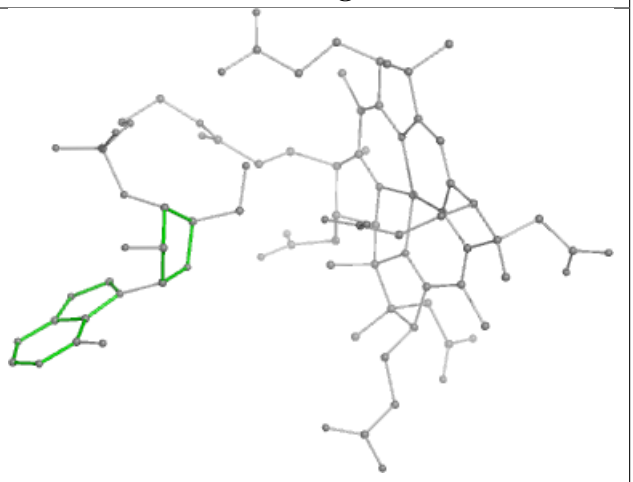
Bond lengths



Bond angles

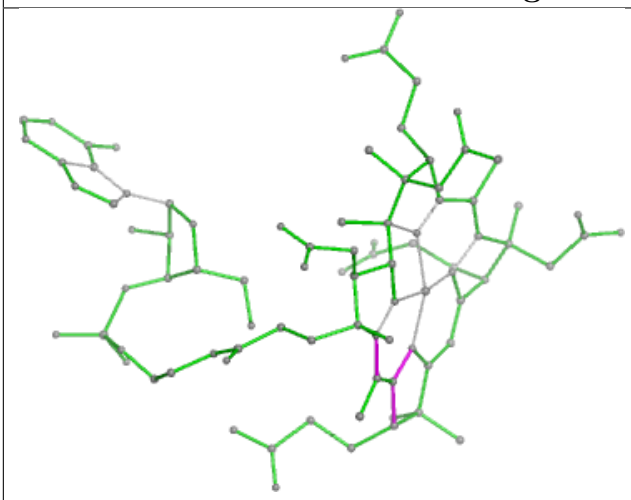


Torsions

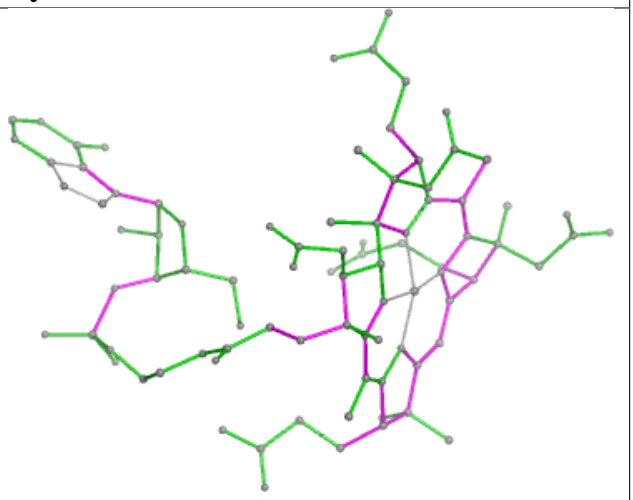


Rings

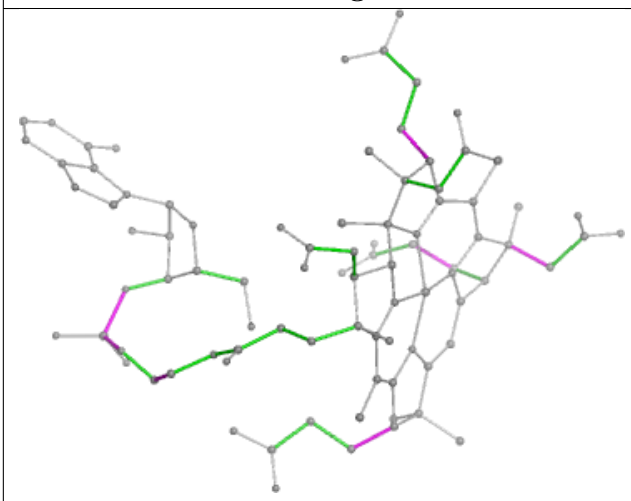
Ligand BVQ E 503



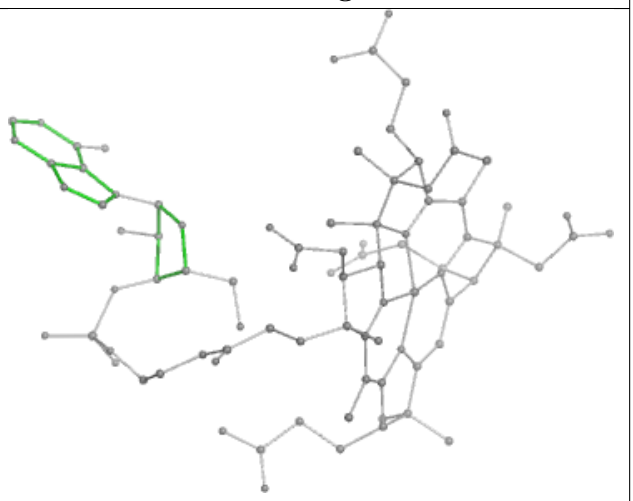
Bond lengths



Bond angles



Torsions



Rings

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

6.1 Protein, DNA and RNA chains

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, 95^{th} 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	458/464 (98%)	0.01	16 (3%)	44	43	20, 35, 53, 67	0
1	B	436/464 (93%)	0.08	33 (7%)	13	13	18, 29, 53, 87	0
1	C	442/464 (95%)	-0.24	4 (0%)	84	84	14, 25, 43, 73	0
1	D	437/464 (94%)	-0.07	19 (4%)	35	34	14, 26, 56, 94	0
1	E	435/464 (93%)	0.34	32 (7%)	14	14	22, 46, 67, 85	0
1	F	429/464 (92%)	-0.12	13 (3%)	50	50	21, 38, 61, 77	0
All	All	2637/2784 (94%)	0.00	117 (4%)	34	34	14, 33, 59, 94	0

All (117) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	410	THR	8.3
1	D	403	VAL	7.2
1	E	396	ASN	6.9
1	E	403	VAL	6.4
1	B	403	VAL	6.4
1	F	396	ASN	6.3
1	D	407	ILE	6.2
1	D	405	TRP	6.2
1	D	399	ILE	6.1
1	F	397	ILE	5.6
1	E	408	ASP	5.6
1	D	396	ASN	5.4
1	D	398	TRP	5.4
1	B	251[A]	MET	5.2
1	D	401	ASP	5.1
1	E	402	GLY	5.0
1	E	395	GLY	4.9
1	B	407	ILE	4.9
1	B	404	GLU	4.8

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Mol	Chain	Res	Type	RSRZ
1	E	26	ASP	4.8
1	B	402	GLY	4.8
1	D	409	ASN	4.4
1	E	399	ILE	4.4
1	D	400	HIS	4.2
1	D	397	ILE	4.1
1	D	6	ASN	4.0
1	D	404	GLU	4.0
1	B	401	ASP	3.9
1	B	400	HIS	3.9
1	E	401	ASP	3.8
1	D	395	GLY	3.7
1	D	406	LEU	3.6
1	E	76	LYS	3.6
1	D	402	GLY	3.6
1	F	405	TRP	3.5
1	E	397	ILE	3.4
1	F	398	TRP	3.4
1	B	399	ILE	3.3
1	E	53	VAL	3.3
1	F	18	ALA	3.3
1	E	24	VAL	3.3
1	A	18	ALA	3.2
1	A	403	VAL	3.2
1	F	76	LYS	3.1
1	F	10	ILE	3.1
1	F	19	GLY	3.1
1	D	394	LYS	3.1
1	B	410	THR	3.0
1	C	76	LYS	3.0
1	E	406	LEU	3.0
1	B	443	TYR	2.9
1	D	408	ASP	2.9
1	E	28	LEU	2.9
1	F	399	ILE	2.9
1	A	154	ALA	2.9
1	B	6	ASN	2.9
1	A	70	ASN	2.8
1	F	255	TRP	2.8
1	C	251[A]	MET	2.7
1	E	409	ASN	2.7
1	F	402	GLY	2.7

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Mol	Chain	Res	Type	RSRZ
1	A	395	GLY	2.7
1	E	59	SER	2.6
1	D	9	GLU	2.6
1	B	249	MET	2.6
1	B	250	CYS	2.6
1	E	51	GLY	2.6
1	E	365	TRP	2.5
1	E	394	LYS	2.5
1	E	23	ILE	2.5
1	B	19	GLY	2.5
1	B	255	TRP	2.5
1	B	244	PHE	2.4
1	B	97	THR	2.4
1	A	69	GLU	2.4
1	E	16	MET	2.4
1	A	26	ASP	2.4
1	B	223	ILE	2.4
1	B	405	TRP	2.4
1	B	98	LEU	2.4
1	B	18	ALA	2.3
1	E	371	LYS	2.3
1	B	76	LYS	2.3
1	B	408	ASP	2.3
1	E	352	GLU	2.3
1	B	26	ASP	2.3
1	B	252	PHE	2.3
1	E	404	GLU	2.2
1	E	354	ARG	2.2
1	A	19	GLY	2.2
1	A	255	TRP	2.2
1	A	98	LEU	2.2
1	B	247	SER	2.2
1	E	328	PHE	2.1
1	B	397	ILE	2.1
1	E	363	LEU	2.1
1	C	415	PRO	2.1
1	E	398	TRP	2.1
1	B	396	ASN	2.1
1	A	443	TYR	2.1
1	A	252	PHE	2.1
1	E	45	PHE	2.1
1	E	405	TRP	2.1

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Mol	Chain	Res	Type	RSRZ
1	B	307	THR	2.1
1	E	400	HIS	2.1
1	B	132	ARG	2.1
1	B	245	CYS	2.1
1	F	53	VAL	2.1
1	A	76	LYS	2.1
1	A	462	LYS	2.0
1	B	50	LYS	2.0
1	F	70	ASN	2.0
1	B	154	ALA	2.0
1	A	50	LYS	2.0
1	C	256	LEU	2.0
1	A	17	THR	2.0
1	E	151	ALA	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, 95^{th} 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
3	BVQ	E	503	89/89	0.94	0.12	29,42,49,59	0
2	SF4	E	502	8/8	0.96	0.06	38,47,52,54	0
3	BVQ	A	503	89/89	0.96	0.11	21,30,36,38	0
3	BVQ	D	503	89/89	0.96	0.12	14,21,26,36	0
2	SF4	E	501	8/8	0.96	0.06	43,51,52,53	0
3	BVQ	B	503	89/89	0.97	0.13	12,22,27,30	0
3	BVQ	C	503	89/89	0.97	0.12	13,21,28,32	0
2	SF4	F	502	8/8	0.97	0.08	32,35,39,39	0
2	SF4	A	501	8/8	0.97	0.06	28,32,34,38	0

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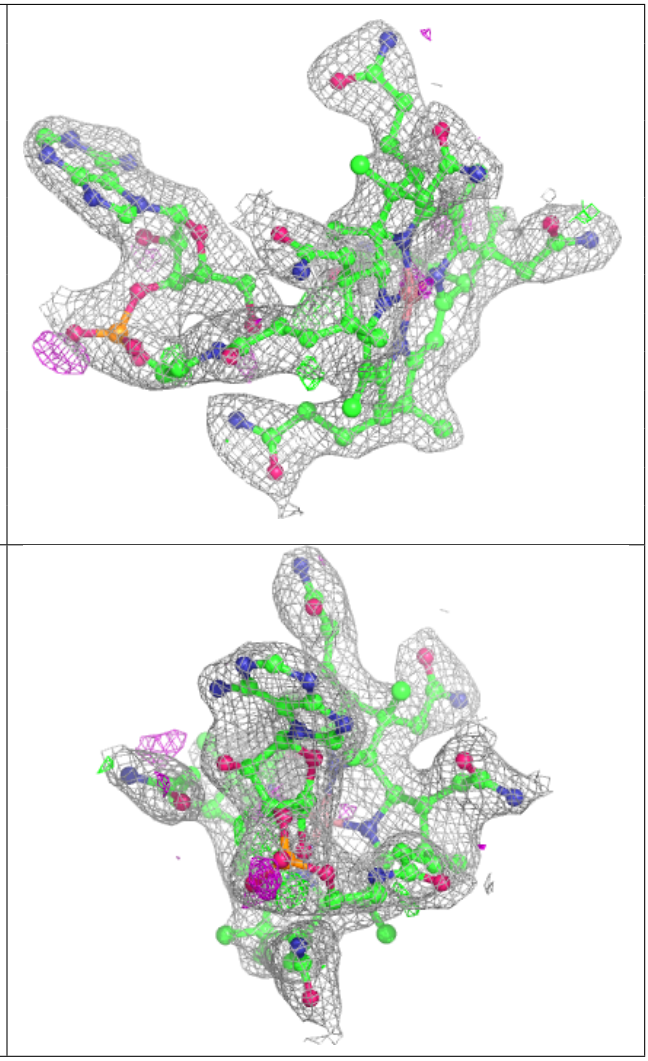
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
3	BVQ	F	503	89/89	0.97	0.11	19,29,36,50	0
2	SF4	C	502	8/8	0.98	0.09	19,23,24,25	0
2	SF4	F	501	8/8	0.98	0.06	33,38,41,44	0
2	SF4	A	502	8/8	0.98	0.06	29,32,35,36	0
2	SF4	B	502	8/8	0.99	0.05	20,23,24,24	0
2	SF4	C	501	8/8	0.99	0.08	19,23,25,28	0
2	SF4	B	501	8/8	0.99	0.06	20,24,25,28	0
2	SF4	D	501	8/8	0.99	0.05	19,26,28,30	0
2	SF4	D	502	8/8	0.99	0.09	22,24,26,29	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.

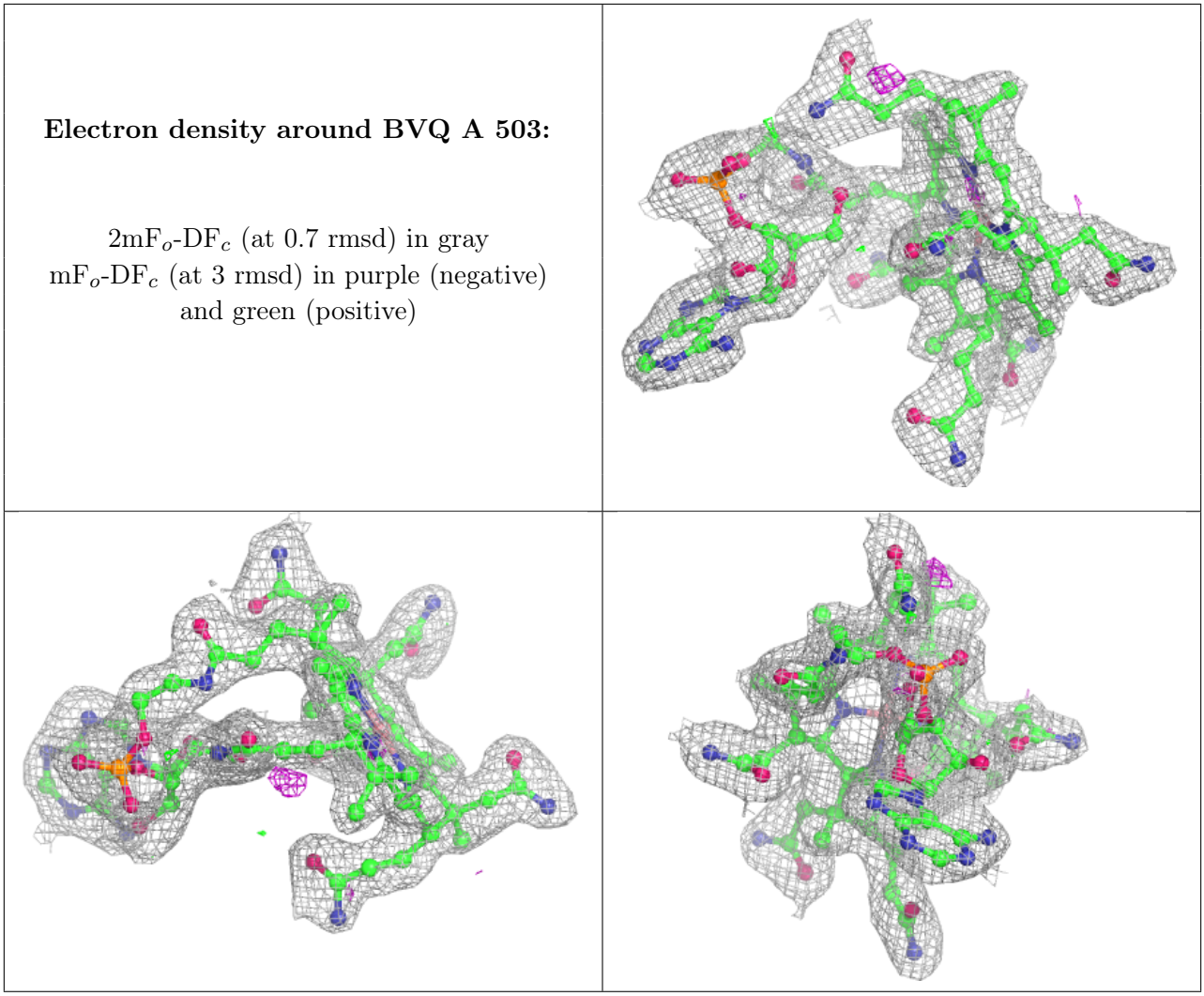
Electron density around BVQ E 503:

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



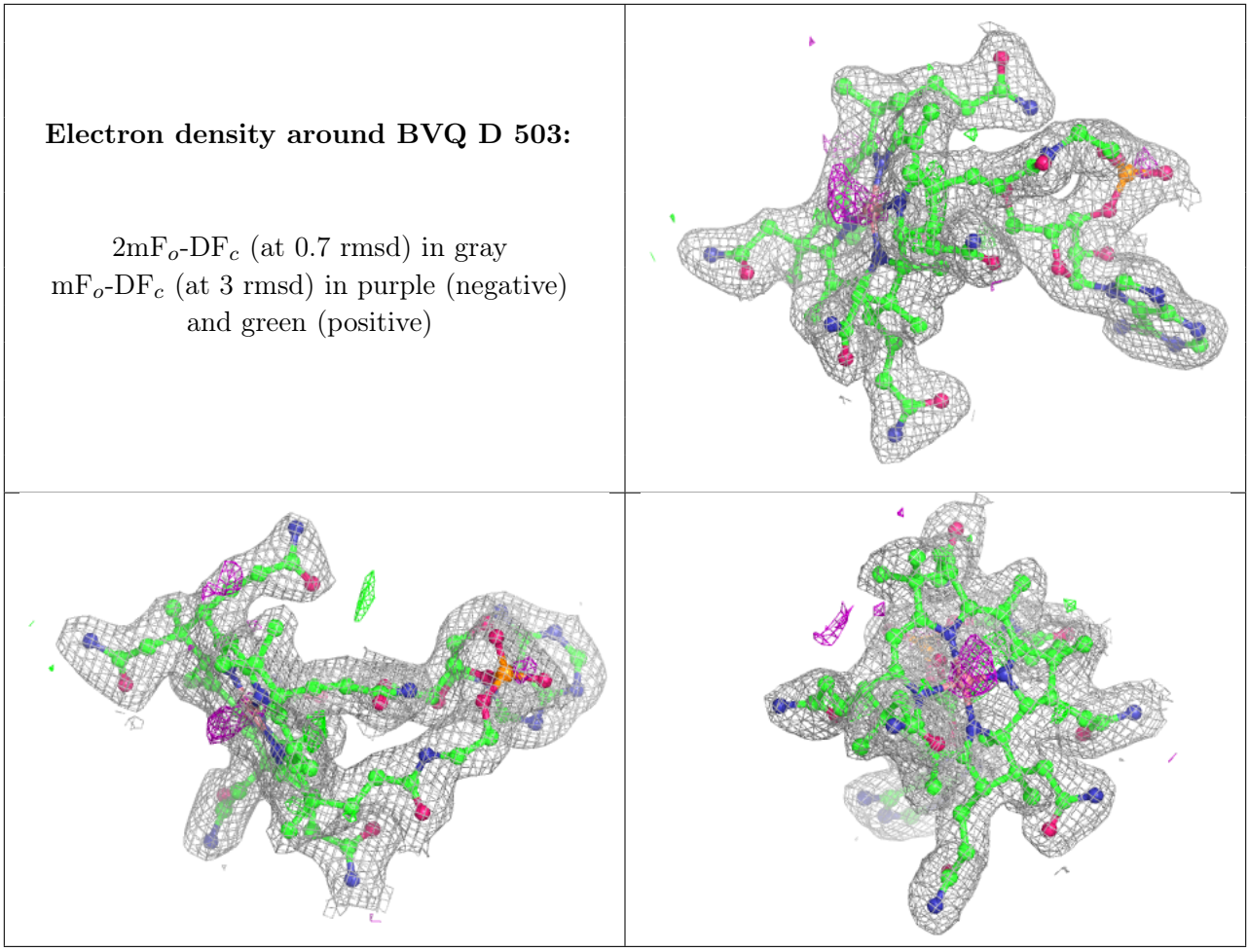
Electron density around BVQ A 503:

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



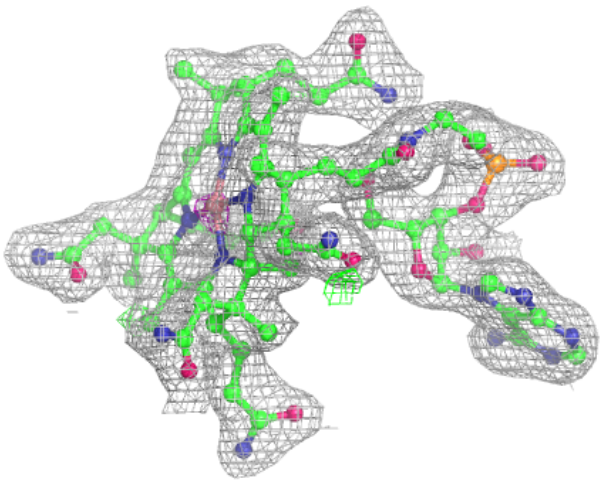
Electron density around BVQ D 503:

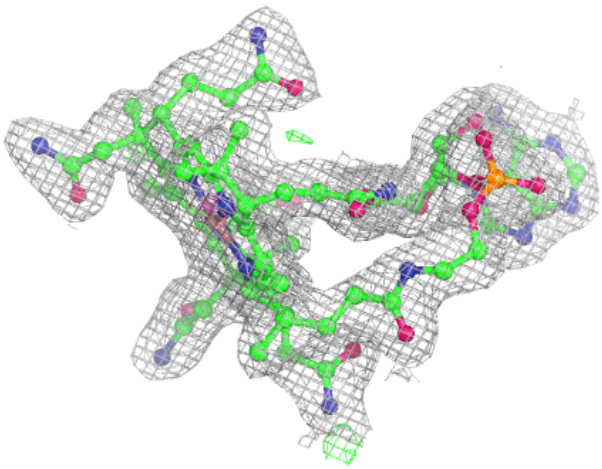
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

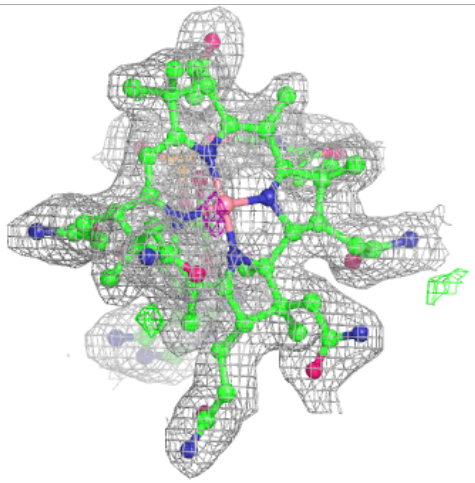


Electron density around BVQ B 503:

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

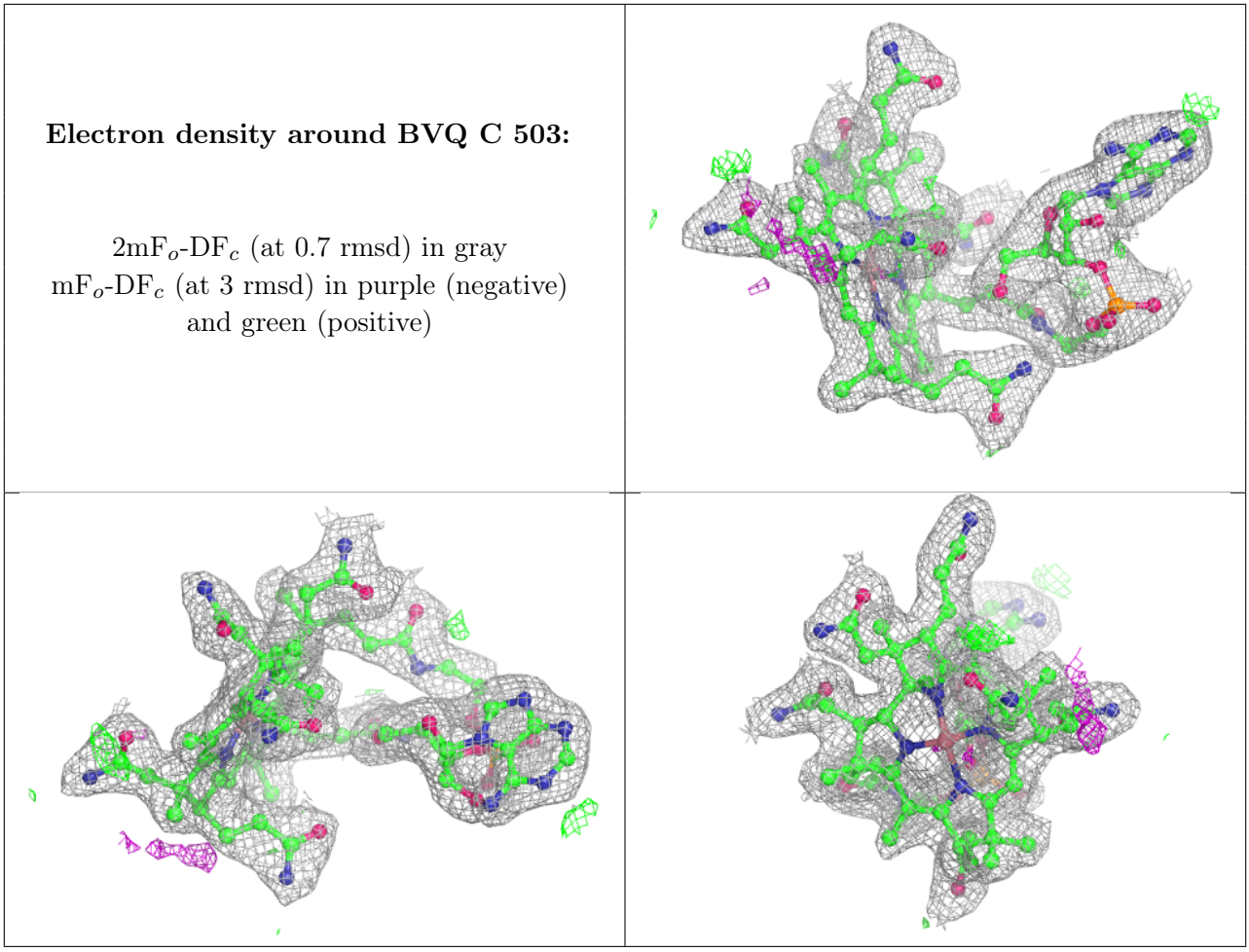






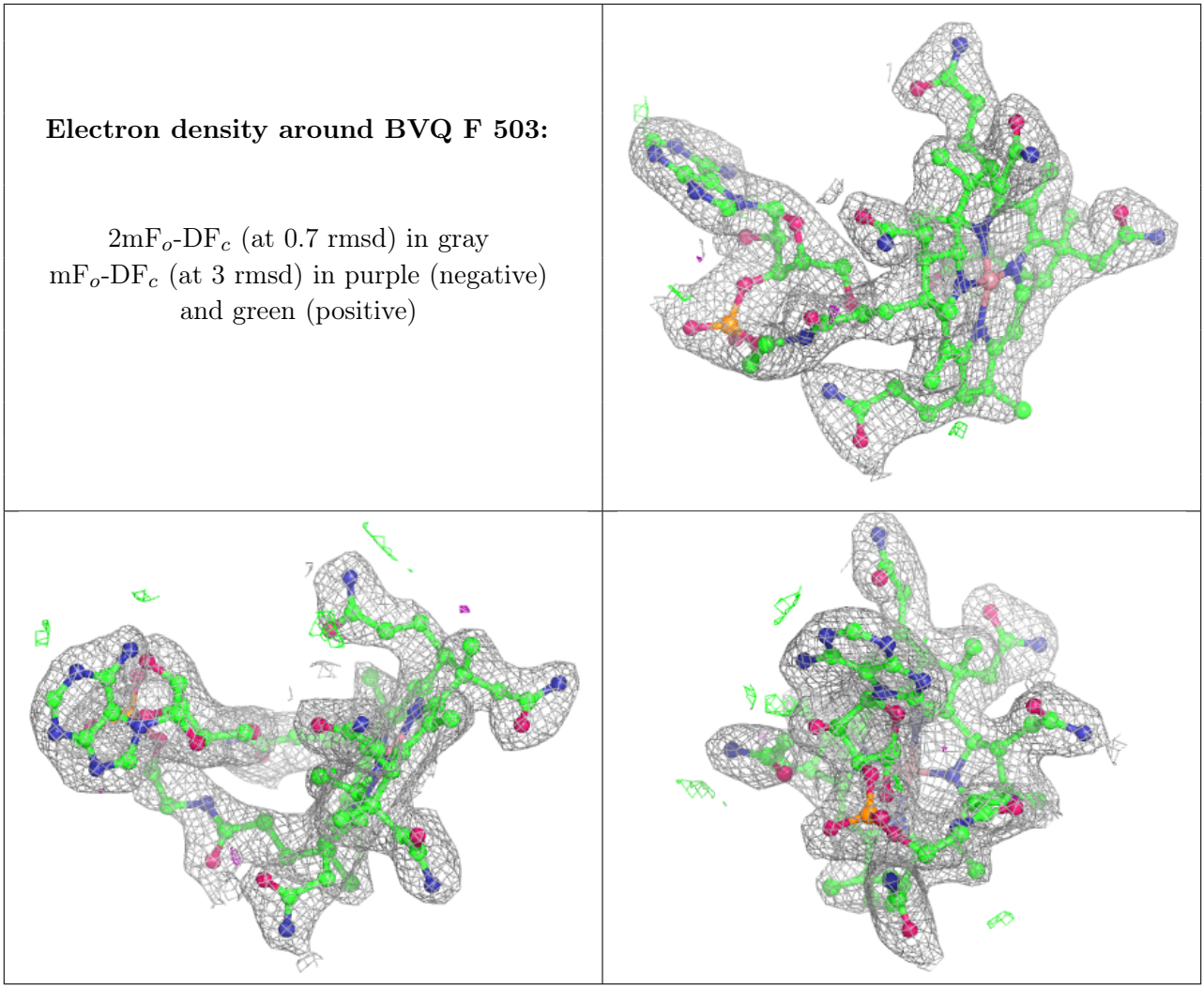
Electron density around BVQ C 503:

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



Electron density around BVQ F 503:

$2mF_o$-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.