



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 05:33 PM UTC

PDB ID : 1O9L / pdb_00001o9l
Title : Succinate:Coenzyme-A Transferase (pig heart)
Authors : Mitchell, E.P.; Lloyd, A.J.; Lewis, G.; Shoolingin-Jordan, P.
Deposited on : 2002-12-17
Resolution : 2.40 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:

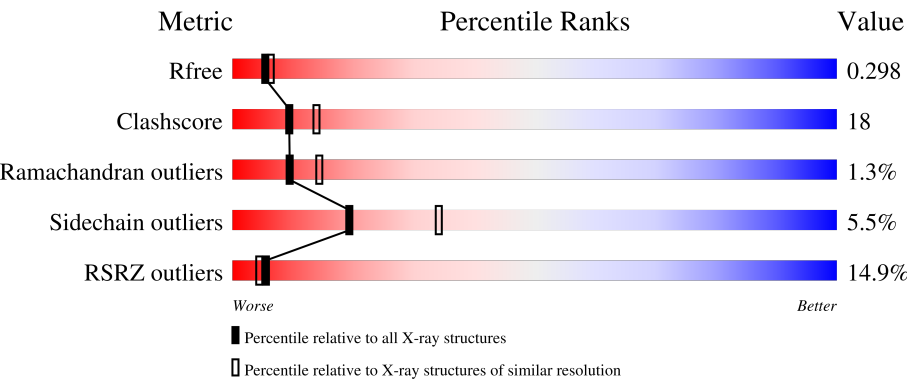
MolProbity : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

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 2.40 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}	180053	4912 (2.40-2.40)
Clashscore	190562	5391 (2.40-2.40)
Ramachandran outliers	187476	5320 (2.40-2.40)
Sidechain outliers	187428	5321 (2.40-2.40)
RSRZ outliers	180081	4916 (2.40-2.40)

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 $\leq 5\%$. 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	481	13% 63%29% . . .
1	B	481	11% 63%22% . 12%
1	C	481	17% 57%27% . 12%
1	D	481	14% 64%26%6% .

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
2	EMC	A	9003	-	-	-	X
2	EMC	B	9004	-	-	-	X
2	EMC	C	9005	-	-	-	X
2	EMC	C	9006	-	-	-	X
2	EMC	D	9000	-	-	-	X
2	EMC	D	9001	-	-	-	X
2	EMC	D	9002	-	-	-	X
3	EMT	A	9007	-	-	-	X
3	EMT	B	9008	-	-	X	X

2 Entry composition [i](#)

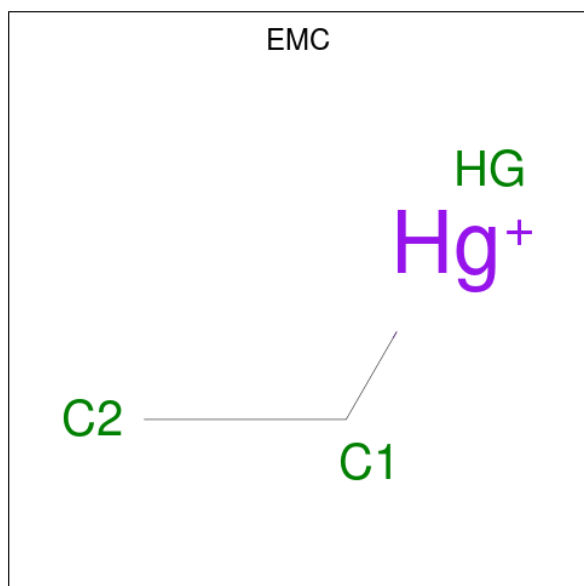
There are 4 unique types of molecules in this entry. The entry contains 14135 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 SUCCINYL-COA\;3-KETOACID-COENZYME A TRANSFERASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	468	Total	C	N	O	S	0	0	0
			3568	2264	612	674	18			
1	B	425	Total	C	N	O	S	0	0	0
			3239	2056	554	616	13			
1	C	425	Total	C	N	O	S	0	0	0
			3234	2053	553	614	14			
1	D	464	Total	C	N	O	S	0	0	0
			3535	2244	604	669	18			

- Molecule 2 is ETHYL MERCURY ION (CCD ID: EMC) (formula: C₂H₅Hg).



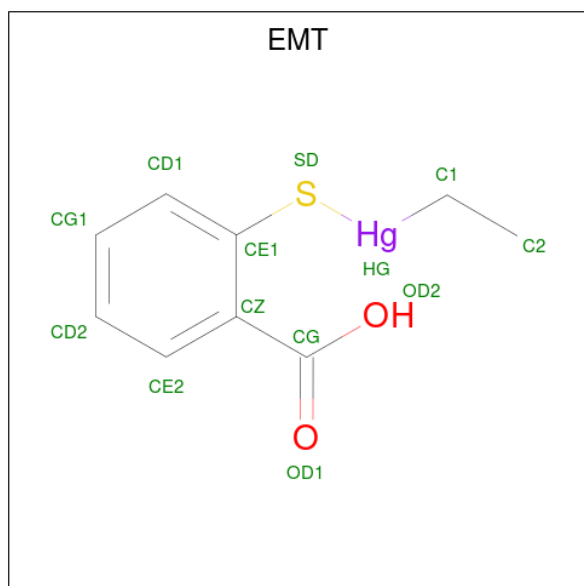
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	C	Hg	0	0
			3	2	1		
2	B	1	Total	C	Hg	0	0
			3	2	1		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	C	1	Total	C	Hg	0	0
			3	2	1		
2	C	1	Total	C	Hg	0	0
			3	2	1		
2	D	1	Total	C	Hg	0	0
			3	2	1		
2	D	1	Total	C	Hg	0	0
			3	2	1		
2	D	1	Total	C	Hg	0	0
			3	2	1		

- Molecule 3 is 2-(ETHYLMERCURI-THIO)-BENZOIC ACID (CCD ID: EMT) (formula: $C_9H_{10}HgO_2S$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	Hg	O	S	0	0
			13	9	1	2	1		
3	B	1	Total	C	Hg	O	S	0	0
			13	9	1	2	1		

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	107	Total	O	0	0
			107	107		
4	B	86	Total	O	0	0
			86	86		

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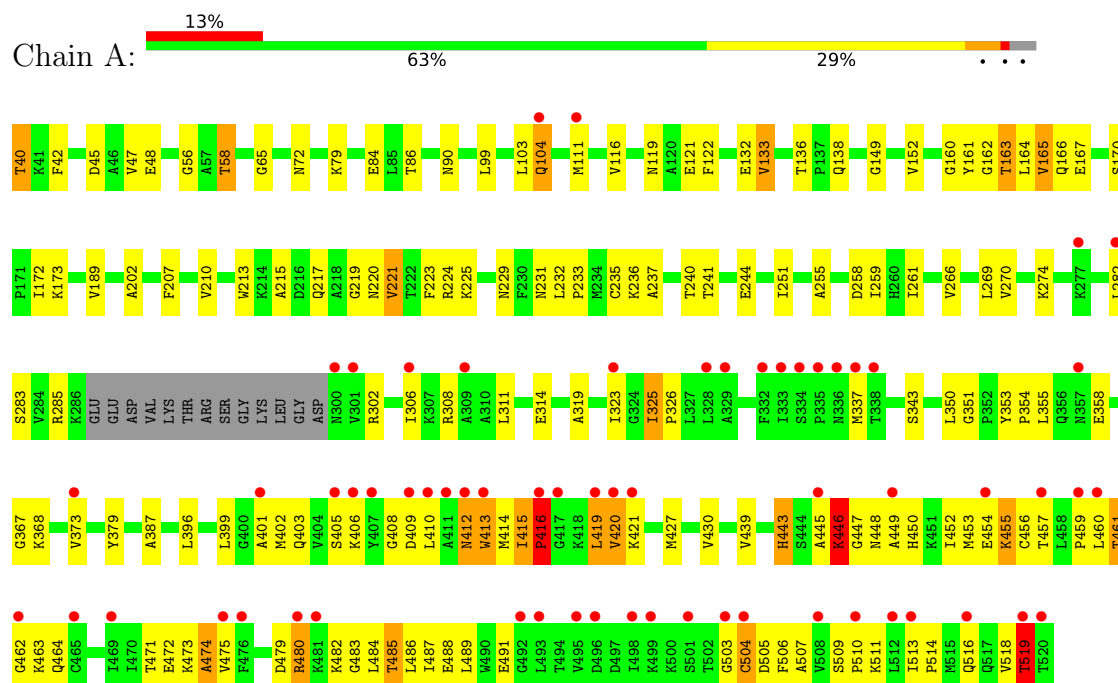
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	C	139	Total 139	O 139	0	0
4	D	180	Total 180	O 180	0	0

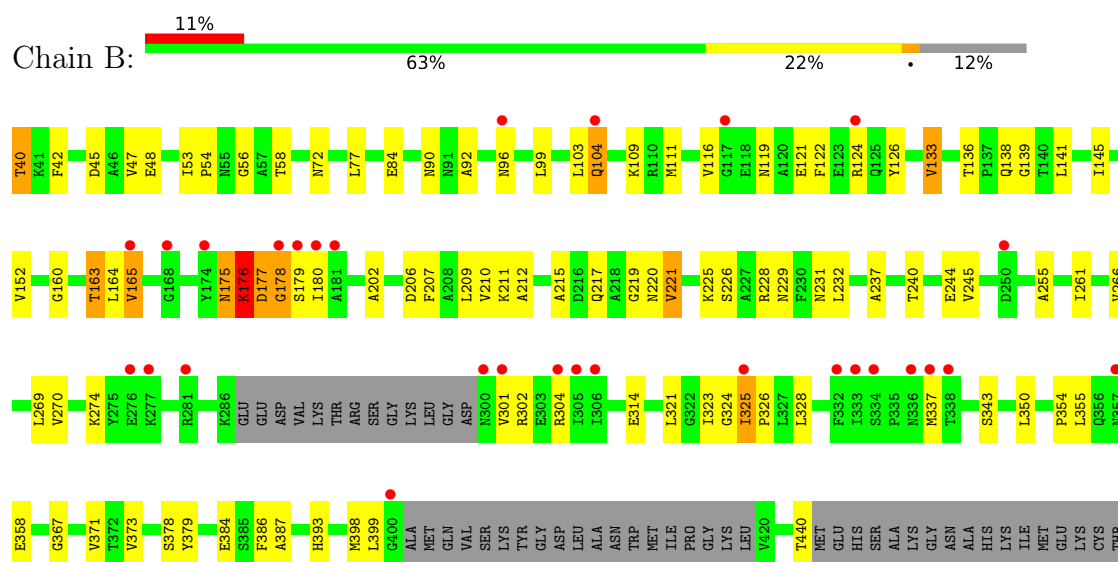
3 Residue-property plots

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: SUCCINYL-COA\3-KETOACID-COENZYME A TRANSFERASE

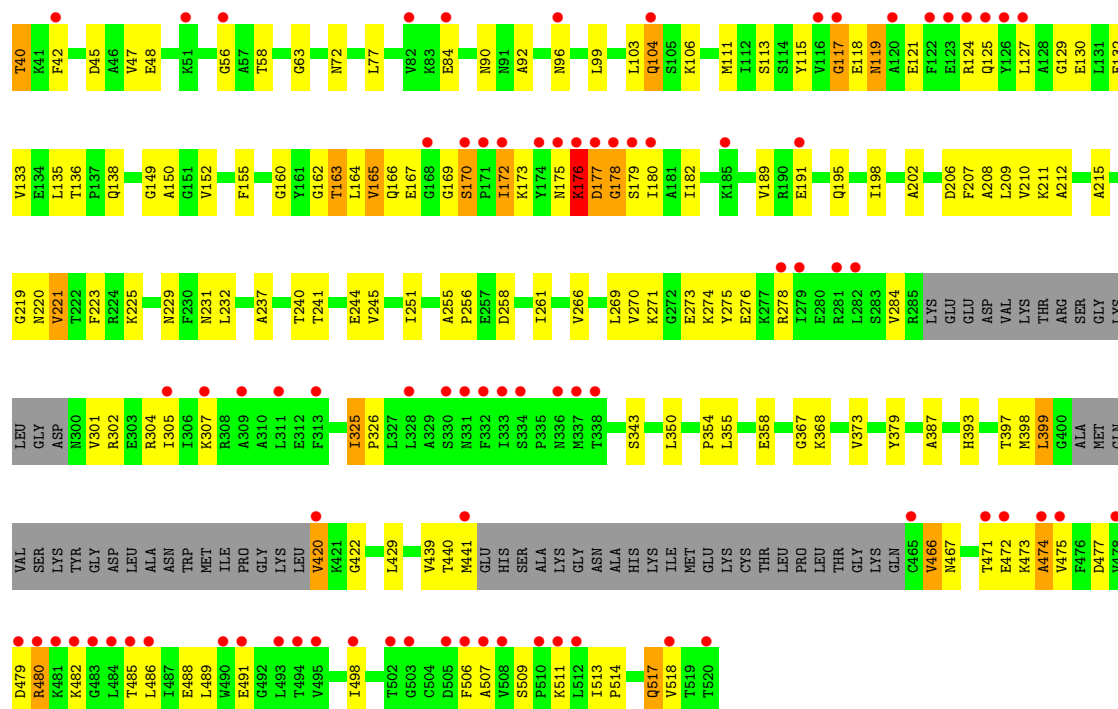


• Molecule 1: SUCCINYL-COA\3-KETOACID-COENZYME A TRANSFERASE

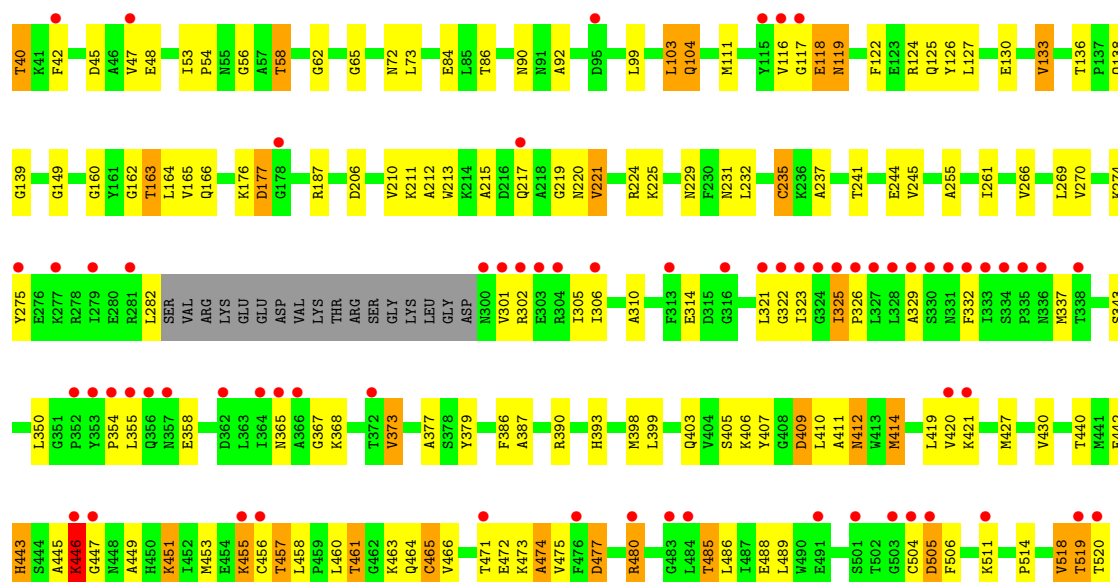




• Molecule 1: SUCCINYL-COA\3-KETOACID-COENZYME A TRANSFERASE



• Molecule 1: SUCCINYL-COA\3-KETOACID-COENZYME A TRANSFERASE



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	74.80Å 133.80Å 101.90Å 90.00° 104.40° 90.00°	Depositor
Resolution (Å)	29.76 – 2.40 29.76 – 2.40	Depositor EDS
% Data completeness (in resolution range)	99.7 (29.76-2.40) 99.7 (29.76-2.40)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.05	Depositor
$\langle I/\sigma(I) \rangle$ ¹	4.06 (at 2.39Å)	Xtriage
Refinement program	CNS 1.0	Depositor
R, R_{free}	0.240 , 0.270 0.278 , 0.298	Depositor DCC
R_{free} test set	1506 reflections (1.99%)	wwPDB-VP
Wilson B-factor (Å ²)	36.8	Xtriage
Anisotropy	0.459	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.38 , 70.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.90	EDS
Total number of atoms	14135	wwPDB-VP
Average B, all atoms (Å ²)	44.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.08% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ 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: EMT, EMC

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	0.43	0/3626	0.97	14/4894 (0.3%)
1	B	0.41	0/3288	0.92	8/4438 (0.2%)
1	C	0.46	0/3283	0.95	13/4431 (0.3%)
1	D	0.50	1/3593 (0.0%)	1.00	15/4851 (0.3%)
All	All	0.45	1/13790 (0.0%)	0.96	50/18614 (0.3%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	414	MET	SD-CE	6.50	1.95	1.79

All (50) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	505	ASP	N-CA-C	-9.42	96.93	110.59
1	D	355	LEU	N-CA-C	-8.57	99.47	110.53
1	A	387	ALA	N-CA-C	-8.07	102.56	111.36
1	B	355	LEU	N-CA-C	-7.80	100.02	110.55
1	B	387	ALA	N-CA-C	-7.79	102.87	111.36
1	B	255	ALA	N-CA-C	-7.61	100.50	109.93
1	C	355	LEU	N-CA-C	-7.49	100.44	110.55
1	A	255	ALA	N-CA-C	-7.44	100.38	109.83
1	D	387	ALA	N-CA-C	-7.44	102.86	112.23
1	D	255	ALA	N-CA-C	-7.43	100.39	109.83
1	C	255	ALA	N-CA-C	-7.42	100.41	109.83
1	A	355	LEU	N-CA-C	-7.19	99.88	110.52
1	D	461	THR	N-CA-C	-7.14	104.70	113.41
1	A	415	ILE	CA-C-N	6.95	128.53	119.84
1	A	415	ILE	C-N-CA	6.95	128.53	119.84
1	C	387	ALA	N-CA-C	-6.80	103.95	111.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	206	ASP	N-CA-C	-6.69	103.47	111.69
1	A	443	HIS	N-CA-C	6.51	118.03	111.07
1	C	474	ALA	N-CA-C	6.16	116.69	108.38
1	D	237	ALA	N-CA-C	6.08	120.28	112.26
1	D	409	ASP	N-CA-C	-6.06	102.53	110.53
1	B	165	VAL	N-CA-C	-6.05	104.84	110.53
1	A	461	THR	N-CA-C	-6.05	104.64	112.68
1	D	443	HIS	N-CA-C	6.03	117.52	111.07
1	D	477	ASP	N-CA-C	-6.02	100.75	110.32
1	C	466	VAL	N-CA-C	6.01	118.10	108.85
1	D	474	ALA	N-CA-C	5.99	117.89	108.96
1	D	206	ASP	N-CA-C	-5.78	104.59	111.69
1	B	206	ASP	N-CA-C	-5.69	104.69	111.69
1	A	165	VAL	N-CA-C	-5.65	104.86	110.62
1	B	237	ALA	N-CA-C	5.61	119.66	112.26
1	B	474	ALA	N-CA-C	5.56	116.41	108.74
1	A	237	ALA	N-CA-C	5.51	119.32	112.59
1	D	466	VAL	N-CA-C	5.38	116.03	109.30
1	B	477	ASP	N-CA-C	-5.37	102.58	110.52
1	A	133	VAL	N-CA-C	5.37	115.62	108.27
1	A	474	ALA	N-CA-C	5.36	116.13	108.74
1	A	258	ASP	N-CA-C	5.33	118.80	112.72
1	C	477	ASP	N-CA-C	-5.32	102.65	110.52
1	C	237	ALA	N-CA-C	5.29	119.24	112.26
1	C	63	GLY	N-CA-C	5.26	118.61	111.72
1	C	165	VAL	N-CA-C	-5.19	105.65	110.53
1	C	251	ILE	N-CA-C	-5.12	102.45	109.37
1	D	225	LYS	CB-CA-C	-5.12	110.65	116.54
1	D	103	LEU	N-CA-C	-5.05	105.47	111.69
1	C	258	ASP	N-CA-C	5.05	118.75	112.59
1	D	451	LYS	N-CA-C	-5.03	107.70	113.88
1	C	172	ILE	N-CA-C	-5.02	107.94	112.96
1	A	351	GLY	CA-C-N	5.00	125.01	120.21
1	A	351	GLY	C-N-CA	5.00	125.01	120.21

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	3568	0	3639	140	0
1	B	3239	0	3296	92	0
1	C	3234	0	3281	127	0
1	D	3535	0	3597	138	0
2	A	3	0	0	0	0
2	B	3	0	0	0	0
2	C	6	0	0	0	0
2	D	9	0	0	1	0
3	A	13	0	4	3	0
3	B	13	0	4	8	0
4	A	107	0	0	6	0
4	B	86	0	0	6	0
4	C	139	0	0	10	0
4	D	180	0	0	5	0
All	All	14135	0	13821	495	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 18.

All (495) 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:B:9008:EMT:HE2	3:B:9008:EMT:CZ	2.07	1.23
3:B:9008:EMT:HE2	3:B:9008:EMT:CD2	2.06	1.23
1:B:163:THR:HG22	1:B:165:VAL:H	1.13	1.10
1:A:163:THR:HG22	1:A:165:VAL:H	1.17	1.10
1:C:163:THR:HG22	1:C:165:VAL:H	1.12	1.06
3:B:9008:EMT:HE2	3:B:9008:EMT:CE2	0.97	1.06
1:A:414:MET:HE2	1:A:459:PRO:HG2	1.34	1.03
1:C:96:ASN:HB3	4:C:2018:HOH:O	1.59	1.02
1:D:163:THR:HG22	1:D:165:VAL:H	1.25	1.01
1:D:325:ILE:HD13	1:D:440:THR:HB	1.41	1.00
1:B:96:ASN:HB3	4:B:2011:HOH:O	1.60	0.99
1:D:446:LYS:HG2	1:D:447:GLY:H	1.26	0.99
1:D:326:PRO:HA	1:D:398:MET:HE3	1.44	0.96
1:C:307:LYS:HE3	1:C:517:GLN:HG3	1.50	0.94
1:D:99:LEU:HD23	1:D:111:MET:HE1	1.50	0.91
1:B:40:THR:HG21	1:B:219:GLY:HA3	1.53	0.90
1:A:445:ALA:HB3	1:A:449:ALA:HB3	1.54	0.90

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:99:LEU:HD23	1:C:111:MET:HE1	1.52	0.89
1:A:325:ILE:HG23	1:A:326:PRO:HD3	1.54	0.88
1:A:450:HIS:ND1	1:A:503:GLY:HA2	1.88	0.88
1:D:306:ILE:HA	1:D:325:ILE:HG13	1.57	0.87
1:D:40:THR:HB	1:D:266:VAL:O	1.75	0.86
1:B:325:ILE:HG23	1:B:326:PRO:HD3	1.57	0.85
1:D:403:GLN:HE22	1:D:457:THR:H	1.23	0.85
1:A:99:LEU:HD23	1:A:111:MET:HE1	1.58	0.85
1:D:40:THR:HG21	1:D:219:GLY:HA3	1.58	0.84
1:C:40:THR:HB	1:C:266:VAL:O	1.76	0.84
1:A:40:THR:HG21	1:A:219:GLY:HA3	1.59	0.84
1:A:162:GLY:H	1:A:166:GLN:NE2	1.76	0.84
1:A:406:LYS:HE3	1:C:273:GLU:HG2	1.60	0.83
1:B:40:THR:HB	1:B:266:VAL:O	1.78	0.83
1:C:325:ILE:HG23	1:C:326:PRO:HD3	1.61	0.82
1:D:116:VAL:HG11	1:D:122:PHE:CZ	2.15	0.82
1:D:471:THR:CG2	1:D:474:ALA:H	1.92	0.81
1:D:445:ALA:HB3	1:D:449:ALA:HB3	1.61	0.81
1:B:221:VAL:HG22	1:B:261:ILE:HB	1.62	0.80
1:A:40:THR:HB	1:A:266:VAL:O	1.81	0.80
1:A:410:LEU:HG	1:A:461:THR:HB	1.63	0.80
1:C:221:VAL:HG22	1:C:261:ILE:HB	1.64	0.79
1:C:40:THR:HG21	1:C:219:GLY:HA3	1.62	0.79
1:C:325:ILE:HG22	4:C:2091:HOH:O	1.82	0.78
1:D:221:VAL:HG22	1:D:261:ILE:HB	1.64	0.77
1:B:99:LEU:HD23	1:B:111:MET:HE1	1.67	0.76
1:A:221:VAL:HG22	1:A:261:ILE:HB	1.67	0.76
1:A:446:LYS:HG2	1:A:447:GLY:H	1.49	0.76
1:D:305:ILE:HB	1:D:325:ILE:HD12	1.67	0.76
1:C:162:GLY:H	1:C:166:GLN:NE2	1.85	0.75
1:A:471:THR:HG23	1:A:474:ALA:H	1.53	0.73
1:A:443:HIS:ND1	1:A:471:THR:HG21	2.02	0.73
1:A:401:ALA:HA	1:A:412:ASN:HB3	1.71	0.72
1:C:56:GLY:HA2	1:C:84:GLU:O	1.89	0.72
1:B:325:ILE:HD13	1:B:440:THR:HB	1.72	0.72
1:D:305:ILE:HG22	1:D:325:ILE:CD1	2.19	0.71
1:D:464:GLN:NE2	1:D:480:ARG:HB2	2.06	0.71
1:C:164:LEU:O	1:C:167:GLU:O	2.09	0.71
1:C:132:GLU:HG2	1:C:173:LYS:HB2	1.73	0.70
1:A:511:LYS:HD2	1:A:511:LYS:N	2.07	0.70
1:A:162:GLY:H	1:A:166:GLN:HE21	1.38	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:456:CYS:SG	1:A:460:LEU:HG	2.33	0.69
1:D:475:VAL:HB	1:D:488:GLU:HB2	1.73	0.69
1:C:511:LYS:HD2	1:C:511:LYS:N	2.09	0.68
1:A:119:ASN:C	1:A:119:ASN:HD22	2.02	0.68
1:A:475:VAL:HB	1:A:488:GLU:HB2	1.74	0.68
1:B:475:VAL:HB	1:B:488:GLU:HB2	1.74	0.68
1:D:305:ILE:CB	1:D:325:ILE:HD12	2.23	0.68
1:C:96:ASN:ND2	4:C:2019:HOH:O	2.27	0.68
1:A:42:PHE:CE2	1:A:269:LEU:HD23	2.29	0.68
1:A:56:GLY:HA2	1:A:84:GLU:O	1.94	0.68
3:B:9008:EMT:HD1	4:B:2075:HOH:O	1.92	0.67
1:D:403:GLN:NE2	1:D:457:THR:H	1.93	0.67
1:A:445:ALA:HB1	1:A:446:LYS:HD3	1.77	0.66
1:D:325:ILE:HG23	1:D:326:PRO:HD3	1.76	0.66
1:B:163:THR:HG22	1:B:165:VAL:N	1.98	0.66
1:B:472:GLU:HG3	1:B:473:LYS:HG3	1.77	0.66
1:D:455:LYS:HD3	1:D:455:LYS:H	1.60	0.66
1:B:42:PHE:CE2	1:B:269:LEU:HD23	2.30	0.66
1:C:475:VAL:HB	1:C:488:GLU:HB2	1.78	0.66
1:C:479:ASP:HB3	1:C:482:LYS:HB2	1.78	0.65
1:D:446:LYS:HG2	1:D:447:GLY:N	2.05	0.65
1:A:172:ILE:HG12	3:A:9007:EMT:HD1	1.77	0.65
1:B:489:LEU:O	1:B:514:PRO:HA	1.95	0.65
1:D:119:ASN:C	1:D:119:ASN:HD22	2.02	0.65
1:D:471:THR:HG22	1:D:474:ALA:H	1.62	0.65
1:A:471:THR:CG2	1:A:474:ALA:H	2.10	0.64
1:A:511:LYS:O	1:A:513:ILE:HG23	1.97	0.64
1:A:403:GLN:HE22	1:A:457:THR:N	1.95	0.64
1:A:450:HIS:CG	1:A:503:GLY:HA2	2.31	0.64
1:D:117:GLY:O	1:D:118:GLU:HB2	1.95	0.64
1:C:471:THR:HG22	1:C:474:ALA:O	1.97	0.64
1:A:160:GLY:O	1:A:163:THR:HB	1.98	0.64
1:A:455:LYS:O	1:A:455:LYS:HE2	1.98	0.64
1:B:119:ASN:C	1:B:119:ASN:HD22	2.05	0.64
1:B:511:LYS:N	1:B:511:LYS:HD2	2.12	0.64
1:C:211:LYS:HE2	1:C:275:TYR:CE1	2.33	0.64
1:C:354:PRO:HB2	1:C:358:GLU:HB2	1.79	0.64
1:D:410:LEU:HD12	1:D:411:ALA:N	2.13	0.63
1:D:116:VAL:HG22	1:D:421:LYS:O	1.99	0.63
1:A:472:GLU:HG3	1:A:473:LYS:HG3	1.80	0.63
1:D:45:ASP:OD2	1:D:48:GLU:HG2	1.99	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:B:9008:EMT:HE2	3:B:9008:EMT:CG	2.67	0.62
1:C:471:THR:HG23	1:C:474:ALA:H	1.64	0.62
1:D:403:GLN:HE22	1:D:457:THR:N	1.97	0.62
1:D:511:LYS:HD2	1:D:511:LYS:N	2.14	0.62
1:A:104:GLN:NE2	1:A:121:GLU:HG2	2.15	0.62
1:B:116:VAL:HG21	1:B:122:PHE:CE2	2.35	0.62
1:A:79:LYS:HE3	4:A:2010:HOH:O	1.98	0.62
1:C:472:GLU:HG3	1:C:473:LYS:HG3	1.80	0.62
1:C:163:THR:HG22	1:C:165:VAL:N	1.98	0.62
1:D:163:THR:HG22	1:D:165:VAL:N	2.08	0.62
1:D:406:LYS:HE3	1:D:407:TYR:CE2	2.35	0.61
1:D:471:THR:HG23	1:D:474:ALA:H	1.65	0.61
1:C:511:LYS:O	1:C:513:ILE:HG23	2.01	0.61
1:D:406:LYS:HE3	1:D:407:TYR:CZ	2.35	0.61
1:D:453:MET:HE2	1:D:455:LYS:O	2.01	0.61
1:C:45:ASP:OD2	1:C:48:GLU:HG2	2.00	0.60
1:A:446:LYS:HD3	1:A:446:LYS:N	2.15	0.60
1:A:104:GLN:HG2	4:A:2015:HOH:O	2.01	0.60
1:C:42:PHE:CE2	1:C:269:LEU:HD23	2.35	0.60
1:B:302:ARG:HG2	4:B:2050:HOH:O	2.01	0.60
1:D:126:TYR:CE1	1:D:133:VAL:HG13	2.37	0.60
1:A:509:SER:C	1:A:511:LYS:H	2.10	0.60
1:B:471:THR:HG22	1:B:474:ALA:O	2.02	0.60
1:D:301:VAL:HG13	1:D:472:GLU:HB3	1.84	0.60
1:A:163:THR:HG22	1:A:165:VAL:N	2.02	0.60
1:C:115:TYR:CZ	1:C:117:GLY:HA3	2.37	0.60
1:B:56:GLY:HA2	1:B:84:GLU:O	2.01	0.59
1:A:401:ALA:HA	1:A:412:ASN:CB	2.33	0.59
1:B:160:GLY:O	1:B:163:THR:HB	2.02	0.59
1:C:441:MET:HE3	1:C:471:THR:OG1	2.02	0.59
1:C:45:ASP:OD1	1:C:47:VAL:HG12	2.02	0.59
1:D:354:PRO:HB2	1:D:358:GLU:HB2	1.85	0.59
1:C:106:LYS:HG2	1:C:125:GLN:HE22	1.67	0.59
1:C:471:THR:CG2	1:C:474:ALA:H	2.16	0.59
1:A:452:ILE:HG22	1:A:484:LEU:HD11	1.85	0.59
1:C:90:ASN:ND2	1:C:138:GLN:HG3	2.18	0.59
1:C:307:LYS:HE3	1:C:517:GLN:CG	2.29	0.59
1:D:116:VAL:HG21	1:D:122:PHE:CE1	2.37	0.58
1:D:412:ASN:C	1:D:412:ASN:HD22	2.11	0.58
1:D:446:LYS:CG	1:D:447:GLY:H	2.05	0.58
1:A:413:TRP:CE3	1:A:414:MET:HB2	2.38	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:454:GLU:HB2	1:A:504:CYS:SG	2.43	0.58
1:A:474:ALA:HB1	1:A:486:LEU:CD1	2.33	0.58
1:B:471:THR:CG2	1:B:474:ALA:H	2.17	0.58
1:D:211:LYS:HE2	1:D:275:TYR:CE1	2.39	0.58
1:D:443:HIS:ND1	1:D:471:THR:HG21	2.19	0.58
1:C:160:GLY:O	1:C:163:THR:HB	2.04	0.57
1:B:211:LYS:HE3	4:B:2006:HOH:O	2.05	0.57
1:A:132:GLU:CG	1:A:173:LYS:HD2	2.35	0.57
1:A:489:LEU:O	1:A:514:PRO:HA	2.03	0.57
1:D:480:ARG:CZ	1:D:480:ARG:H	2.18	0.57
1:C:474:ALA:HB1	1:C:486:LEU:CD1	2.35	0.57
1:D:126:TYR:CD1	1:D:133:VAL:CG1	2.88	0.57
1:B:354:PRO:HB2	1:B:358:GLU:HB2	1.85	0.57
1:D:310:ALA:HA	1:D:329:ALA:HB1	1.86	0.57
1:C:90:ASN:HD21	1:C:138:GLN:HG3	1.70	0.56
1:A:45:ASP:OD1	1:A:47:VAL:HG12	2.05	0.56
1:B:104:GLN:NE2	1:B:121:GLU:HG2	2.20	0.56
1:C:325:ILE:HD13	1:C:440:THR:HB	1.87	0.56
1:D:124:ARG:HH12	1:D:125:GLN:HG2	1.70	0.56
1:A:45:ASP:OD2	1:A:48:GLU:HG2	2.06	0.56
1:B:471:THR:HG23	1:B:474:ALA:H	1.70	0.56
1:D:472:GLU:HG3	1:D:473:LYS:HG3	1.87	0.56
1:C:118:GLU:O	1:C:119:ASN:HB2	2.05	0.55
1:C:169:GLY:O	1:C:170:SER:C	2.49	0.55
1:C:367:GLY:O	1:C:368:LYS:HB2	2.06	0.55
1:C:106:LYS:HG2	1:C:125:GLN:NE2	2.21	0.55
1:C:326:PRO:HA	1:C:398:MET:HE3	1.86	0.55
1:D:471:THR:HG23	1:D:473:LYS:H	1.71	0.55
1:A:446:LYS:HD3	1:A:446:LYS:H	1.72	0.55
1:A:455:LYS:H	1:A:455:LYS:HZ3	1.54	0.55
1:A:455:LYS:H	1:A:455:LYS:NZ	2.04	0.54
1:D:305:ILE:CG2	1:D:325:ILE:HD12	2.37	0.54
1:D:310:ALA:CA	1:D:329:ALA:HB1	2.37	0.54
1:D:471:THR:HG22	1:D:474:ALA:O	2.08	0.54
1:A:408:GLY:HA3	1:A:464:GLN:HA	1.89	0.54
1:A:232:LEU:HG	1:A:261:ILE:HD11	1.89	0.54
1:C:343:SER:HB2	1:C:350:LEU:HD11	1.89	0.54
1:B:490:TRP:HB3	1:B:493:LEU:HD12	1.89	0.54
1:C:397:THR:HG21	1:C:429:LEU:HB3	1.89	0.54
1:C:489:LEU:O	1:C:514:PRO:HA	2.08	0.54
1:A:164:LEU:HA	1:A:167:GLU:HB2	1.89	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:325:ILE:CD1	1:B:440:THR:HB	2.36	0.53
1:D:90:ASN:ND2	1:D:138:GLN:HG3	2.23	0.53
1:D:90:ASN:HD21	1:D:138:GLN:HG3	1.74	0.53
1:D:305:ILE:CG2	1:D:325:ILE:CD1	2.87	0.53
1:A:72:ASN:HD21	1:A:274:LYS:H	1.54	0.53
1:D:211:LYS:HE3	4:D:2015:HOH:O	2.08	0.53
1:D:343:SER:HB2	1:D:350:LEU:HD11	1.91	0.53
1:C:176:LYS:HD3	1:C:176:LYS:N	2.23	0.53
1:A:456:CYS:SG	1:A:456:CYS:O	2.66	0.53
1:D:405:SER:OG	1:D:409:ASP:HB2	2.09	0.53
1:A:406:LYS:NZ	1:A:454:GLU:HG3	2.24	0.53
1:B:509:SER:C	1:B:511:LYS:H	2.16	0.53
1:A:90:ASN:HD21	1:A:138:GLN:HG3	1.73	0.53
1:D:446:LYS:NZ	1:D:449:ALA:HB2	2.24	0.53
1:D:489:LEU:O	1:D:514:PRO:HA	2.09	0.52
1:D:42:PHE:CE2	1:D:269:LEU:HD23	2.44	0.52
1:D:412:ASN:C	1:D:412:ASN:ND2	2.66	0.52
1:B:474:ALA:HB1	1:B:486:LEU:CD1	2.40	0.52
1:A:474:ALA:HB1	1:A:486:LEU:HD11	1.91	0.52
1:C:176:LYS:HG2	1:C:177:ASP:N	2.24	0.52
1:D:72:ASN:HD21	1:D:274:LYS:H	1.56	0.52
1:B:511:LYS:O	1:B:513:ILE:HG23	2.08	0.52
1:C:180:ILE:N	1:C:180:ILE:HD12	2.23	0.52
1:D:306:ILE:HG12	1:D:325:ILE:HA	1.92	0.52
1:D:367:GLY:O	1:D:368:LYS:HB2	2.09	0.52
1:B:176:LYS:N	1:B:176:LYS:HD3	2.25	0.52
1:B:177:ASP:CG	1:B:178:GLY:H	2.18	0.52
1:A:479:ASP:OD2	1:A:482:LYS:HG3	2.09	0.52
1:C:480:ARG:HG3	1:C:480:ARG:HH11	1.74	0.52
1:D:471:THR:HG23	1:D:473:LYS:N	2.25	0.52
1:A:354:PRO:HB2	1:A:358:GLU:HB2	1.92	0.51
1:C:301:VAL:HG13	1:C:472:GLU:HB3	1.93	0.51
1:D:455:LYS:HD3	1:D:455:LYS:N	2.25	0.51
3:B:9008:EMT:HE2	3:B:9008:EMT:OD2	2.48	0.51
1:C:135:LEU:HD13	1:C:422:GLY:HA2	1.91	0.51
1:B:72:ASN:HD21	1:B:274:LYS:H	1.59	0.51
1:C:393:HIS:HE1	1:D:149:GLY:O	1.93	0.51
1:A:166:GLN:OE1	1:A:189:VAL:HG21	2.11	0.51
1:C:302:ARG:HG2	4:C:2084:HOH:O	2.10	0.51
1:D:235:CYS:O	1:D:241:THR:HG21	2.11	0.51
1:A:132:GLU:HG2	1:A:173:LYS:HB2	1.93	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:119:ASN:HD21	1:B:121:GLU:HB3	1.76	0.51
1:A:163:THR:CG2	1:A:164:LEU:N	2.73	0.51
1:D:119:ASN:C	1:D:119:ASN:ND2	2.69	0.51
1:B:232:LEU:HG	1:B:261:ILE:HD11	1.92	0.50
1:C:163:THR:CG2	1:C:164:LEU:N	2.74	0.50
1:D:160:GLY:O	1:D:163:THR:HB	2.11	0.50
1:B:45:ASP:OD2	1:B:48:GLU:HG2	2.11	0.50
1:B:504:CYS:SG	1:B:505:ASP:N	2.84	0.50
1:D:122:PHE:CD1	1:D:122:PHE:C	2.89	0.50
1:A:472:GLU:HG3	1:A:473:LYS:N	2.27	0.50
1:B:163:THR:CG2	1:B:164:LEU:N	2.75	0.50
1:A:446:LYS:HG2	1:A:447:GLY:N	2.24	0.50
1:C:124:ARG:C	1:C:124:ARG:HD3	2.36	0.50
1:C:474:ALA:HB1	1:C:486:LEU:HD11	1.94	0.50
1:A:65:GLY:HA3	1:A:368:LYS:HD2	1.94	0.50
1:A:518:VAL:O	1:A:519:THR:HG23	2.12	0.50
1:B:302:ARG:NH1	4:B:2049:HOH:O	2.43	0.50
1:D:163:THR:HG21	1:D:427:MET:CE	2.41	0.50
1:C:149:GLY:O	1:D:393:HIS:HE1	1.94	0.49
1:D:430:VAL:HB	1:D:465:CYS:HB3	1.94	0.49
1:A:410:LEU:HD11	1:A:430:VAL:HG11	1.94	0.49
1:D:124:ARG:NH2	1:D:130:GLU:OE2	2.43	0.49
1:A:510:PRO:C	1:A:511:LYS:HD2	2.37	0.49
1:B:45:ASP:OD1	1:B:47:VAL:HG12	2.13	0.49
1:A:415:ILE:HB	1:A:419:LEU:HB2	1.95	0.49
1:C:276:GLU:O	1:C:278:ARG:N	2.44	0.49
1:D:176:LYS:O	1:D:177:ASP:HB3	2.11	0.49
1:A:149:GLY:O	1:B:393:HIS:HE1	1.96	0.49
1:A:406:LYS:HA	1:A:484:LEU:HG	1.94	0.49
1:C:127:LEU:C	1:C:129:GLY:H	2.19	0.49
1:B:180:ILE:HD12	1:B:180:ILE:N	2.27	0.49
1:B:244:GLU:HA	1:B:270:VAL:O	2.12	0.49
1:D:176:LYS:O	1:D:177:ASP:CB	2.61	0.49
1:C:121:GLU:O	1:C:125:GLN:HG3	2.13	0.49
1:C:420:VAL:HB	4:C:2121:HOH:O	2.13	0.49
1:C:479:ASP:OD2	1:C:482:LYS:HG3	2.12	0.49
1:D:45:ASP:OD2	1:D:47:VAL:HG13	2.12	0.49
1:A:302:ARG:O	1:A:306:ILE:HG13	2.12	0.49
1:C:368:LYS:HG3	4:C:2010:HOH:O	2.13	0.49
1:A:325:ILE:CG2	1:A:326:PRO:HD3	2.35	0.49
1:C:175:ASN:HB2	1:C:179:SER:OG	2.12	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:480:ARG:HG3	1:C:480:ARG:NH1	2.28	0.49
1:D:213:TRP:CE2	1:D:224:ARG:HD2	2.47	0.49
1:A:319:ALA:HA	1:A:396:LEU:O	2.12	0.48
1:D:326:PRO:CA	1:D:398:MET:HE3	2.29	0.48
1:C:176:LYS:HZ2	1:C:178:GLY:N	2.12	0.48
1:C:215:ALA:HA	1:C:220:ASN:O	2.13	0.48
1:D:65:GLY:HA2	4:D:2123:HOH:O	2.14	0.48
1:D:504:CYS:SG	1:D:505:ASP:N	2.86	0.48
1:A:480:ARG:H	1:A:480:ARG:CZ	2.26	0.48
1:D:325:ILE:HD13	1:D:440:THR:CB	2.29	0.48
1:A:90:ASN:ND2	1:A:138:GLN:HG3	2.28	0.48
1:A:343:SER:HB2	1:A:350:LEU:HD11	1.95	0.48
1:C:99:LEU:CD2	1:C:111:MET:HE1	2.35	0.48
1:D:99:LEU:HD23	1:D:111:MET:CE	2.35	0.48
1:A:215:ALA:HA	1:A:220:ASN:O	2.13	0.48
1:A:471:THR:HG22	1:A:474:ALA:O	2.14	0.48
1:D:92:ALA:HB2	1:D:111:MET:HE2	1.96	0.48
1:D:163:THR:CG2	1:D:164:LEU:N	2.76	0.48
1:A:213:TRP:CE2	1:A:224:ARG:HD2	2.48	0.48
1:B:175:ASN:O	1:B:177:ASP:N	2.47	0.48
1:C:393:HIS:HD2	4:D:2121:HOH:O	1.97	0.48
1:D:323:ILE:HG21	1:D:367:GLY:HA3	1.95	0.48
1:D:104:GLN:CA	1:D:104:GLN:HE21	2.27	0.48
1:A:450:HIS:HB3	1:A:503:GLY:CA	2.44	0.48
1:B:480:ARG:CZ	1:B:480:ARG:H	2.26	0.48
1:C:176:LYS:HE3	1:C:179:SER:OG	2.13	0.47
1:C:304:ARG:HA	1:C:517:GLN:OE1	2.14	0.47
1:D:56:GLY:HA2	1:D:84:GLU:O	2.13	0.47
1:C:284:VAL:HG13	1:C:354:PRO:O	2.14	0.47
1:C:325:ILE:CG2	1:C:326:PRO:HD3	2.41	0.47
1:A:99:LEU:HD23	1:A:111:MET:CE	2.37	0.47
1:B:314:GLU:HA	1:B:337:MET:HE2	1.97	0.47
1:D:162:GLY:HA3	1:D:463:LYS:HD3	1.97	0.47
1:D:456:CYS:SG	1:D:460:LEU:HD21	2.55	0.47
1:A:161:TYR:CE2	1:A:463:LYS:HE2	2.50	0.47
1:A:170:SER:HB3	3:A:9007:EMT:SD	2.54	0.47
1:A:414:MET:HE3	1:A:416:PRO:HA	1.95	0.47
1:A:410:LEU:O	1:A:461:THR:N	2.41	0.47
1:C:72:ASN:HD21	1:C:274:LYS:H	1.63	0.47
1:C:176:LYS:O	1:C:177:ASP:HB2	2.14	0.47
1:D:442:GLU:HG2	1:D:451:LYS:HZ2	1.80	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:403:GLN:HE22	1:A:457:THR:H	1.59	0.47
1:A:509:SER:C	1:A:511:LYS:N	2.73	0.47
1:D:480:ARG:HH11	1:D:480:ARG:HB3	1.80	0.47
1:B:215:ALA:CB	1:B:269:LEU:HD21	2.44	0.47
1:D:215:ALA:HA	1:D:220:ASN:O	2.15	0.47
1:C:166:GLN:OE1	1:C:189:VAL:HG21	2.15	0.46
1:A:302:ARG:HG2	4:A:2067:HOH:O	2.13	0.46
1:B:465:CYS:SG	3:B:9008:EMT:CE2	3.03	0.46
1:A:406:LYS:O	1:A:483:GLY:HA2	2.15	0.46
1:C:212:ALA:HB3	1:C:245:VAL:HG12	1.97	0.46
1:C:399:LEU:HD12	1:C:439:VAL:HG22	1.96	0.46
1:D:99:LEU:CD2	1:D:111:MET:HE1	2.34	0.46
1:D:477:ASP:HB2	1:D:485:THR:HG23	1.97	0.46
1:C:441:MET:HE2	4:C:2135:HOH:O	2.15	0.46
1:D:163:THR:HG21	1:D:427:MET:SD	2.56	0.46
1:A:402:MET:HE3	1:A:412:ASN:HA	1.98	0.46
1:A:419:LEU:HD22	1:A:421:LYS:HE3	1.96	0.46
1:D:325:ILE:N	1:D:326:PRO:CD	2.78	0.46
1:A:244:GLU:HA	1:A:270:VAL:O	2.16	0.46
1:B:92:ALA:HB2	1:B:111:MET:HE2	1.97	0.46
1:B:215:ALA:HA	1:B:220:ASN:O	2.15	0.46
1:D:302:ARG:O	1:D:306:ILE:HG13	2.15	0.46
1:B:152:VAL:O	1:B:202:ALA:HB2	2.16	0.46
1:B:301:VAL:HG13	1:B:472:GLU:HB3	1.98	0.46
1:C:127:LEU:C	1:C:129:GLY:N	2.74	0.46
1:A:368:LYS:HG3	4:A:2006:HOH:O	2.15	0.46
1:B:175:ASN:N	1:B:179:SER:O	2.42	0.46
1:D:322:GLY:O	1:D:326:PRO:HB2	2.15	0.46
1:A:402:MET:HE1	1:A:414:MET:O	2.16	0.45
1:B:45:ASP:OD2	1:B:47:VAL:HG13	2.16	0.45
1:B:90:ASN:HD21	1:B:138:GLN:HG3	1.81	0.45
1:C:466:VAL:HG12	1:C:467:ASN:N	2.30	0.45
1:A:259:ILE:HD12	1:B:378:SER:HB3	1.98	0.45
1:D:58:THR:HA	1:D:86:THR:O	2.16	0.45
1:D:511:LYS:HD2	1:D:511:LYS:H	1.82	0.45
1:D:519:THR:OG1	1:D:520:THR:N	2.49	0.45
1:A:225:LYS:HA	1:A:379:TYR:CD2	2.51	0.45
1:B:119:ASN:C	1:B:119:ASN:ND2	2.75	0.45
1:C:509:SER:C	1:C:511:LYS:H	2.24	0.45
1:A:485:THR:O	1:A:487:ILE:HG23	2.16	0.45
1:B:301:VAL:HG13	1:B:472:GLU:CB	2.47	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:150:ALA:O	1:D:390:ARG:HD2	2.17	0.45
1:D:212:ALA:HB3	1:D:245:VAL:HG12	1.99	0.45
1:A:323:ILE:HG21	1:A:367:GLY:HA3	1.98	0.45
1:B:104:GLN:HE22	1:B:121:GLU:HG2	1.82	0.45
1:D:244:GLU:HA	1:D:270:VAL:O	2.16	0.45
1:D:326:PRO:HB3	1:D:398:MET:HG2	1.98	0.45
1:C:472:GLU:HG3	1:C:473:LYS:N	2.32	0.45
1:A:235:CYS:O	1:A:241:THR:HG21	2.17	0.45
1:C:191:GLU:HA	1:C:195:GLN:O	2.17	0.45
1:C:232:LEU:HG	1:C:261:ILE:HD11	1.98	0.45
1:C:244:GLU:HA	1:C:270:VAL:O	2.17	0.44
1:C:486:LEU:HD11	1:C:488:GLU:O	2.17	0.44
1:C:152:VAL:O	1:C:202:ALA:HB2	2.17	0.44
1:C:155:PHE:CD1	1:C:155:PHE:C	2.94	0.44
1:D:321:LEU:HD22	1:D:398:MET:HE2	1.98	0.44
1:D:472:GLU:HG3	1:D:473:LYS:N	2.32	0.44
1:B:90:ASN:ND2	1:B:138:GLN:HG3	2.32	0.44
1:D:474:ALA:HB1	1:D:486:LEU:CD1	2.48	0.44
1:A:308:ARG:HD3	1:A:516:GLN:O	2.17	0.44
1:C:399:LEU:CD1	1:C:439:VAL:HG22	2.47	0.44
1:A:311:LEU:HG	1:A:518:VAL:HG13	1.99	0.44
1:B:40:THR:CG2	1:B:219:GLY:HA3	2.35	0.44
1:B:228:ARG:HB3	4:B:2065:HOH:O	2.16	0.44
1:B:465:CYS:SG	3:B:9008:EMT:CZ	3.06	0.44
1:A:223:PHE:HE1	1:A:261:ILE:HG12	1.82	0.44
1:A:163:THR:HG21	1:A:427:MET:HE1	1.99	0.44
1:B:343:SER:HB2	1:B:350:LEU:HD11	1.99	0.44
1:D:332:PHE:CG	1:D:518:VAL:HG21	2.53	0.44
1:B:489:LEU:O	1:B:515:MET:N	2.51	0.44
1:D:373:VAL:HG22	1:D:377:ALA:CB	2.48	0.44
1:C:180:ILE:N	1:C:180:ILE:CD1	2.80	0.44
1:A:408:GLY:CA	1:A:464:GLN:HA	2.47	0.43
3:A:9007:EMT:HE2	4:A:2025:HOH:O	2.55	0.43
1:C:441:MET:HE1	1:C:472:GLU:OE2	2.17	0.43
1:D:127:LEU:HD21	1:D:420:VAL:HG21	1.99	0.43
1:D:163:THR:CG2	1:D:165:VAL:H	2.13	0.43
1:C:132:GLU:HA	1:C:172:ILE:O	2.18	0.43
1:A:236:LYS:NZ	1:B:384:GLU:OE1	2.50	0.43
1:A:410:LEU:HD23	1:A:462:GLY:O	2.18	0.43
1:B:217:GLN:HE21	1:B:217:GLN:HB2	1.66	0.43
1:B:304:ARG:HG2	1:B:490:TRP:CH2	2.54	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:210:VAL:HG13	1:C:231:ASN:HB3	2.00	0.43
1:D:365:ASN:HB2	4:D:2139:HOH:O	2.19	0.43
1:D:73:LEU:HG	1:D:244:GLU:OE1	2.18	0.43
1:D:314:GLU:HA	1:D:337:MET:HE2	1.99	0.43
1:B:509:SER:C	1:B:511:LYS:N	2.75	0.43
1:D:511:LYS:N	1:D:511:LYS:CD	2.81	0.43
1:A:314:GLU:HA	1:A:337:MET:HE2	2.00	0.43
1:A:401:ALA:HB3	1:A:439:VAL:HG11	2.01	0.43
1:A:405:SER:HB3	1:A:409:ASP:HB2	2.00	0.43
1:A:414:MET:HG2	1:A:415:ILE:N	2.34	0.43
1:A:455:LYS:HE2	1:A:455:LYS:C	2.44	0.43
1:B:126:TYR:CE1	1:B:133:VAL:CG1	3.01	0.43
1:C:301:VAL:HG13	1:C:472:GLU:CB	2.48	0.43
1:D:139:GLY:HA2	1:D:386:PHE:CG	2.54	0.43
1:A:410:LEU:HD23	1:A:410:LEU:N	2.34	0.43
1:B:210:VAL:HG13	1:B:231:ASN:HB3	2.00	0.43
1:A:406:LYS:HZ1	1:A:454:GLU:HG3	1.83	0.43
1:B:474:ALA:HB1	1:B:486:LEU:HD11	2.00	0.43
1:C:305:ILE:HG22	1:C:325:ILE:HD11	1.99	0.43
1:C:509:SER:C	1:C:511:LYS:N	2.77	0.43
1:D:104:GLN:HE21	1:D:104:GLN:N	2.17	0.43
1:D:232:LEU:HG	1:D:261:ILE:HD11	2.00	0.43
1:A:232:LEU:HB3	1:A:233:PRO:CD	2.49	0.43
1:A:446:LYS:C	1:A:448:ASN:H	2.27	0.43
1:C:45:ASP:OD2	1:C:47:VAL:CG1	2.67	0.43
1:C:354:PRO:CB	1:C:358:GLU:HB2	2.48	0.42
1:A:482:LYS:O	1:C:271:LYS:HE3	2.20	0.42
1:B:323:ILE:HG21	1:B:367:GLY:HA3	2.01	0.42
1:A:480:ARG:HH11	1:A:480:ARG:HB3	1.84	0.42
1:C:173:LYS:HE2	1:C:182:ILE:HG13	2.01	0.42
1:C:92:ALA:HB2	1:C:111:MET:HE2	2.00	0.42
1:C:225:LYS:HA	1:C:379:TYR:CD2	2.53	0.42
1:A:325:ILE:N	1:A:326:PRO:CD	2.83	0.42
1:A:506:PHE:HD1	1:A:507:ALA:O	2.02	0.42
1:D:301:VAL:HG13	1:D:472:GLU:CB	2.48	0.42
1:D:506:PHE:HA	2:D:9000:EMC:C1	2.49	0.42
1:A:45:ASP:OD2	1:A:47:VAL:HG13	2.18	0.42
1:B:104:GLN:CA	1:B:104:GLN:HE21	2.31	0.42
1:B:141:LEU:O	1:B:145:ILE:HG13	2.19	0.42
1:C:130:GLU:HA	1:C:130:GLU:OE1	2.20	0.42
1:C:189:VAL:HG22	1:C:198:ILE:HG22	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:210:VAL:HG13	1:D:231:ASN:HB3	2.01	0.42
1:B:471:THR:HG23	1:B:473:LYS:H	1.84	0.42
1:C:480:ARG:NE	1:C:480:ARG:H	2.17	0.42
1:D:414:MET:HE2	1:D:420:VAL:HG12	2.01	0.42
1:A:207:PHE:HA	1:A:240:THR:O	2.20	0.42
1:B:84:GLU:HA	1:B:109:LYS:HB2	2.02	0.42
1:B:139:GLY:HA2	1:B:386:PHE:CG	2.55	0.42
1:B:176:LYS:O	1:B:177:ASP:HB3	2.20	0.42
1:C:45:ASP:OD2	1:C:47:VAL:HG13	2.19	0.42
1:C:420:VAL:CB	4:C:2121:HOH:O	2.68	0.42
1:D:166:GLN:HA	1:D:187:ARG:HB2	2.02	0.42
1:D:472:GLU:HG3	1:D:473:LYS:H	1.83	0.42
1:A:152:VAL:O	1:A:202:ALA:HB2	2.19	0.42
1:A:215:ALA:CB	1:A:269:LEU:HD21	2.49	0.42
1:B:45:ASP:OD2	1:B:47:VAL:CG1	2.68	0.42
1:B:321:LEU:HD22	1:B:398:MET:HE2	2.01	0.42
1:A:283:SER:O	1:A:354:PRO:HD2	2.20	0.41
1:B:53:ILE:HA	1:B:54:PRO:HD3	1.85	0.41
1:B:226:SER:C	1:B:228:ARG:H	2.28	0.41
1:B:472:GLU:HG3	1:B:473:LYS:N	2.35	0.41
1:C:99:LEU:HD23	1:C:111:MET:CE	2.36	0.41
1:C:208:ALA:HB3	1:C:241:THR:HG22	2.02	0.41
1:C:489:LEU:CD1	1:C:498:ILE:HD11	2.50	0.41
1:A:210:VAL:HG13	1:A:231:ASN:HB3	2.03	0.41
1:A:511:LYS:N	1:A:511:LYS:CD	2.80	0.41
1:B:77:LEU:HD11	1:B:209:LEU:HD11	2.02	0.41
1:C:121:GLU:OE1	1:C:121:GLU:HA	2.19	0.41
1:C:138:GLN:NE2	4:C:2111:HOH:O	2.53	0.41
1:A:58:THR:HA	1:A:86:THR:O	2.20	0.41
1:A:311:LEU:CD2	1:A:518:VAL:HG12	2.50	0.41
1:A:409:ASP:HB3	1:A:460:LEU:CD2	2.50	0.41
1:A:413:TRP:CZ3	1:A:414:MET:HB2	2.55	0.41
1:C:325:ILE:N	1:C:326:PRO:CD	2.84	0.41
1:C:441:MET:HA	4:C:2130:HOH:O	2.20	0.41
1:B:207:PHE:HA	1:B:240:THR:O	2.21	0.41
1:B:354:PRO:HD3	1:B:371:VAL:HA	2.03	0.41
1:C:163:THR:CG2	1:C:165:VAL:HG23	2.51	0.41
1:C:367:GLY:O	1:C:368:LYS:CB	2.68	0.41
1:D:367:GLY:O	1:D:368:LYS:CB	2.69	0.41
1:D:412:ASN:ND2	1:D:461:THR:OG1	2.54	0.41
1:A:420:VAL:HG23	4:A:2093:HOH:O	2.19	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:77:LEU:HD11	1:C:209:LEU:HD11	2.03	0.41
1:D:53:ILE:HA	1:D:54:PRO:HD3	1.86	0.41
1:C:223:PHE:HE1	1:C:261:ILE:HG12	1.86	0.41
1:C:479:ASP:O	1:C:480:ARG:C	2.63	0.41
1:D:47:VAL:HG13	4:D:2003:HOH:O	2.21	0.41
1:D:65:GLY:HA3	1:D:368:LYS:HD2	2.02	0.41
1:D:217:GLN:HE21	1:D:217:GLN:HB2	1.62	0.41
1:A:40:THR:CG2	1:A:219:GLY:HA3	2.39	0.41
1:A:116:VAL:HG21	1:A:122:PHE:CZ	2.56	0.41
1:A:217:GLN:HB2	1:A:251:ILE:HG13	2.03	0.40
1:A:402:MET:CE	1:A:412:ASN:HA	2.51	0.40
1:A:453:MET:HA	1:A:504:CYS:H	1.86	0.40
1:B:354:PRO:CB	1:B:358:GLU:HB2	2.50	0.40
1:C:256:PRO:HB2	1:D:379:TYR:CE2	2.57	0.40
1:D:403:GLN:NE2	1:D:458:LEU:H	2.19	0.40
1:A:285:ARG:HG2	1:A:353:TYR:O	2.21	0.40
1:B:324:GLY:O	1:B:328:LEU:HG	2.22	0.40
1:C:104:GLN:CA	1:C:104:GLN:HE21	2.35	0.40
1:C:207:PHE:HA	1:C:240:THR:O	2.21	0.40
1:D:62:GLY:HA3	1:D:231:ASN:OD1	2.21	0.40
1:A:42:PHE:CD1	1:A:42:PHE:N	2.90	0.40
1:B:225:LYS:HA	1:B:379:TYR:CD2	2.56	0.40
1:C:90:ASN:O	1:C:113:SER:HB3	2.21	0.40
1:C:506:PHE:HD1	1:C:507:ALA:O	2.03	0.40
1:D:442:GLU:CG	1:D:451:LYS:HZ2	2.34	0.40
1:B:212:ALA:HB3	1:B:245:VAL:HG12	2.02	0.40
1:B:326:PRO:HA	1:B:398:MET:HE3	2.02	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	464/481 (96%)	438 (94%)	18 (4%)	8 (2%)	7	10
1	B	417/481 (87%)	397 (95%)	16 (4%)	4 (1%)	12	20
1	C	417/481 (87%)	397 (95%)	13 (3%)	7 (2%)	7	10
1	D	460/481 (96%)	438 (95%)	18 (4%)	4 (1%)	14	22
All	All	1758/1924 (91%)	1670 (95%)	65 (4%)	23 (1%)	9	14

All (23) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	413	TRP
1	A	416	PRO
1	A	519	THR
1	B	177	ASP
1	C	177	ASP
1	D	177	ASP
1	D	446	LYS
1	D	519	THR
1	A	419	LEU
1	A	505	ASP
1	B	176	LYS
1	C	119	ASN
1	A	229	ASN
1	A	446	LYS
1	C	176	LYS
1	C	229	ASN
1	D	229	ASN
1	A	412	ASN
1	B	178	GLY
1	B	229	ASN
1	C	170	SER
1	C	178	GLY
1	C	117	GLY

5.3.2 Protein sidechains ⓘ

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	382/393 (97%)	361 (94%)	21 (6%)	19	34
1	B	347/393 (88%)	330 (95%)	17 (5%)	22	39
1	C	345/393 (88%)	327 (95%)	18 (5%)	21	36
1	D	378/393 (96%)	354 (94%)	24 (6%)	16	29
All	All	1452/1572 (92%)	1372 (94%)	80 (6%)	19	34

All (80) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	40	THR
1	A	58	THR
1	A	103	LEU
1	A	104	GLN
1	A	133	VAL
1	A	136	THR
1	A	163	THR
1	A	221	VAL
1	A	282	LEU
1	A	325	ILE
1	A	373	VAL
1	A	399	LEU
1	A	416	PRO
1	A	420	VAL
1	A	446	LYS
1	A	455	LYS
1	A	480	ARG
1	A	485	THR
1	A	491	GLU
1	A	504	CYS
1	A	519	THR
1	B	40	THR
1	B	58	THR
1	B	103	LEU
1	B	104	GLN
1	B	124	ARG
1	B	133	VAL
1	B	136	THR
1	B	163	THR
1	B	175	ASN
1	B	176	LYS
1	B	221	VAL
1	B	325	ILE

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Mol	Chain	Res	Type
1	B	373	VAL
1	B	399	LEU
1	B	480	ARG
1	B	485	THR
1	B	491	GLU
1	C	40	THR
1	C	58	THR
1	C	103	LEU
1	C	104	GLN
1	C	133	VAL
1	C	136	THR
1	C	163	THR
1	C	176	LYS
1	C	221	VAL
1	C	325	ILE
1	C	373	VAL
1	C	399	LEU
1	C	420	VAL
1	C	480	ARG
1	C	485	THR
1	C	491	GLU
1	C	517	GLN
1	C	518	VAL
1	D	40	THR
1	D	58	THR
1	D	103	LEU
1	D	104	GLN
1	D	118	GLU
1	D	119	ASN
1	D	133	VAL
1	D	136	THR
1	D	163	THR
1	D	221	VAL
1	D	235	CYS
1	D	282	LEU
1	D	325	ILE
1	D	373	VAL
1	D	399	LEU
1	D	412	ASN
1	D	419	LEU
1	D	446	LYS
1	D	455	LYS

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Mol	Chain	Res	Type
1	D	457	THR
1	D	465	CYS
1	D	480	ARG
1	D	485	THR
1	D	518	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (43) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	72	ASN
1	A	90	ASN
1	A	104	GLN
1	A	119	ASN
1	A	125	GLN
1	A	166	GLN
1	A	175	ASN
1	A	217	GLN
1	A	393	HIS
1	A	403	GLN
1	A	464	GLN
1	B	72	ASN
1	B	90	ASN
1	B	104	GLN
1	B	119	ASN
1	B	125	GLN
1	B	175	ASN
1	B	196	HIS
1	B	217	GLN
1	B	393	HIS
1	C	72	ASN
1	C	90	ASN
1	C	104	GLN
1	C	125	GLN
1	C	138	GLN
1	C	166	GLN
1	C	193	ASN
1	C	217	GLN
1	C	393	HIS
1	C	516	GLN
1	D	72	ASN
1	D	90	ASN
1	D	104	GLN

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Mol	Chain	Res	Type
1	D	119	ASN
1	D	125	GLN
1	D	175	ASN
1	D	193	ASN
1	D	217	GLN
1	D	336	ASN
1	D	393	HIS
1	D	403	GLN
1	D	412	ASN
1	D	464	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

9 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	EMC	B	9004	1	1,2,2	0.49	0	-		
2	EMC	A	9003	1	1,2,2	0.38	0	-		
2	EMC	D	9001	1	1,2,2	3.63	1 (100%)	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	EMT	B	9008	-	12,13,13	1.11	1 (8%)	13,16,16	0.57	0
3	EMT	A	9007	-	12,13,13	1.10	1 (8%)	13,16,16	0.87	1 (7%)
2	EMC	C	9005	4,1	1,2,2	1.54	0	-		
2	EMC	D	9002	1	1,2,2	0.42	0	-		
2	EMC	C	9006	1	1,2,2	0.52	0	-		
2	EMC	D	9000	1	1,2,2	0.55	0	-		

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
3	EMT	A	9007	-	-	0/4/8/8	0/1/1/1
3	EMT	B	9008	-	-	0/4/8/8	0/1/1/1

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	9001	EMC	C2-C1	-3.63	1.30	1.49
3	B	9008	EMT	CZ-CG	2.24	1.54	1.49
3	A	9007	EMT	CE1-SD	2.14	1.82	1.78

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	9007	EMT	CZ-CE1-SD	-2.33	120.34	124.18

There are no chirality outliers.

There are no torsion outliers.

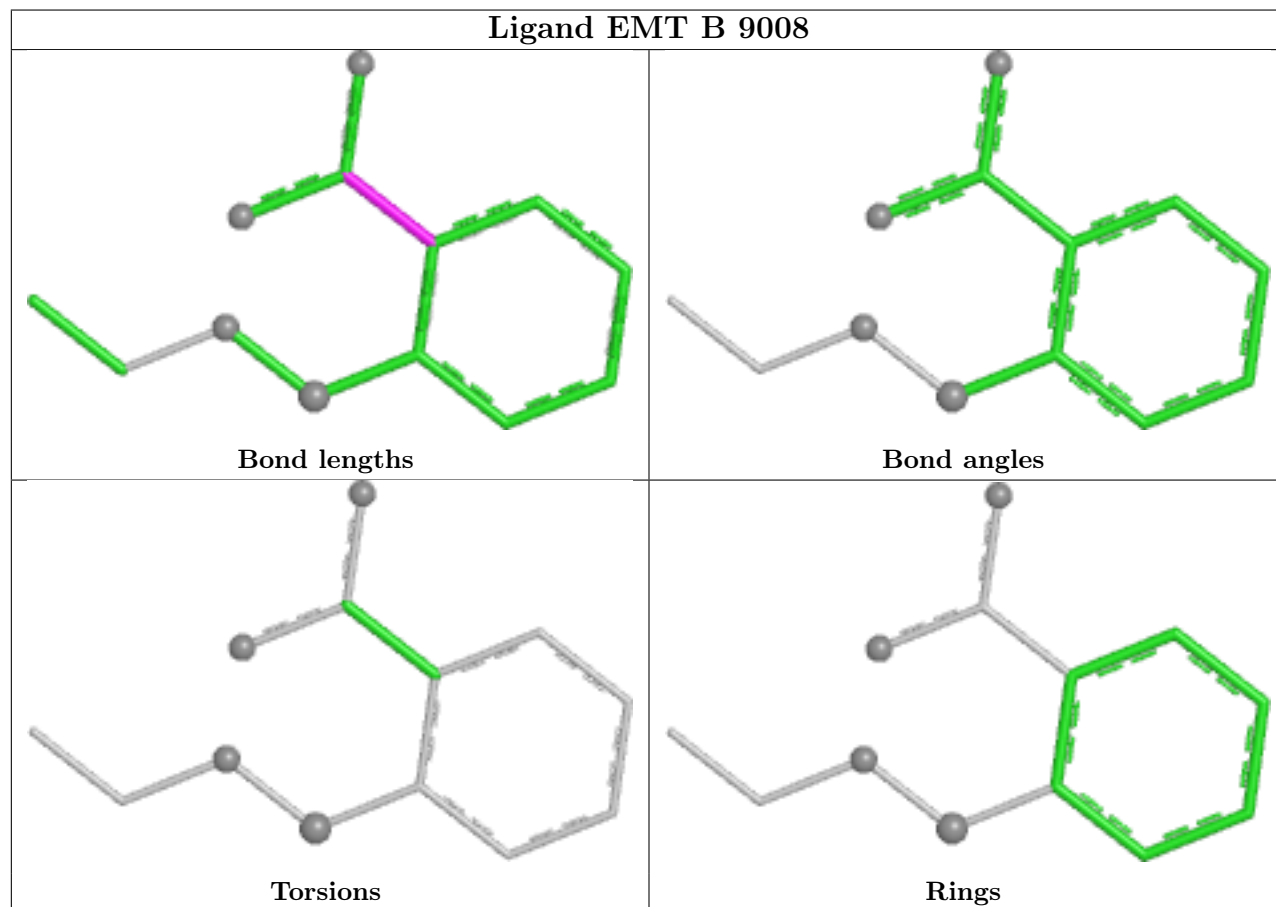
There are no ring outliers.

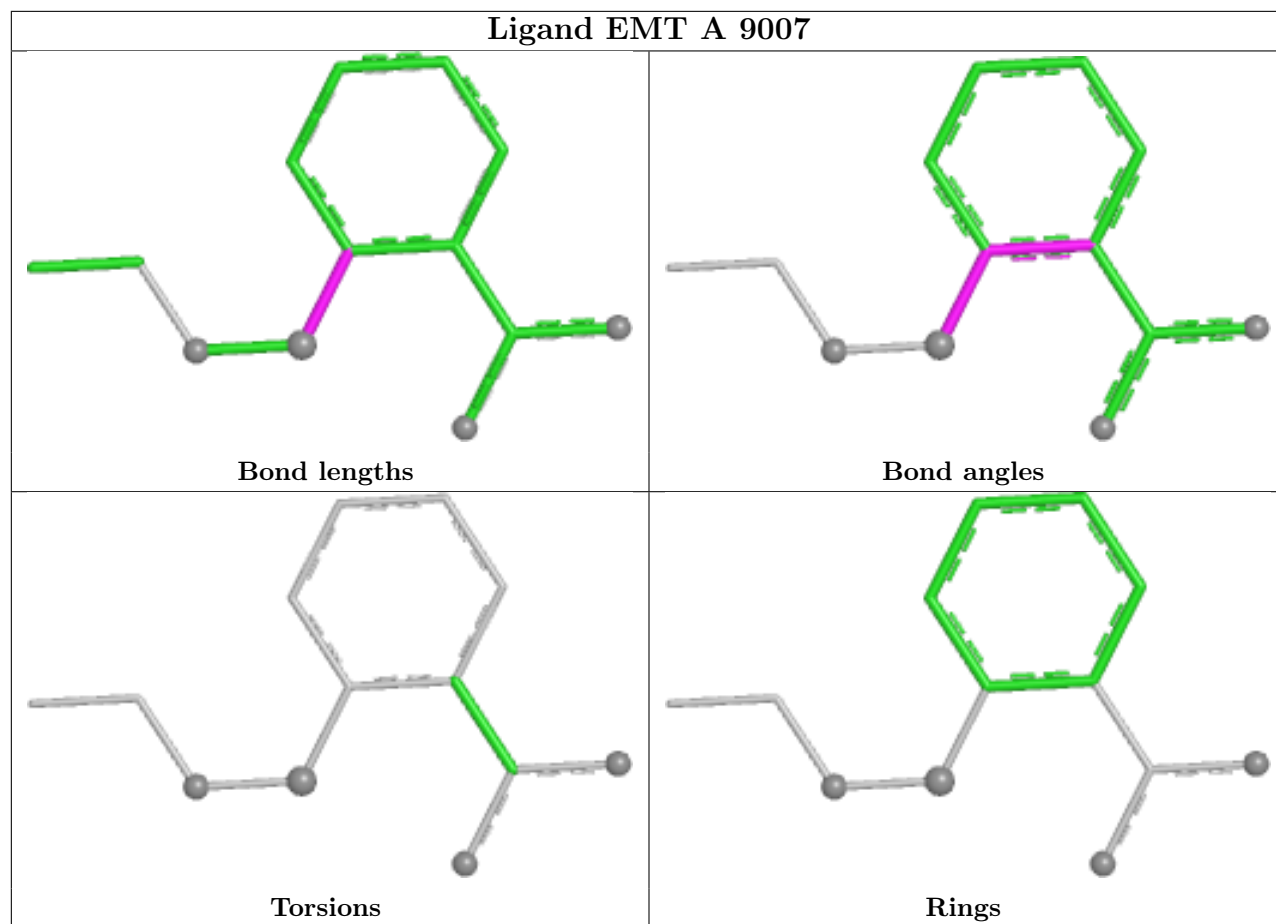
3 monomers are involved in 12 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	9008	EMT	8	0
3	A	9007	EMT	3	0
2	D	9000	EMC	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 than 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, 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	468/481 (97%)	0.79	63 (13%) 7 5	23, 41, 73, 83	0
1	B	425/481 (88%)	0.81	55 (12%) 7 5	24, 44, 76, 82	0
1	C	425/481 (88%)	0.88	80 (18%) 3 3	19, 40, 77, 86	0
1	D	464/481 (96%)	0.76	67 (14%) 6 4	18, 36, 62, 80	0
All	All	1782/1924 (92%)	0.81	265 (14%) 5 4	18, 40, 75, 86	0

All (265) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	465	CYS	6.2
1	D	332	PHE	5.2
1	D	326	PRO	5.0
1	D	329	ALA	5.0
1	D	325	ILE	4.9
1	C	480	ARG	4.8
1	C	485	THR	4.7
1	B	465	CYS	4.6
1	A	520	THR	4.6
1	A	336	ASN	4.4
1	D	117	GLY	4.4
1	C	503	GLY	4.2
1	D	301	VAL	4.1
1	C	479	ASP	4.0
1	D	420	VAL	4.0
1	D	335	PRO	4.0
1	A	335	PRO	4.0
1	A	419	LEU	3.9
1	D	327	LEU	3.9
1	D	328	LEU	3.9
1	D	352	PRO	3.9

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Mol	Chain	Res	Type	RSRZ
1	D	116	VAL	3.8
1	A	496	ASP	3.8
1	C	512	LEU	3.8
1	C	494	THR	3.7
1	D	323	ILE	3.7
1	C	126	TYR	3.7
1	C	334	SER	3.6
1	A	457	THR	3.6
1	D	338	THR	3.6
1	A	357	ASN	3.6
1	A	449	ALA	3.5
1	A	421	LYS	3.5
1	C	332	PHE	3.5
1	B	481	LYS	3.5
1	A	504	CYS	3.5
1	B	480	ARG	3.4
1	C	125	GLN	3.4
1	C	420	VAL	3.4
1	D	365	ASN	3.4
1	C	506	PHE	3.4
1	D	178	GLY	3.4
1	C	176	LYS	3.4
1	B	300	ASN	3.3
1	A	519	THR	3.3
1	C	122	PHE	3.3
1	D	324	GLY	3.3
1	A	460	LEU	3.3
1	D	520	THR	3.3
1	B	250	ASP	3.2
1	D	336	ASN	3.2
1	A	462	GLY	3.2
1	B	490	TRP	3.2
1	D	484	LEU	3.2
1	B	333	ILE	3.2
1	C	472	GLU	3.2
1	A	409	ASP	3.2
1	D	303	GLU	3.2
1	D	421	LYS	3.2
1	C	510	PRO	3.1
1	D	353	TYR	3.1
1	D	483	GLY	3.1
1	C	333	ILE	3.1

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Mol	Chain	Res	Type	RSRZ
1	B	491	GLU	3.1
1	C	170	SER	3.1
1	D	322	GLY	3.1
1	A	513	ILE	3.1
1	D	356	GLN	3.1
1	A	337	MET	3.1
1	A	332	PHE	3.1
1	B	96	ASN	3.1
1	A	420	VAL	3.1
1	D	471	THR	3.0
1	C	484	LEU	3.0
1	A	412	ASN	3.0
1	D	321	LEU	3.0
1	D	511	LYS	3.0
1	B	507	ALA	3.0
1	D	366	ALA	3.0
1	D	115	TYR	3.0
1	B	476	PHE	3.0
1	D	330	SER	3.0
1	D	504	CYS	3.0
1	C	336	ASN	3.0
1	A	333	ILE	2.9
1	A	475	VAL	2.9
1	D	333	ILE	2.9
1	A	338	THR	2.9
1	C	174	TYR	2.9
1	A	104	GLN	2.9
1	A	300	ASN	2.9
1	B	332	PHE	2.9
1	A	417	GLY	2.9
1	B	168	GLY	2.9
1	D	491	GLU	2.9
1	C	180	ILE	2.9
1	C	478	VAL	2.9
1	B	104	GLN	2.9
1	A	465	CYS	2.8
1	D	334	SER	2.8
1	C	171	PRO	2.8
1	B	276	GLU	2.8
1	B	506	PHE	2.8
1	C	116	VAL	2.8
1	D	362	ASP	2.8

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Mol	Chain	Res	Type	RSRZ
1	C	127	LEU	2.8
1	B	334	SER	2.7
1	B	508	VAL	2.7
1	C	486	LEU	2.7
1	A	416	PRO	2.7
1	A	111	MET	2.7
1	C	172	ILE	2.7
1	B	336	ASN	2.7
1	B	301	VAL	2.7
1	B	471	THR	2.7
1	D	277	LYS	2.7
1	D	357	ASN	2.7
1	B	478	VAL	2.7
1	C	502	THR	2.7
1	C	441	MET	2.6
1	A	410	LEU	2.6
1	A	493	LEU	2.6
1	C	123	GLU	2.6
1	B	306	ILE	2.6
1	C	42	PHE	2.6
1	B	475	VAL	2.6
1	C	520	THR	2.6
1	A	459	PRO	2.6
1	C	104	GLN	2.6
1	B	498	ILE	2.6
1	C	498	ILE	2.6
1	A	476	PHE	2.6
1	D	313	PHE	2.6
1	A	508	VAL	2.6
1	B	400	GLY	2.5
1	A	323	ILE	2.5
1	D	355	LEU	2.5
1	D	95	ASP	2.5
1	D	42	PHE	2.5
1	B	485	THR	2.5
1	D	47	VAL	2.5
1	B	117	GLY	2.5
1	A	413	TRP	2.5
1	D	300	ASN	2.5
1	C	120	ALA	2.5
1	A	334	SER	2.5
1	A	405	SER	2.5

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Mol	Chain	Res	Type	RSRZ
1	C	330	SER	2.5
1	A	512	LEU	2.4
1	A	469	ILE	2.4
1	C	124	ARG	2.4
1	D	304	ARG	2.4
1	C	495	VAL	2.4
1	C	474	ALA	2.4
1	B	277	LYS	2.4
1	B	500	LYS	2.4
1	C	482	LYS	2.4
1	A	516	GLN	2.4
1	C	331	ASN	2.4
1	B	482	LYS	2.4
1	B	484	LEU	2.4
1	C	177	ASP	2.4
1	A	406	LYS	2.4
1	C	481	LYS	2.4
1	C	168	GLY	2.3
1	C	483	GLY	2.3
1	B	325	ILE	2.3
1	B	469	ILE	2.3
1	A	495	VAL	2.3
1	C	508	VAL	2.3
1	A	411	ALA	2.3
1	B	179	SER	2.3
1	D	503	GLY	2.3
1	D	364	ILE	2.3
1	D	456	CYS	2.3
1	C	56	GLY	2.3
1	C	178	GLY	2.3
1	C	305	ILE	2.3
1	D	306	ILE	2.3
1	C	337	MET	2.3
1	C	491	GLU	2.3
1	D	275	TYR	2.3
1	A	329	ALA	2.3
1	C	507	ALA	2.3
1	B	494	THR	2.3
1	A	503	GLY	2.3
1	A	501	SER	2.3
1	C	518	VAL	2.3
1	C	175	ASN	2.2

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Mol	Chain	Res	Type	RSRZ
1	C	278	ARG	2.3
1	D	354	PRO	2.3
1	C	309	ALA	2.2
1	D	455	LYS	2.2
1	B	165	VAL	2.2
1	B	304	ARG	2.2
1	D	372	THR	2.2
1	A	492	GLY	2.2
1	B	337	MET	2.2
1	C	117	GLY	2.2
1	C	282	LEU	2.2
1	A	306	ILE	2.2
1	D	279	ILE	2.2
1	B	479	ASP	2.2
1	C	490	TRP	2.2
1	D	480	ARG	2.2
1	A	301	VAL	2.2
1	B	357	ASN	2.2
1	D	519	THR	2.2
1	C	311	LEU	2.2
1	C	328	LEU	2.2
1	B	180	ILE	2.2
1	B	501	SER	2.2
1	D	505	ASP	2.2
1	C	191	GLU	2.2
1	C	82	VAL	2.2
1	A	401	ALA	2.2
1	B	181	ALA	2.2
1	D	331	ASN	2.2
1	A	328	LEU	2.2
1	C	505	ASP	2.2
1	A	480	ARG	2.2
1	B	124	ARG	2.2
1	D	281	ARG	2.2
1	B	338	THR	2.1
1	C	338	THR	2.1
1	C	279	ILE	2.1
1	A	277	LYS	2.1
1	C	313	PHE	2.1
1	C	471	THR	2.1
1	C	493	LEU	2.1
1	D	316	GLY	2.1

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Mol	Chain	Res	Type	RSRZ
1	D	447	GLY	2.1
1	B	281	ARG	2.1
1	C	84	GLU	2.1
1	D	302	ARG	2.1
1	C	179	SER	2.1
1	A	481	LYS	2.1
1	C	185	LYS	2.1
1	C	307	LYS	2.1
1	A	282	LEU	2.1
1	B	486	LEU	2.1
1	C	281	ARG	2.1
1	A	454	GLU	2.1
1	B	305	ILE	2.1
1	C	475	VAL	2.1
1	B	178	GLY	2.1
1	A	498	ILE	2.1
1	A	499	LYS	2.1
1	C	51	LYS	2.1
1	A	407	TYR	2.1
1	B	174	TYR	2.1
1	A	309	ALA	2.0
1	B	499	LYS	2.0
1	C	511	LYS	2.0
1	B	505	ASP	2.0
1	A	510	PRO	2.0
1	D	501	SER	2.0
1	D	217	GLN	2.0
1	A	373	VAL	2.0
1	D	476	PHE	2.0
1	A	445	ALA	2.0
1	B	489	LEU	2.0
1	C	96	ASN	2.0
1	D	446	LYS	2.0
1	B	520	THR	2.0

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

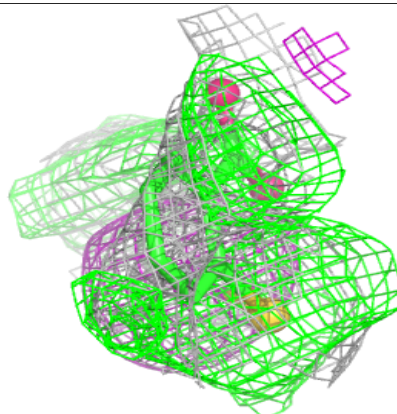
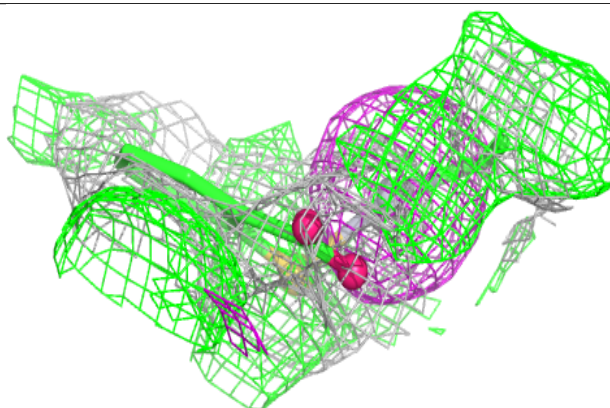
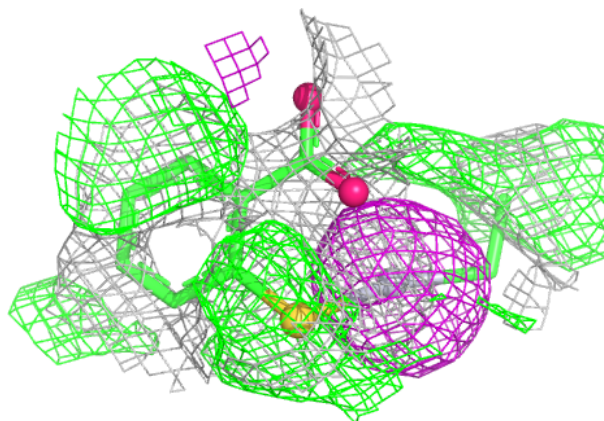
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	EMC	D	9001	3/3	-0.38	0.70	2,2,2,11	3
3	EMT	B	9008	13/13	0.27	0.52	32,41,45,47	13
2	EMC	C	9006	3/3	0.49	0.48	65,65,65,69	3
2	EMC	C	9005	3/3	0.54	0.60	2,2,2,5	3
2	EMC	D	9000	3/3	0.58	0.48	46,46,47,48	3
3	EMT	A	9007	13/13	0.59	0.41	5,11,12,13	13
2	EMC	D	9002	3/3	0.69	0.60	25,25,25,27	3
2	EMC	B	9004	3/3	0.71	0.56	42,42,44,45	3
2	EMC	A	9003	3/3	0.73	0.57	23,23,23,25	3

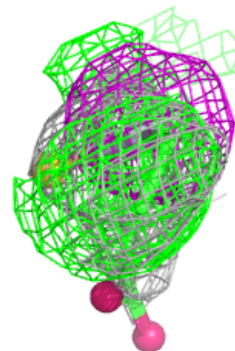
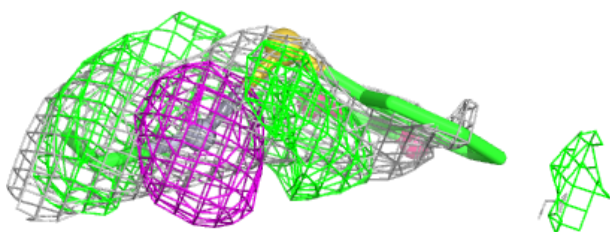
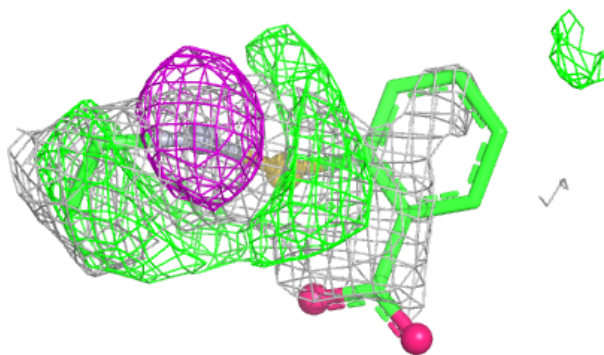
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around EMT B 9008:

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

**Electron density around EMT A 9007:**

$2mF_o-DF_c$ (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.