Full wwPDB X-ray Structure Validation Report (i)

Nov 21, 2023 – 06:28 PM JST

PDB ID	:	7XAY
Title	:	Crystal structure of Hat1-Hat2-Asf1-H3-H4
Authors	:	Yue, Y.; Yang, W.S.; Xu, R.M.
Deposited on	:	2022-03-19
Resolution	:	3.30 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:

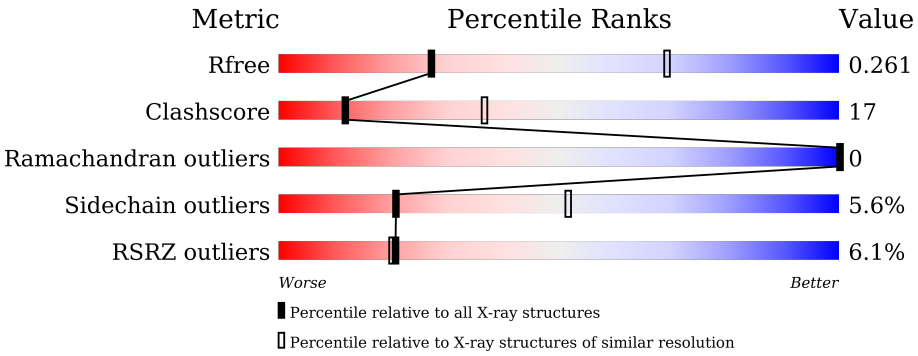
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

1 Overall quality at a glance (i)

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

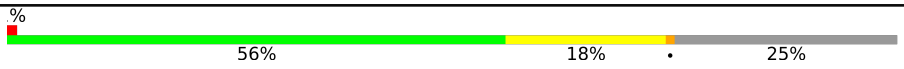
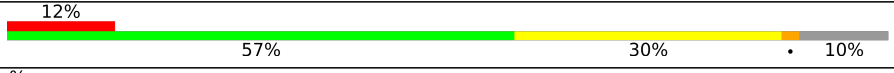
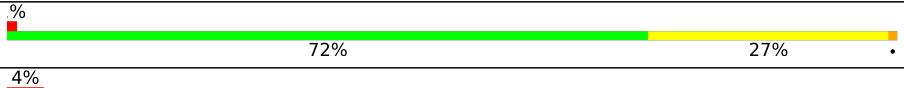
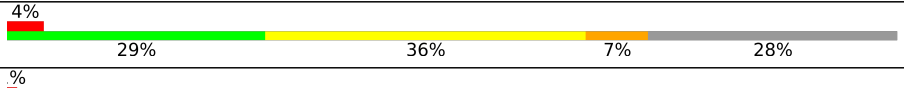
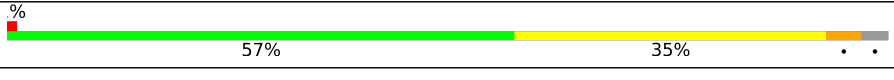
The reported resolution of this entry is 3.30 Å.

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	1149 (3.34-3.26)
Clashscore	141614	1205 (3.34-3.26)
Ramachandran outliers	138981	1183 (3.34-3.26)
Sidechain outliers	138945	1182 (3.34-3.26)
RSRZ outliers	127900	1115 (3.34-3.26)

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	416	
2	B	401	
3	C	154	
4	D	135	
5	E	96	

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 8299 atoms, of which 32 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 Soluble cytochrome b562,Histone acetyltransferase type B catalytic subunit.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	311	Total	C	N	O	S	0	0	0
			2592	1676	423	489	4			

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-89	TRP	MET	conflict	UNP P0ABE7
A	6	ILE	HIS	conflict	UNP P0ABE7
A	10	LEU	-	linker	UNP P0ABE7

- Molecule 2 is a protein called Histone acetyltransferase type B subunit 2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	360	Total	C	N	O	S	0	0	0
			2859	1801	483	565	10			

- Molecule 3 is a protein called Histone chaperone asf1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	154	Total	C	N	O	S	0	0	0
			1237	800	199	235	3			

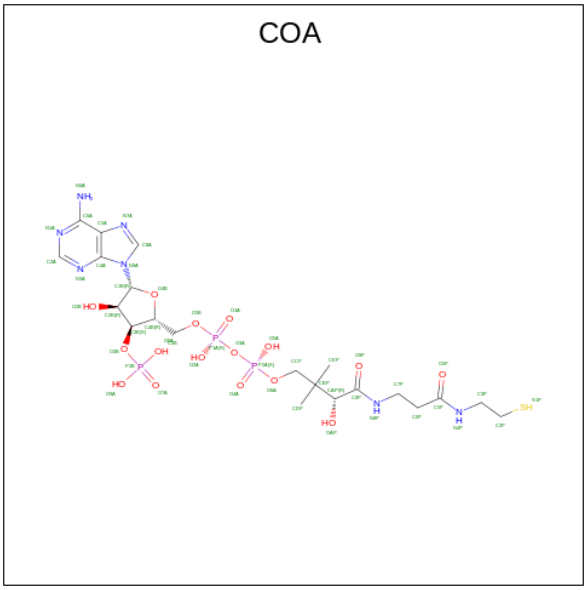
- Molecule 4 is a protein called Histone H3.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
4	D	97	Total	C	N	O	0	0	0
			789	494	156	139			

- Molecule 5 is a protein called Histone H4.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
5	E	93	742	468	149	125	0	0	0

- Molecule 6 is COENZYME A (three-letter code: COA) (formula: $C_{21}H_{36}N_7O_{16}P_3S$) (labeled as "Ligand of Interest" by depositor).



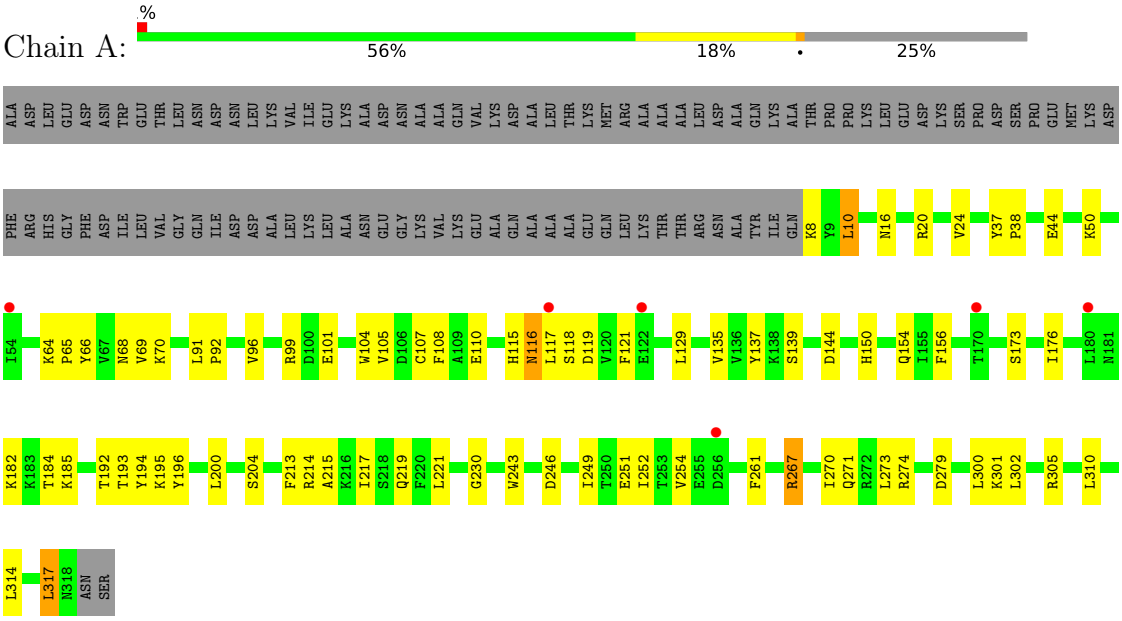
Mol	Chain	Residues	Atoms							ZeroOcc	AltConf
			Total	C	H	N	O	P	S		
6	A	1	80	21	32	7	16	3	1	0	0

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.

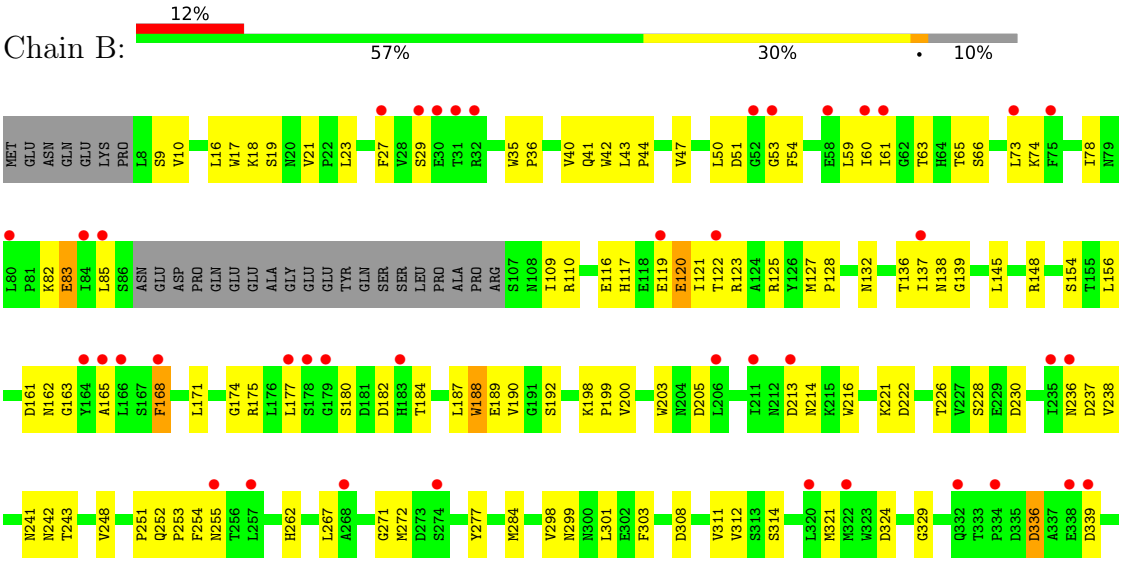
• Molecule 1: Soluble cytochrome b562,Histone acetyltransferase type B catalytic subunit

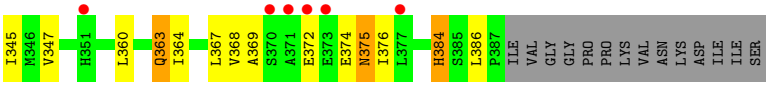
Chain A:



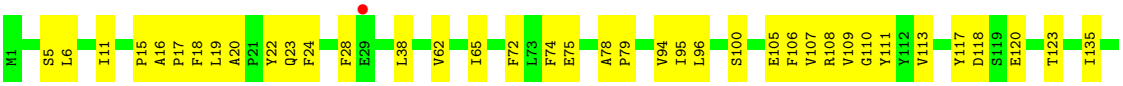
• Molecule 2: Histone acetyltransferase type B subunit 2

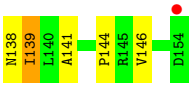
Chain B:



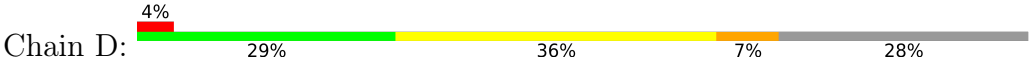


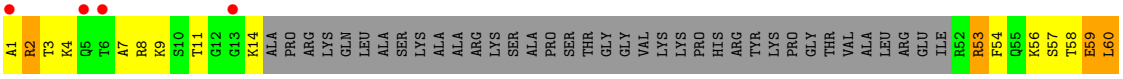
• Molecule 3: Histone chaperone asf1





• Molecule 4: Histone H3





• Molecule 5: Histone H4

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	96.41Å 124.68Å 161.07Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	22.40 – 3.30 82.72 – 3.30	Depositor EDS
% Data completeness (in resolution range)	98.8 (22.40-3.30) 95.3 (82.72-3.30)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.62 (at 3.33Å)	Xtriage
Refinement program	PHENIX 1.19.2_4158	Depositor
R, R_{free}	0.230 , 0.256 0.232 , 0.261	Depositor DCC
R_{free} test set	2000 reflections (6.77%)	wwPDB-VP
Wilson B-factor (Å^2)	79.7	Xtriage
Anisotropy	0.045	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.31 , 26.4	EDS
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.88	EDS
Total number of atoms	8299	wwPDB-VP
Average B, all atoms (Å^2)	77.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.99% 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: COA

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	0.30	0/2654	0.42	0/3586
2	B	0.25	0/2929	0.45	0/3988
3	C	0.25	0/1265	0.43	0/1723
4	D	0.26	0/795	0.42	0/1057
5	E	0.24	0/750	0.41	0/999
All	All	0.27	0/8393	0.43	0/11353

There are no bond length outliers.

There are no bond angle outliers.

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	2592	0	2544	58	0
2	B	2859	0	2731	111	0
3	C	1237	0	1244	36	0
4	D	789	0	846	66	0
5	E	742	0	806	46	0
6	A	48	32	32	4	0
All	All	8267	32	8203	285	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 17.

All (285) 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)
3:C:11:ILE:HG12	3:C:139:ILE:HD11	1.28	1.15
5:E:26:ILE:HG13	5:E:59:LYS:HD2	1.40	1.04
4:D:128:ARG:HD2	5:E:57:VAL:HG23	1.47	0.94
4:D:100:LEU:HD11	5:E:58:LEU:HD12	1.50	0.94
3:C:100:SER:HB3	3:C:105:GLU:HA	1.58	0.86
4:D:60:LEU:H	4:D:60:LEU:HD22	1.39	0.85
2:B:145:LEU:HD11	2:B:190:VAL:HG11	1.57	0.84
2:B:47:VAL:HG11	2:B:85:LEU:HD11	1.58	0.83
2:B:324:ASP:HB2	2:B:345:ILE:HD11	1.59	0.83
2:B:53:GLY:HA2	2:B:82:LYS:HD2	1.62	0.80
2:B:236:ASN:HB3	2:B:243:THR:O	1.83	0.78
4:D:62:ILE:HD11	5:E:29:ILE:HD12	1.65	0.78
3:C:11:ILE:CG1	3:C:139:ILE:HD11	2.11	0.78
5:E:26:ILE:CG1	5:E:59:LYS:HD2	2.15	0.76
5:E:30:THR:OG1	5:E:32:PRO:HD2	1.85	0.76
2:B:83:GLU:HG2	4:D:56:LYS:HE3	1.68	0.76
2:B:214:ASN:HB3	2:B:226:THR:HG22	1.69	0.74
2:B:360:LEU:HD13	2:B:368:VAL:HG22	1.69	0.74
3:C:11:ILE:HG12	3:C:139:ILE:CD1	2.14	0.74
6:A:401:COA:S1P	5:E:12:LYS:NZ	2.59	0.72
2:B:321:MET:HG2	2:B:347:VAL:HG22	1.71	0.72
2:B:78:ILE:HD13	2:B:109:ILE:HG23	1.72	0.71
4:D:83:ARG:HB3	5:E:80:THR:HG23	1.72	0.70
2:B:120:GLU:O	2:B:138:ASN:HA	1.92	0.69
2:B:18:LYS:HA	2:B:21:VAL:HG23	1.74	0.69
4:D:59:GLU:HA	4:D:59:GLU:OE1	1.91	0.69
4:D:70:LEU:O	4:D:74:ILE:HG12	1.92	0.69
4:D:71:VAL:HG11	4:D:89:ILE:HD12	1.74	0.69
2:B:384:HIS:HB3	2:B:386:LEU:CD2	2.23	0.69
2:B:187:LEU:O	2:B:200:VAL:HG22	1.93	0.68
3:C:17:PRO:HG2	3:C:20:ALA:HB2	1.74	0.68
1:A:274:ARG:HE	1:A:317:LEU:CD1	2.07	0.68
5:E:46:ILE:HD11	5:E:51:TYR:OH	1.94	0.68
2:B:360:LEU:CD1	2:B:368:VAL:HG22	2.23	0.68
1:A:10:LEU:HD21	1:A:50:LYS:NZ	2.08	0.68
3:C:18:PHE:HB2	3:C:135:ILE:HG22	1.76	0.67
4:D:60:LEU:HD23	4:D:60:LEU:C	2.15	0.67
1:A:105:VAL:HA	1:A:108:PHE:CE2	2.29	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:94:VAL:HG13	4:D:126:LEU:HD22	1.77	0.67
1:A:195:LYS:HE3	1:A:249:ILE:HD11	1.75	0.67
2:B:384:HIS:HB3	2:B:386:LEU:HD23	1.77	0.66
5:E:59:LYS:O	5:E:63:GLU:HG3	1.95	0.66
2:B:324:ASP:HB2	2:B:345:ILE:CD1	2.24	0.66
4:D:97:GLU:O	4:D:101:VAL:HG23	1.95	0.65
1:A:270:ILE:O	1:A:274:ARG:HG3	1.96	0.65
4:D:60:LEU:H	4:D:60:LEU:CD2	2.09	0.65
3:C:6:LEU:HD12	3:C:107:VAL:HG11	1.78	0.65
1:A:267:ARG:NH1	1:A:271:GLN:OE1	2.30	0.64
2:B:53:GLY:HA2	2:B:82:LYS:CD	2.28	0.64
2:B:174:GLY:O	2:B:189:GLU:HA	1.98	0.64
2:B:198:LYS:HG2	2:B:199:PRO:HD2	1.78	0.64
3:C:96:LEU:HD23	3:C:110:GLY:HA2	1.80	0.63
2:B:127:MET:HA	2:B:168:PHE:CD2	2.34	0.63
1:A:173:SER:HB2	1:A:194:TYR:CE1	2.34	0.62
2:B:35:TRP:CD2	2:B:65:THR:HG22	2.34	0.62
4:D:68:GLN:OE1	4:D:72:ARG:NH2	2.32	0.62
2:B:163:GLY:HA2	2:B:180:SER:HA	1.82	0.62
2:B:214:ASN:CB	2:B:226:THR:HG22	2.30	0.62
2:B:251:PRO:HG2	2:B:277:TYR:CZ	2.34	0.61
2:B:372:GLU:HG2	2:B:376:ILE:HB	1.81	0.61
3:C:23:GLN:HG2	3:C:75:GLU:HG2	1.83	0.61
3:C:108:ARG:NH1	4:D:131:ARG:O	2.33	0.61
4:D:128:ARG:HG3	4:D:133:GLU:OE2	2.00	0.61
2:B:119:GLU:HA	2:B:119:GLU:OE1	2.00	0.61
1:A:192:THR:OG1	1:A:219:GLN:HB2	2.01	0.60
1:A:118:SER:HB2	1:A:137:TYR:OH	2.00	0.60
4:D:56:LYS:HG2	4:D:57:SER:H	1.66	0.60
1:A:68:ASN:ND2	1:A:70:LYS:HE2	2.17	0.60
1:A:135:VAL:HG23	1:A:182:LYS:HB2	1.82	0.60
2:B:123:ARG:HH11	2:B:125:ARG:HH12	1.49	0.59
5:E:31:LYS:HB3	5:E:32:PRO:HD3	1.84	0.59
1:A:37:TYR:N	1:A:38:PRO:HD2	2.16	0.59
1:A:69:VAL:O	1:A:99:ARG:NH2	2.34	0.59
3:C:11:ILE:HD13	3:C:141:ALA:HB2	1.83	0.59
2:B:228:SER:HB3	2:B:230:ASP:OD1	2.02	0.59
3:C:106:PHE:CD2	3:C:107:VAL:HG23	2.37	0.59
2:B:177:LEU:HB3	2:B:214:ASN:ND2	2.16	0.58
1:A:267:ARG:HH21	6:A:401:COA:C6A	2.16	0.58
3:C:65:ILE:HD12	3:C:65:ILE:H	1.68	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:91:LYS:HE2	5:E:95:ARG:HH22	1.68	0.58
3:C:78:ALA:HB1	3:C:79:PRO:HD2	1.86	0.58
1:A:8:LYS:HB2	1:A:8:LYS:NZ	2.19	0.58
1:A:273:LEU:HD21	1:A:300:LEU:HD13	1.85	0.57
4:D:73:GLU:HG3	5:E:22:LEU:HB3	1.87	0.57
1:A:65:PRO:HG2	1:A:96:VAL:HG22	1.84	0.57
2:B:63:THR:CG2	2:B:74:LYS:HE3	2.34	0.57
2:B:23:LEU:HD23	4:D:65:LEU:HD23	1.87	0.57
3:C:11:ILE:HD13	3:C:141:ALA:CB	2.34	0.57
1:A:185:LYS:HD2	1:A:185:LYS:N	2.20	0.57
4:D:71:VAL:HG21	4:D:89:ILE:CD1	2.35	0.56
4:D:100:LEU:CD1	5:E:58:LEU:HD12	2.31	0.56
3:C:100:SER:CB	3:C:105:GLU:HA	2.32	0.56
2:B:35:TRP:CE2	2:B:65:THR:HG22	2.41	0.56
2:B:42:TRP:HA	2:B:59:LEU:HD23	1.87	0.55
4:D:75:ALA:O	4:D:80:THR:HG22	2.05	0.55
4:D:78:PHE:CZ	5:E:67:ARG:HB2	2.42	0.55
2:B:205:ASP:OD1	2:B:205:ASP:N	2.40	0.55
3:C:100:SER:HB3	3:C:105:GLU:CA	2.33	0.55
2:B:18:LYS:HE2	4:D:53:ARG:HG3	1.88	0.55
3:C:113:VAL:HG13	3:C:139:ILE:HG22	1.88	0.55
2:B:36:PRO:HD3	2:B:375:ASN:ND2	2.22	0.55
2:B:222:ASP:O	2:B:238:VAL:HG22	2.07	0.54
4:D:67:PHE:O	4:D:71:VAL:HG12	2.07	0.54
2:B:251:PRO:HG2	2:B:277:TYR:OH	2.08	0.54
3:C:109:VAL:HG13	3:C:146:VAL:HG22	1.90	0.54
2:B:324:ASP:HB2	2:B:345:ILE:CG1	2.38	0.53
4:D:95:SER:HB3	5:E:90:LEU:HD11	1.90	0.53
1:A:37:TYR:CD1	1:A:38:PRO:HD3	2.44	0.53
1:A:279:ASP:OD1	1:A:279:ASP:N	2.41	0.53
2:B:203:TRP:NE1	2:B:243:THR:HG21	2.23	0.53
2:B:145:LEU:HB2	2:B:154:SER:HB2	1.90	0.53
4:D:128:ARG:HD2	5:E:57:VAL:CG2	2.32	0.53
2:B:66:SER:HB2	4:D:7:ALA:HB3	1.91	0.52
2:B:35:TRP:CH2	4:D:9:LYS:HB2	2.45	0.52
2:B:139:GLY:O	2:B:162:ASN:HB2	2.09	0.52
1:A:37:TYR:CE1	5:E:17:ARG:HB2	2.44	0.52
2:B:42:TRP:CZ2	2:B:369:ALA:HB2	2.44	0.52
5:E:49:LEU:HD23	5:E:49:LEU:H	1.74	0.52
1:A:66:TYR:OH	1:A:101:GLU:HG3	2.08	0.52
2:B:18:LYS:HA	2:B:21:VAL:CG2	2.39	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:41:GLN:OE1	2:B:125:ARG:HA	2.09	0.52
1:A:16:ASN:ND2	1:A:44:GLU:OE1	2.40	0.51
2:B:254:PHE:HA	2:B:271:GLY:HA3	1.91	0.51
4:D:67:PHE:CD2	4:D:93:GLN:HG3	2.45	0.51
1:A:215:ALA:HB2	1:A:249:ILE:HD12	1.93	0.51
2:B:242:ASN:O	2:B:243:THR:HB	2.11	0.51
5:E:26:ILE:HG23	5:E:55:ARG:HG3	1.92	0.51
4:D:96:VAL:HG21	5:E:62:LEU:HD13	1.92	0.51
1:A:91:LEU:HB3	1:A:92:PRO:HD2	1.92	0.51
5:E:10:LEU:O	5:E:10:LEU:HD12	2.10	0.51
1:A:150:HIS:O	1:A:154:GLN:HB2	2.11	0.51
2:B:272:MET:SD	4:D:1:ALA:HB3	2.51	0.51
2:B:187:LEU:HG	2:B:200:VAL:HG22	1.93	0.50
1:A:195:LYS:HE3	1:A:249:ILE:CD1	2.40	0.50
4:D:3:THR:HG23	4:D:3:THR:O	2.11	0.50
2:B:61:ILE:HG13	2:B:74:LYS:HB2	1.94	0.50
2:B:171:LEU:HD12	2:B:221:LYS:HA	1.93	0.50
2:B:187:LEU:HG	2:B:200:VAL:CG2	2.42	0.50
4:D:108:ASN:O	4:D:112:ILE:HG12	2.11	0.50
3:C:11:ILE:N	3:C:11:ILE:HD12	2.27	0.50
2:B:237:ASP:O	2:B:243:THR:HA	2.11	0.50
4:D:68:GLN:HA	4:D:71:VAL:HG12	1.93	0.49
5:E:30:THR:HG23	5:E:33:ALA:HB2	1.94	0.49
1:A:65:PRO:CG	1:A:96:VAL:HG22	2.42	0.49
1:A:116:ASN:HB2	1:A:119:ASP:OD2	2.12	0.49
4:D:71:VAL:HG23	5:E:66:ILE:HD11	1.93	0.49
1:A:214:ARG:HD3	2:B:329:GLY:O	2.12	0.49
2:B:255:ASN:H	2:B:271:GLY:HA2	1.77	0.49
4:D:93:GLN:O	4:D:97:GLU:HG3	2.12	0.49
2:B:372:GLU:OE2	2:B:374:GLU:HB3	2.12	0.49
4:D:60:LEU:CD2	4:D:60:LEU:N	2.72	0.49
4:D:56:LYS:HG2	4:D:57:SER:N	2.27	0.49
4:D:71:VAL:HG23	5:E:66:ILE:CD1	2.43	0.49
2:B:253:PRO:O	2:B:271:GLY:HA3	2.12	0.49
2:B:44:PRO:HA	2:B:363:GLN:OE1	2.12	0.48
2:B:175:ARG:HG2	2:B:216:TRP:CZ2	2.48	0.48
4:D:67:PHE:CG	4:D:93:GLN:HG3	2.49	0.48
4:D:108:ASN:HB2	5:E:43:VAL:HG22	1.93	0.48
1:A:221:LEU:HD12	6:A:401:COA:H72	1.95	0.48
2:B:161:ASP:OD1	2:B:162:ASN:N	2.45	0.48
1:A:10:LEU:HD21	1:A:50:LYS:HZ2	1.79	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:54:VAL:HA	5:E:57:VAL:HG12	1.96	0.48
2:B:123:ARG:HH11	2:B:125:ARG:NH1	2.12	0.47
3:C:16:ALA:HB1	3:C:17:PRO:HD2	1.96	0.47
2:B:66:SER:HB2	4:D:7:ALA:CB	2.45	0.47
2:B:299:ASN:HB3	4:D:2:ARG:HD2	1.95	0.47
2:B:122:THR:OG1	2:B:137:ILE:HG23	2.13	0.47
4:D:78:PHE:O	4:D:79:LYS:HG2	2.13	0.47
4:D:103:LEU:HA	4:D:131:ARG:NH2	2.30	0.47
2:B:36:PRO:HD3	2:B:375:ASN:HD21	1.80	0.47
2:B:51:ASP:OD1	2:B:51:ASP:N	2.48	0.47
1:A:184:THR:O	1:A:185:LYS:HB2	2.15	0.47
1:A:274:ARG:HE	1:A:317:LEU:HD11	1.77	0.47
2:B:177:LEU:HB3	2:B:214:ASN:HD21	1.77	0.47
5:E:78:ARG:NH2	5:E:85:ASP:OD2	2.48	0.47
4:D:95:SER:CB	5:E:90:LEU:HD11	2.45	0.47
2:B:175:ARG:HD3	2:B:216:TRP:CH2	2.50	0.47
5:E:8:LYS:O	5:E:8:LYS:HG3	2.15	0.47
2:B:248:VAL:HG21	2:B:284:MET:HE3	1.97	0.46
1:A:176:ILE:HG12	1:A:192:THR:HG22	1.96	0.46
2:B:40:VAL:HG22	2:B:61:ILE:HG22	1.98	0.46
2:B:132:ASN:ND2	2:B:148:ARG:HB2	2.30	0.46
4:D:68:GLN:HA	4:D:71:VAL:CG1	2.45	0.46
1:A:310:LEU:O	1:A:314:LEU:HG	2.14	0.46
3:C:11:ILE:HD12	3:C:11:ILE:H	1.79	0.46
3:C:11:ILE:HG13	3:C:24:PHE:CD1	2.51	0.46
3:C:95:ILE:CG1	3:C:111:TYR:HB2	2.45	0.46
3:C:5:SER:O	3:C:28:PHE:HB2	2.16	0.46
3:C:111:TYR:CE1	3:C:144:PRO:HB3	2.51	0.46
4:D:79:LYS:O	4:D:79:LYS:HG3	2.14	0.46
4:D:99:TYR:OH	4:D:133:GLU:OE2	2.34	0.46
2:B:63:THR:HG21	2:B:74:LYS:HE3	1.98	0.45
2:B:262:HIS:CD2	2:B:308:ASP:HB2	2.52	0.45
2:B:375:ASN:OD1	2:B:375:ASN:N	2.49	0.45
1:A:37:TYR:N	1:A:38:PRO:CD	2.80	0.45
2:B:117:HIS:CE1	2:B:121:ILE:HG12	2.51	0.45
1:A:300:LEU:HB3	1:A:302:LEU:HG	1.98	0.45
2:B:163:GLY:CA	2:B:180:SER:HA	2.46	0.45
2:B:386:LEU:HD23	2:B:386:LEU:H	1.80	0.45
3:C:15:PRO:HB3	3:C:138:ASN:HB2	1.98	0.45
2:B:78:ILE:CD1	2:B:109:ILE:HG23	2.44	0.45
1:A:37:TYR:CG	1:A:38:PRO:HD3	2.52	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:301:LEU:HD12	2:B:312:VAL:O	2.17	0.45
5:E:30:THR:CG2	5:E:33:ALA:HB2	2.46	0.45
1:A:68:ASN:HD21	1:A:70:LYS:HE2	1.81	0.45
1:A:254:VAL:HG11	1:A:261:PHE:CE2	2.52	0.45
1:A:10:LEU:C	1:A:10:LEU:HD23	2.38	0.45
2:B:123:ARG:NH1	2:B:125:ARG:HH12	2.13	0.45
3:C:38:LEU:HG	3:C:65:ILE:HG12	1.99	0.45
1:A:8:LYS:HD2	1:A:10:LEU:CD1	2.48	0.44
2:B:43:LEU:HD21	2:B:60:ILE:HD11	1.97	0.44
4:D:116:ARG:NH2	4:D:123:ASP:OD1	2.44	0.44
2:B:243:THR:O	2:B:243:THR:HG22	2.17	0.44
3:C:72:PHE:CE2	3:C:74:PHE:HB2	2.53	0.44
3:C:117:TYR:HB2	3:C:123:THR:CG2	2.47	0.44
1:A:8:LYS:HB2	1:A:8:LYS:HZ2	1.83	0.44
5:E:30:THR:HG23	5:E:33:ALA:CB	2.48	0.44
5:E:54:VAL:O	5:E:57:VAL:HG12	2.18	0.44
1:A:24:VAL:HG21	1:A:104:TRP:HH2	1.82	0.44
1:A:305:ARG:HD3	5:E:27:GLN:HG2	1.98	0.44
2:B:27:PHE:CZ	2:B:29:SER:HB2	2.53	0.44
4:D:60:LEU:C	4:D:60:LEU:CD2	2.85	0.44
2:B:109:ILE:N	2:B:109:ILE:HD12	2.32	0.43
3:C:18:PHE:HD2	3:C:19:LEU:CD1	2.31	0.43
1:A:115:HIS:CE1	1:A:117:LEU:HB2	2.53	0.43
2:B:128:PRO:HD3	2:B:168:PHE:HB3	1.99	0.43
4:D:101:VAL:O	4:D:105:GLU:HG3	2.18	0.43
1:A:156:PHE:HB3	1:A:221:LEU:CD2	2.48	0.43
2:B:156:LEU:HD23	2:B:188:TRP:CD2	2.54	0.43
5:E:26:ILE:HD11	5:E:59:LYS:HB2	2.00	0.43
2:B:16:LEU:O	2:B:19:SER:OG	2.30	0.43
1:A:246:ASP:O	1:A:301:LYS:NZ	2.52	0.43
2:B:50:LEU:HB2	2:B:54:PHE:O	2.19	0.43
2:B:248:VAL:HG21	2:B:284:MET:CE	2.49	0.43
1:A:121:PHE:CD1	1:A:139:SER:HB3	2.53	0.43
3:C:11:ILE:HG13	3:C:24:PHE:CE1	2.53	0.43
1:A:156:PHE:HB3	1:A:221:LEU:HD21	2.00	0.43
2:B:298:VAL:HG13	2:B:314:SER:O	2.19	0.43
2:B:336:ASP:HA	2:B:339:ASP:OD2	2.18	0.43
3:C:22:TYR:O	3:C:75:GLU:HA	2.19	0.43
4:D:92:LEU:O	4:D:96:VAL:HG23	2.19	0.43
3:C:118:ASP:OD1	3:C:118:ASP:N	2.48	0.42
5:E:78:ARG:HH22	5:E:85:ASP:CG	2.22	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:84:LEU:HG	5:E:88:TYR:CE2	2.54	0.42
2:B:121:ILE:HG23	2:B:136:THR:HB	2.00	0.42
2:B:364:ILE:HD12	2:B:367:LEU:HD23	2.01	0.42
4:D:62:ILE:HG22	4:D:93:GLN:OE1	2.19	0.42
4:D:128:ARG:HG2	4:D:133:GLU:HB2	2.00	0.42
4:D:70:LEU:CD1	5:E:62:LEU:HD23	2.50	0.42
4:D:119:ILE:CD1	5:E:43:VAL:HG11	2.49	0.42
1:A:64:LYS:HE2	1:A:107:CYS:SG	2.59	0.42
4:D:119:ILE:HD13	5:E:43:VAL:HG11	2.02	0.42
2:B:156:LEU:HD12	2:B:156:LEU:N	2.35	0.42
3:C:62:VAL:HG21	3:C:72:PHE:CE1	2.55	0.42
4:D:124:ILE:HG13	5:E:50:ILE:HD11	2.02	0.42
5:E:26:ILE:CD1	5:E:59:LYS:HB2	2.50	0.42
2:B:128:PRO:HD3	2:B:168:PHE:CB	2.50	0.41
2:B:363:GLN:HE21	2:B:363:GLN:HB2	1.73	0.41
4:D:114:ALA:O	4:D:115:LYS:HB2	2.19	0.41
2:B:162:ASN:OD1	4:D:4:LYS:NZ	2.37	0.41
1:A:193:THR:HG22	1:A:217:ILE:HA	2.02	0.41
2:B:182:ASP:O	2:B:184:THR:HG23	2.19	0.41
2:B:303:PHE:CE2	2:B:311:VAL:HG22	2.55	0.41
2:B:360:LEU:N	2:B:360:LEU:HD22	2.35	0.41
5:E:50:ILE:HG12	5:E:50:ILE:O	2.20	0.41
4:D:106:ASP:OD2	4:D:131:ARG:NH2	2.53	0.41
2:B:165:ALA:HB2	2:B:213:ASP:HA	2.02	0.41
4:D:3:THR:O	4:D:3:THR:CG2	2.69	0.41
5:E:46:ILE:HD11	5:E:51:TYR:CZ	2.54	0.41
2:B:241:ASN:OD1	2:B:241:ASN:N	2.54	0.41
4:D:121:LYS:HE2	4:D:121:LYS:HB3	1.86	0.41
1:A:214:ARG:HG2	1:A:251:GLU:HB2	2.03	0.41
1:A:230:GLY:N	6:A:401:COA:O1A	2.52	0.41
2:B:128:PRO:CD	2:B:168:PHE:HB3	2.50	0.41
5:E:26:ILE:CG2	5:E:55:ARG:HG3	2.50	0.41
2:B:165:ALA:HB1	2:B:214:ASN:OD1	2.21	0.41
2:B:252:GLN:HB3	2:B:253:PRO:CD	2.51	0.41
1:A:10:LEU:HD21	1:A:50:LYS:HZ3	1.84	0.40
2:B:17:TRP:O	2:B:21:VAL:HG23	2.21	0.40
2:B:372:GLU:CG	2:B:376:ILE:HB	2.47	0.40
4:D:61:LEU:HD22	4:D:61:LEU:H	1.86	0.40
2:B:60:ILE:HG23	2:B:73:LEU:HD11	2.03	0.40
1:A:196:TYR:O	1:A:213:PHE:HA	2.22	0.40
1:A:243:TRP:HE3	1:A:252:ILE:HD12	1.86	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:58:LEU:HD23	5:E:58:LEU:C	2.42	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	309/416 (74%)	303 (98%)	6 (2%)	0	100	100
2	B	356/401 (89%)	345 (97%)	11 (3%)	0	100	100
3	C	152/154 (99%)	150 (99%)	2 (1%)	0	100	100
4	D	93/135 (69%)	89 (96%)	4 (4%)	0	100	100
5	E	91/96 (95%)	89 (98%)	2 (2%)	0	100	100
All	All	1001/1202 (83%)	976 (98%)	25 (2%)	0	100	100

There are no Ramachandran outliers to report.

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	286/371 (77%)	276 (96%)	10 (4%)	36	64
2	B	322/358 (90%)	308 (96%)	14 (4%)	29	59
3	C	139/139 (100%)	137 (99%)	2 (1%)	67	82

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
4	D	83/112 (74%)	66 (80%)	17 (20%)	1 4
5	E	77/77 (100%)	69 (90%)	8 (10%)	7 25
All	All	907/1057 (86%)	856 (94%)	51 (6%)	21 52

All (51) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	10	LEU
1	A	20	ARG
1	A	110	GLU
1	A	116	ASN
1	A	129	LEU
1	A	144	ASP
1	A	200	LEU
1	A	204	SER
1	A	267	ARG
1	A	317	LEU
2	B	9	SER
2	B	10	VAL
2	B	83	GLU
2	B	110	ARG
2	B	116	GLU
2	B	120	GLU
2	B	168	PHE
2	B	188	TRP
2	B	192	SER
2	B	267	LEU
2	B	336	ASP
2	B	363	GLN
2	B	375	ASN
2	B	384	HIS
3	C	120	GLU
3	C	139	ILE
4	D	2	ARG
4	D	8	ARG
4	D	11	THR
4	D	14	LYS
4	D	53	ARG
4	D	54	PHE
4	D	58	THR
4	D	59	GLU

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Mol	Chain	Res	Type
4	D	60	LEU
4	D	65	LEU
4	D	78	PHE
4	D	83	ARG
4	D	102	SER
4	D	103	LEU
4	D	128	ARG
4	D	129	ARG
4	D	131	ARG
5	E	10	LEU
5	E	19	ARG
5	E	20	LYS
5	E	22	LEU
5	E	23	ARG
5	E	35	ARG
5	E	49	LEU
5	E	55	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
2	B	214	ASN

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)

1 ligand is 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	$\#\|Z\| > 2$
6	COA	A	401	-	41,50,50	0.65	1 (2%)	52,75,75	1.01	2 (3%)

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
6	COA	A	401	-	-	6/44/64/64	0/3/3/3

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	A	401	COA	P3B-O3B	2.17	1.63	1.59

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
6	A	401	COA	O4B-C1B-C2B	-3.62	101.63	106.93
6	A	401	COA	C5A-C6A-N6A	2.07	123.50	120.35

There are no chirality outliers.

All (6) torsion outliers are listed below:

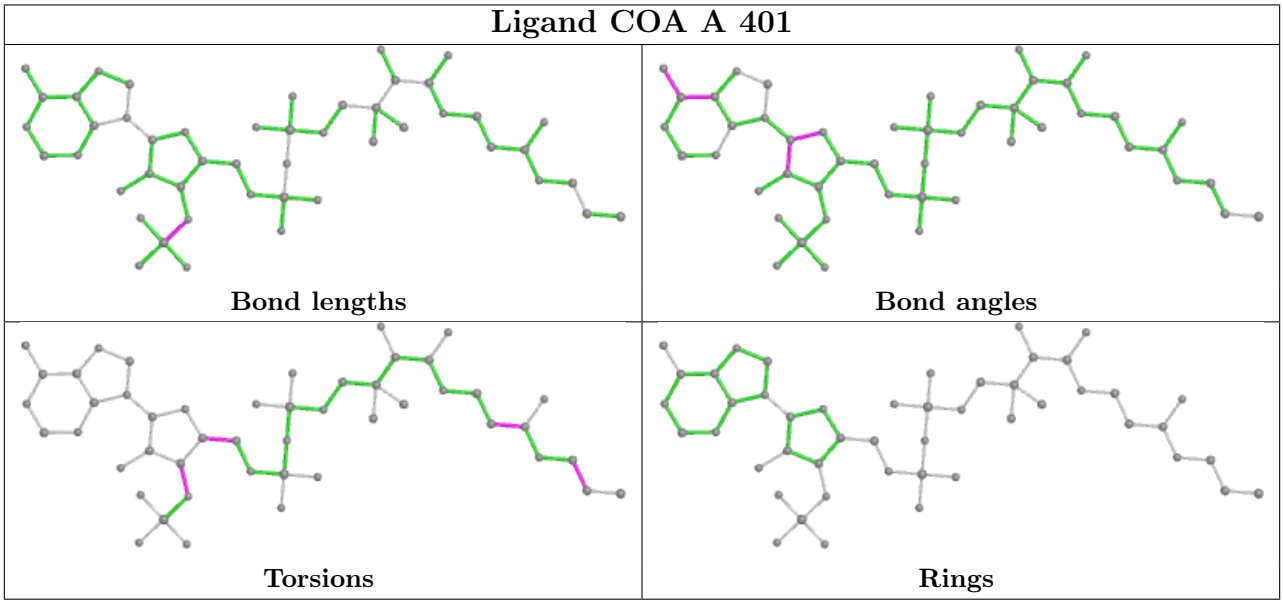
Mol	Chain	Res	Type	Atoms
6	A	401	COA	C4B-C3B-O3B-P3B
6	A	401	COA	S1P-C2P-C3P-N4P
6	A	401	COA	O5P-C5P-C6P-C7P
6	A	401	COA	N4P-C5P-C6P-C7P
6	A	401	COA	C3B-C4B-C5B-O5B
6	A	401	COA	O4B-C4B-C5B-O5B

There are no ring outliers.

1 monomer is involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	A	401	COA	4	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.



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	311/416 (74%)	0.59	6 (1%) 66 65	57, 69, 84, 96	0
2	B	360/401 (89%)	1.06	47 (13%) 3 3	64, 84, 108, 123	0
3	C	154/154 (100%)	0.53	2 (1%) 77 77	59, 69, 86, 89	0
4	D	97/135 (71%)	0.72	6 (6%) 20 20	67, 83, 104, 111	0
5	E	93/96 (96%)	0.51	1 (1%) 80 81	62, 76, 97, 104	0
All	All	1015/1202 (84%)	0.75	62 (6%) 21 20	57, 76, 103, 123	0

All (62) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	211	ILE	3.6
2	B	370	SER	3.3
2	B	31	THR	3.1
2	B	339	ASP	3.0
2	B	320	LEU	2.9
2	B	206	LEU	2.9
1	A	256	ASP	2.8
2	B	73	LEU	2.8
2	B	213	ASP	2.8
2	B	178	SER	2.8
2	B	52	GLY	2.8
2	B	168	PHE	2.8
2	B	372	GLU	2.7
1	A	117	LEU	2.7
2	B	30	GLU	2.7
2	B	179	GLY	2.6
2	B	183	HIS	2.6
2	B	85	LEU	2.6
2	B	177	LEU	2.6
2	B	334	PRO	2.6

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Mol	Chain	Res	Type	RSRZ
2	B	61	ILE	2.5
2	B	164	TYR	2.5
4	D	1	ALA	2.5
2	B	119	GLU	2.4
2	B	75	PHE	2.4
3	C	29	GLU	2.4
2	B	274	SER	2.4
2	B	268	ALA	2.4
2	B	122	THR	2.3
4	D	133	GLU	2.3
2	B	257	LEU	2.3
2	B	58	GLU	2.3
5	E	79	LYS	2.3
4	D	5	GLN	2.3
2	B	351	HIS	2.3
2	B	60	ILE	2.3
2	B	371	ALA	2.2
2	B	377	LEU	2.2
2	B	27	PHE	2.2
2	B	338	GLU	2.2
1	A	54	ILE	2.2
2	B	255	ASN	2.2
4	D	13	GLY	2.2
2	B	332	GLN	2.2
2	B	53	GLY	2.1
2	B	322	MET	2.1
4	D	83	ARG	2.1
1	A	122	GLU	2.1
2	B	84	ILE	2.1
1	A	170	THR	2.1
2	B	165	ALA	2.1
3	C	154	ASP	2.1
2	B	137	ILE	2.1
4	D	6	THR	2.1
1	A	180	LEU	2.1
2	B	29	SER	2.1
2	B	236	ASN	2.0
2	B	235	ILE	2.0
2	B	32	ARG	2.0
2	B	80	LEU	2.0
2	B	166	LEU	2.0
2	B	373	GLU	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)

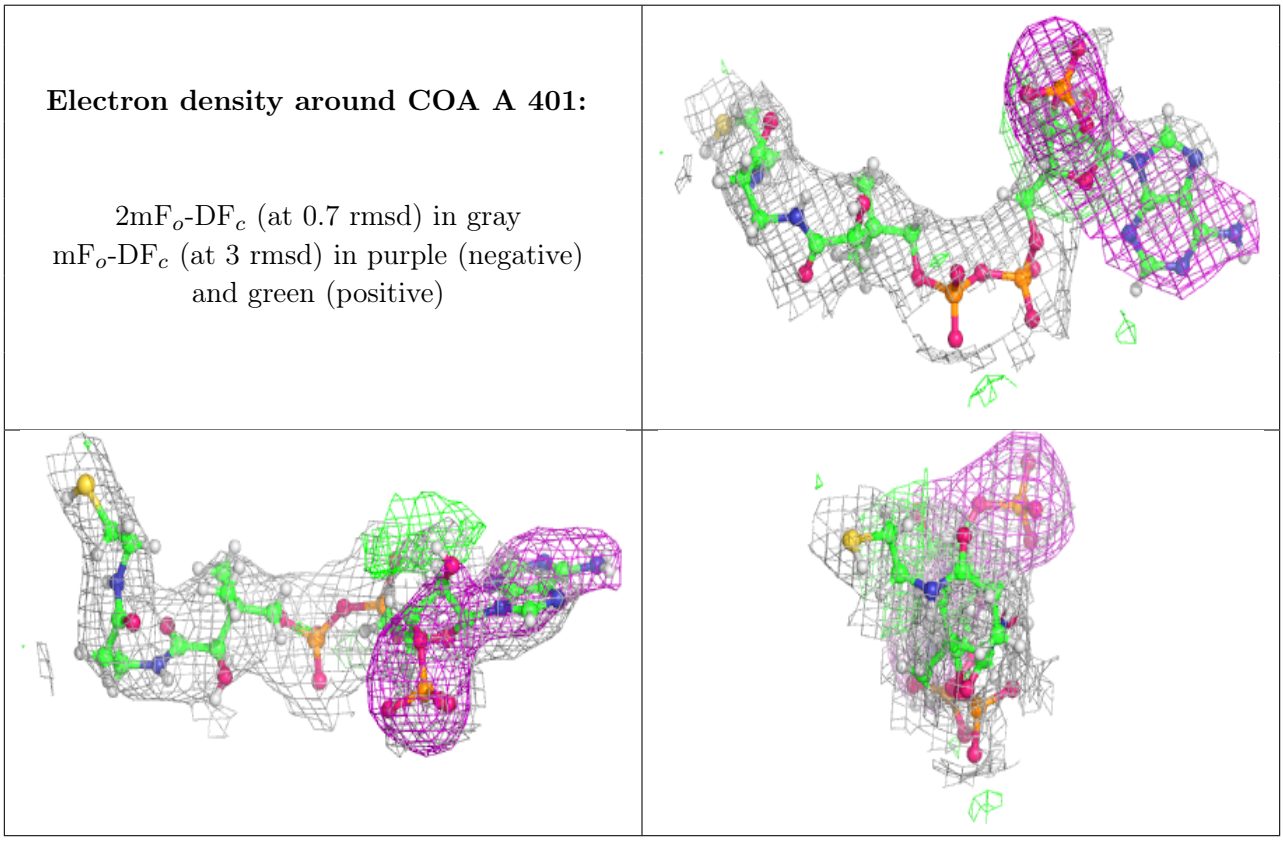
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' 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
6	COA	A	401	48/48	0.82	0.35	67,67,67,67	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 COA 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)



6.5 Other polymers (i)

There are no such residues in this entry.