



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 02:36 AM UTC

PDB ID : 4IXZ / pdb_00004ixz
Title : Native structure of cystathionine gamma lyase (XometC) from xanthomonas oryzae pv. oryzae at pH 9.0
Authors : Ngo, H.P.T.; Kim, J.K.; Kang, L.W.
Deposited on : 2013-01-28
Resolution : 2.07 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
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

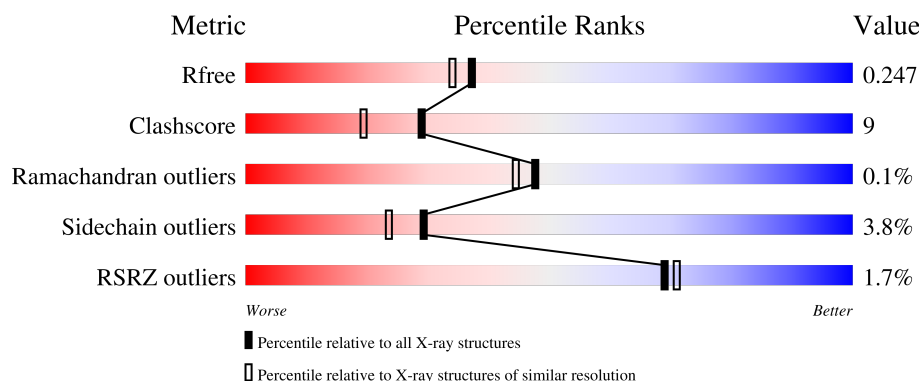
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.07 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	3774 (2.08-2.04)
Clashscore	190562	3883 (2.08-2.04)
Ramachandran outliers	187476	3860 (2.08-2.04)
Sidechain outliers	187428	3860 (2.08-2.04)
RSRZ outliers	180081	3775 (2.08-2.04)

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	397	79% 15% ...
1	B	397	72% 22% ..
1	C	397	3% 75% 18% 5%
1	D	397	2% 77% 15% 5%

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	BCT	A	401	-	-	X	-

2 Entry composition [i](#)

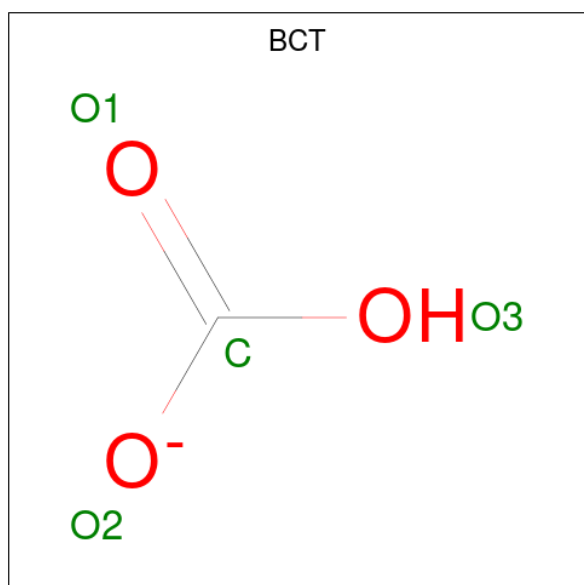
There are 5 unique types of molecules in this entry. The entry contains 12425 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 Cystathionine gamma-lyase-like protein.

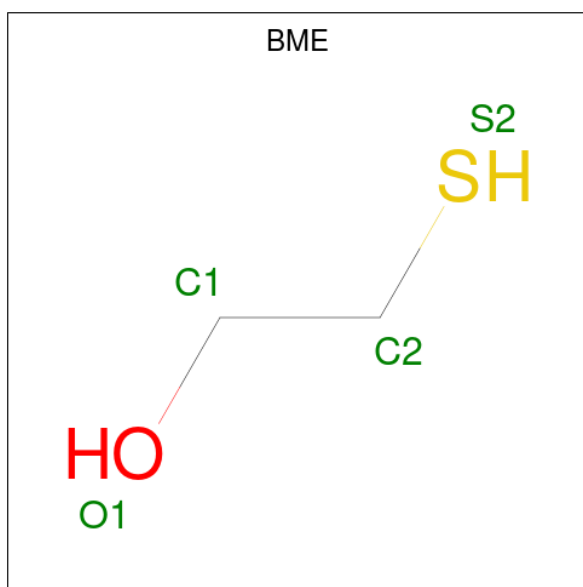
Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	381	Total	C	N	O	P	S	0	1	0
			2881	1822	506	537	1	15			
1	B	381	Total	C	N	O	P	S	0	2	0
			2889	1827	509	537	1	15			
1	C	378	Total	C	N	O	P	S	0	1	0
			2855	1805	501	533	1	15			
1	D	378	Total	C	N	O	P	S	0	2	0
			2860	1808	503	533	1	15			

- Molecule 2 is BICARBONATE ION (CCD ID: BCT) (formula: CHO_3).



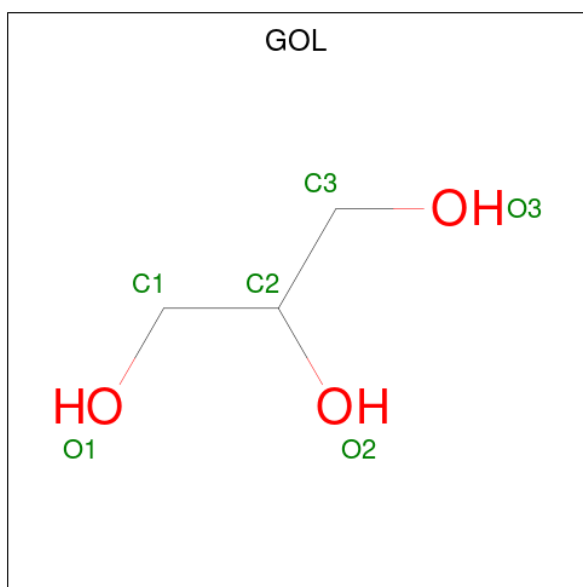
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	C	O	0	0
			4	1	3		

- Molecule 3 is BETA-MERCAPTOETHANOL (CCD ID: BME) (formula: $\text{C}_2\text{H}_6\text{OS}$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	O	S	0	0
			4	2	1	1		
3	B	1	Total	C	O	S	0	0
			4	2	1	1		
3	C	1	Total	C	O	S	0	0
			4	2	1	1		

- Molecule 4 is GLYCEROL (CCD ID: GOL) (formula: $C_3H_8O_3$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	D	1	Total	C	O	0	0
			6	3	3		

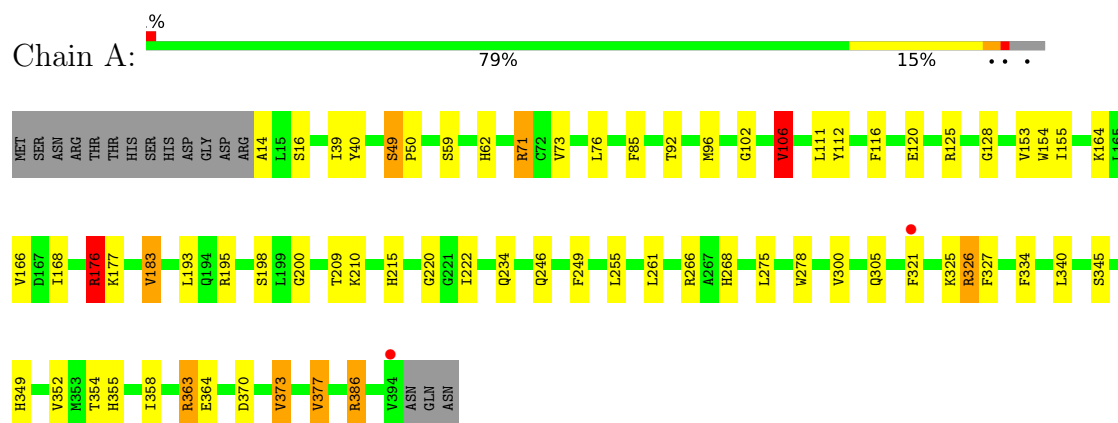
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	239	Total 239	O 239	0	0
5	B	238	Total 238	O 238	0	0
5	C	211	Total 211	O 211	0	0
5	D	230	Total 230	O 230	0	0

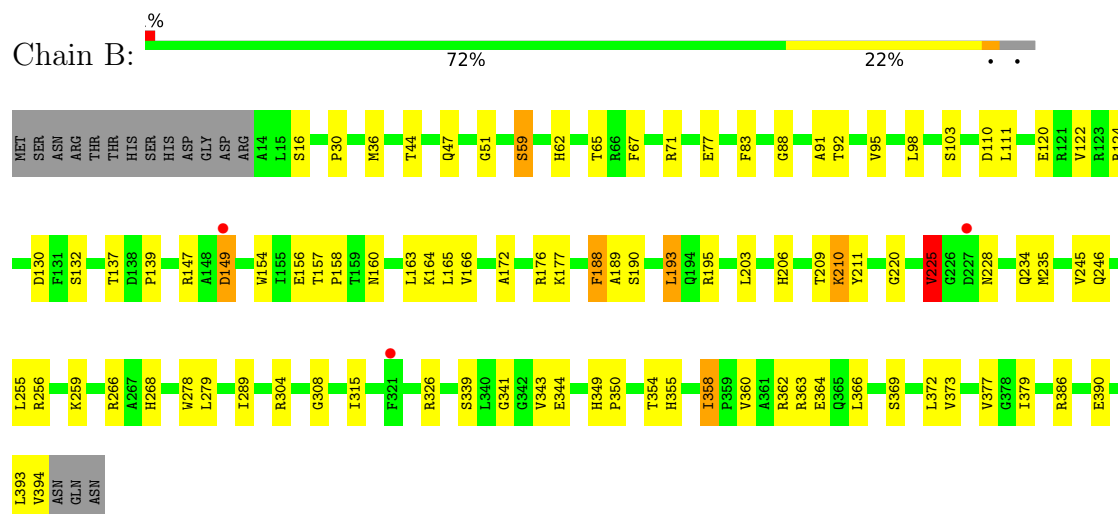
3 Residue-property plots [i](#)

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.

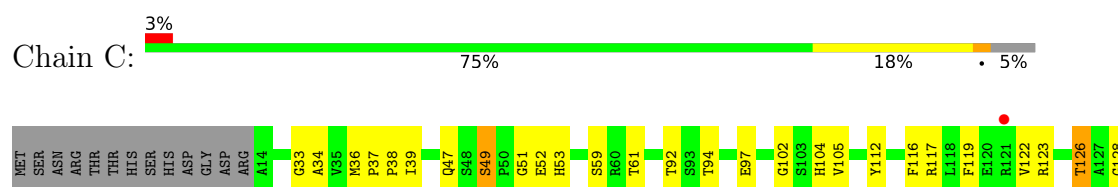
- Molecule 1: Cystathionine gamma-lyase-like protein

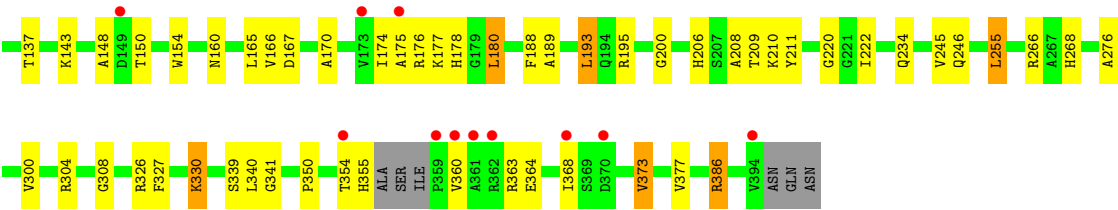


- Molecule 1: Cystathionine gamma-lyase-like protein

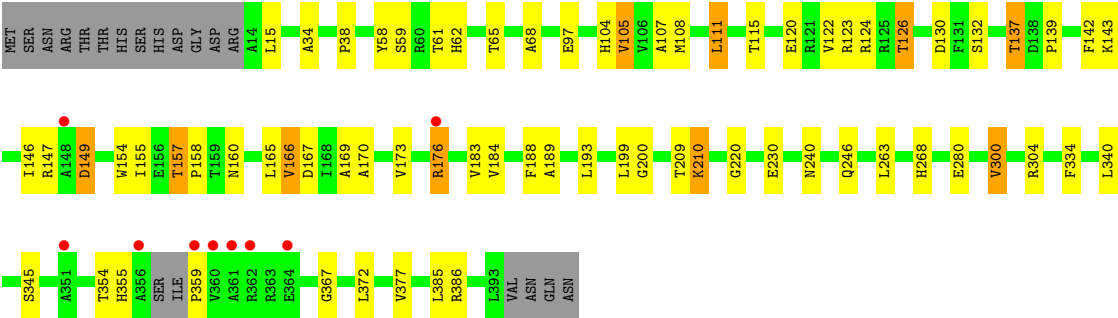
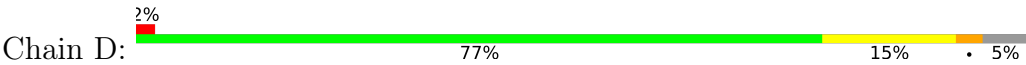


- Molecule 1: Cystathionine gamma-lyase-like protein





● Molecule 1: Cystathionine gamma-lyase-like protein



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	78.82Å 86.31Å 223.35Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	40.25 – 2.07 40.25 – 2.07	Depositor EDS
% Data completeness (in resolution range)	99.5 (40.25-2.07) 99.5 (40.25-2.07)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	9.00 (at 2.06Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.181 , 0.247 0.182 , 0.247	Depositor DCC
R_{free} test set	4705 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å ²)	21.4	Xtriage
Anisotropy	0.199	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 41.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	12425	wwPDB-VP
Average B, all atoms (Å ²)	23.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.89% 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: GOL, BCT, LLP, BME

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	1.41	7/2917 (0.2%)	1.24	14/3958 (0.4%)
1	B	1.41	13/2928 (0.4%)	1.24	12/3973 (0.3%)
1	C	1.30	10/2888 (0.3%)	1.23	13/3916 (0.3%)
1	D	1.35	10/2898 (0.3%)	1.22	6/3930 (0.2%)
All	All	1.37	40/11631 (0.3%)	1.23	45/15777 (0.3%)

All (40) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	209	THR	C-O	8.84	1.41	1.23
1	D	105	VAL	CA-CB	7.36	1.65	1.54
1	A	209	THR	C-O	6.50	1.36	1.23
1	B	343	VAL	CA-CB	6.48	1.64	1.54
1	D	300	VAL	CA-CB	6.44	1.63	1.54
1	C	104	HIS	CG-ND1	-6.16	1.31	1.38
1	A	76	LEU	C-O	-5.98	1.17	1.24
1	D	386	ARG	C-O	-5.91	1.17	1.24
1	C	368	ILE	CA-C	5.83	1.57	1.52
1	A	106	VAL	C-O	-5.83	1.17	1.24
1	D	68	ALA	CA-CB	5.83	1.62	1.53
1	C	208	ALA	N-CA	5.80	1.53	1.46
1	C	37	PRO	CA-C	5.76	1.57	1.52
1	A	377	VAL	N-CA	-5.68	1.39	1.46
1	C	61	THR	CA-CB	5.60	1.62	1.53
1	B	209	THR	C-O	5.59	1.34	1.23
1	B	44	THR	CA-CB	5.58	1.62	1.53
1	D	38	PRO	C-O	5.58	1.30	1.23
1	C	104	HIS	CD2-NE2	-5.56	1.31	1.37
1	C	94	THR	C-O	5.46	1.30	1.24
1	B	122	VAL	CA-CB	5.36	1.61	1.54
1	A	261	LEU	CA-C	5.34	1.58	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	156	GLU	CA-C	5.33	1.58	1.52
1	B	289	ILE	CA-CB	-5.31	1.47	1.53
1	B	228	ASN	CA-C	-5.28	1.47	1.53
1	C	166	VAL	C-O	5.28	1.29	1.24
1	C	276	ALA	N-CA	5.27	1.52	1.46
1	D	189	ALA	CA-CB	5.25	1.61	1.53
1	B	172	ALA	CA-CB	5.19	1.61	1.53
1	B	88	GLY	C-O	5.16	1.29	1.23
1	B	103	SER	CA-C	-5.14	1.46	1.53
1	A	215	HIS	N-CA	5.14	1.52	1.46
1	B	30	PRO	C-O	-5.12	1.17	1.24
1	D	157	THR	CA-CB	5.09	1.61	1.53
1	B	71	ARG	CA-C	-5.07	1.46	1.52
1	A	155	ILE	CA-CB	5.06	1.61	1.54
1	B	245	VAL	CA-C	-5.05	1.47	1.53
1	D	385	LEU	C-O	-5.05	1.18	1.24
1	D	34	ALA	N-CA	5.03	1.52	1.46
1	C	116	PHE	C-O	-5.02	1.18	1.24

All (45) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	368	ILE	N-CA-C	8.53	115.33	106.21
1	D	149	ASP	N-CA-C	7.93	120.83	111.71
1	B	67	PHE	N-CA-C	-7.12	103.60	111.36
1	A	176	ARG	NE-CZ-NH1	-7.06	114.44	121.50
1	D	137	THR	N-CA-C	-6.87	103.85	111.82
1	A	71	ARG	NE-CZ-NH2	-6.65	113.22	119.20
1	A	176	ARG	NE-CZ-NH2	6.54	125.08	119.20
1	A	275	LEU	N-CA-C	6.51	118.04	111.07
1	B	349	HIS	CA-C-N	6.43	126.19	119.05
1	B	349	HIS	C-N-CA	6.43	126.19	119.05
1	B	195[A]	ARG	CA-C-N	-6.28	113.22	119.56
1	B	195[A]	ARG	C-N-CA	-6.28	113.22	119.56
1	B	195[B]	ARG	CA-C-N	-6.28	113.22	119.56
1	B	195[B]	ARG	C-N-CA	-6.28	113.22	119.56
1	C	112	TYR	CA-C-N	6.00	126.64	119.98
1	C	112	TYR	C-N-CA	6.00	126.64	119.98
1	A	49	SER	CA-C-N	-5.92	113.60	119.93
1	A	49	SER	C-N-CA	-5.92	113.60	119.93
1	B	225	VAL	N-CA-C	5.88	117.47	108.71
1	B	65	THR	N-CA-C	-5.65	105.20	111.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	91	ALA	N-CA-C	-5.63	104.83	110.97
1	C	49	SER	CA-C-N	-5.58	113.81	119.83
1	C	49	SER	C-N-CA	-5.58	113.81	119.83
1	C	245	VAL	N-CA-C	5.57	116.12	110.05
1	D	263	LEU	N-CA-C	5.52	117.38	111.36
1	A	183	VAL	CA-C-N	-5.45	116.01	123.14
1	A	183	VAL	C-N-CA	-5.45	116.01	123.14
1	D	15	LEU	N-CA-C	5.38	118.08	110.50
1	A	363	ARG	NE-CZ-NH2	5.31	123.98	119.20
1	B	379	ILE	N-CA-C	5.30	116.63	111.91
1	C	148	ALA	CA-C-N	5.28	128.34	120.31
1	C	148	ALA	C-N-CA	5.28	128.34	120.31
1	A	125	ARG	N-CA-C	5.28	116.84	111.14
1	C	360	VAL	N-CA-C	5.22	117.57	111.05
1	B	149	ASP	N-CA-CB	-5.16	102.59	110.33
1	C	119	PHE	N-CA-C	-5.15	105.31	111.03
1	A	198	SER	N-CA-C	-5.12	107.04	113.28
1	C	105	VAL	N-CA-C	5.11	115.47	108.12
1	D	115	THR	N-CA-C	-5.10	105.80	111.36
1	D	65	THR	N-CA-C	-5.05	105.48	111.69
1	A	85	PHE	CA-C-N	5.04	127.54	120.28
1	A	85	PHE	C-N-CA	5.04	127.54	120.28
1	C	59	SER	N-CA-C	5.03	118.67	112.54
1	A	255	LEU	N-CA-C	-5.02	105.89	111.36
1	C	330	LYS	N-CA-C	5.02	119.67	113.50

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	2881	0	2881	40	0
1	B	2889	0	2893	62	0
1	C	2855	0	2848	58	0
1	D	2860	0	2851	46	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	A	4	0	0	2	0
3	A	4	0	5	3	0
3	B	4	0	5	2	0
3	C	4	0	5	2	0
4	D	6	0	8	0	0
5	A	239	0	0	9	0
5	B	238	0	0	8	0
5	C	211	0	0	10	0
5	D	230	0	0	5	0
All	All	12425	0	11496	200	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 9.

All (200) 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:B:98:LEU:HD11	1:B:235:MET:CE	1.78	1.14
1:B:98:LEU:HD11	1:B:235:MET:HE2	1.06	1.04
1:C:150:THR:HG22	1:C:180:LEU:CD1	1.89	1.03
1:B:98:LEU:CD1	1:B:235:MET:HE2	1.90	1.01
1:C:126:THR:HG21	1:D:97:GLU:OE1	1.62	1.00
1:C:180:LEU:CD2	1:C:180:LEU:N	2.29	0.95
1:D:160:ASN:HB3	5:D:682:HOH:O	1.66	0.95
1:C:97:GLU:OE1	1:D:126:THR:HG21	1.69	0.92
1:C:180:LEU:HD23	1:C:180:LEU:H	1.35	0.91
1:D:220:GLY:HA3	1:D:246:GLN:HE22	1.40	0.83
1:B:220:GLY:HA3	1:B:246:GLN:HE22	1.44	0.82
2:A:401:BCT:O2	5:A:680:HOH:O	1.99	0.81
1:C:300:VAL:HG12	5:C:635:HOH:O	1.81	0.80
1:B:158:PRO:HG2	1:B:188:PHE:CE2	2.17	0.80
1:A:266:ARG:HA	3:A:402:BME:H12	1.64	0.78
1:C:180:LEU:N	1:C:180:LEU:HD22	1.99	0.78
1:C:150:THR:HG22	1:C:180:LEU:HD11	1.64	0.77
1:B:266:ARG:HA	3:B:401:BME:H11	1.67	0.77
1:C:220:GLY:HA3	1:C:246:GLN:HE22	1.49	0.77
1:D:142:PHE:O	1:D:146:ILE:HD12	1.86	0.76
1:D:210:LLP:HD3	1:D:340:LEU:HG	1.69	0.74
1:D:280:GLU:OE2	5:D:651:HOH:O	2.06	0.73
1:B:124:ARG:NH2	1:B:130:ASP:OD1	2.21	0.73
1:D:124:ARG:NH2	1:D:130:ASP:OD1	2.23	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:98:LEU:CD1	1:B:235:MET:CE	2.59	0.72
1:A:112:TYR:HE1	2:A:401:BCT:O2	1.72	0.71
1:B:36:MET:CE	5:C:659:HOH:O	2.37	0.71
1:C:304:ARG:NH1	5:C:674:HOH:O	2.22	0.71
1:A:249:PHE:HD1	5:A:737:HOH:O	1.72	0.71
1:B:130:ASP:OD2	1:B:147:ARG:NH2	2.24	0.70
1:A:168:ILE:H	1:A:305:GLN:HE22	1.38	0.70
1:D:268:HIS:HD2	1:D:377:VAL:O	1.74	0.70
1:C:150:THR:HG22	1:C:180:LEU:HD12	1.71	0.69
1:C:167:ASP:OD2	1:C:304:ARG:NH2	2.27	0.68
1:D:160:ASN:HB2	1:D:188:PHE:CZ	2.29	0.68
1:A:268:HIS:HE1	5:A:647:HOH:O	1.76	0.68
1:A:349:HIS:HD2	1:A:352:VAL:H	1.40	0.67
1:B:203:LEU:CD2	1:B:235:MET:HE3	2.24	0.67
5:B:708:HOH:O	1:C:36:MET:SD	2.51	0.67
1:A:326:ARG:HH11	1:A:326:ARG:HG3	1.59	0.66
1:C:350:PRO:HB3	1:C:354:THR:OG1	1.96	0.66
1:D:137:THR:O	1:D:139:PRO:HD3	1.95	0.66
1:A:327:PHE:HE2	1:A:373:VAL:HG21	1.61	0.66
1:B:160:ASN:CG	5:B:668:HOH:O	2.38	0.65
1:B:203:LEU:HD22	1:B:235:MET:HE3	1.78	0.65
1:D:268:HIS:CD2	1:D:377:VAL:O	2.51	0.63
1:B:354:THR:OG1	1:B:355:HIS:HD2	1.82	0.63
1:C:176:ARG:NH1	1:C:200:GLY:O	2.27	0.62
1:C:364:GLU:HA	1:C:364:GLU:OE2	1.97	0.62
1:D:354:THR:OG1	1:D:355:HIS:HD2	1.82	0.62
1:D:367:GLY:O	5:D:683:HOH:O	2.16	0.62
1:A:71:ARG:NH2	5:A:580:HOH:O	2.25	0.62
1:C:355:HIS:CB	1:C:363:ARG:HD3	2.29	0.62
1:C:150:THR:CG2	1:C:180:LEU:HD11	2.28	0.61
1:A:193:LEU:HD21	3:A:402:BME:S2	2.39	0.61
1:B:36:MET:HE3	5:C:659:HOH:O	1.99	0.61
1:B:158:PRO:HG2	1:B:188:PHE:CD2	2.35	0.61
1:A:327:PHE:CE2	1:A:373:VAL:HG21	2.35	0.61
1:A:220:GLY:HA3	1:A:246:GLN:HE22	1.66	0.60
1:B:358:ILE:HD12	1:B:358:ILE:N	2.16	0.60
1:C:180:LEU:N	1:C:180:LEU:HD23	1.98	0.59
1:A:268:HIS:HD2	1:A:377:VAL:O	1.84	0.59
1:C:189:ALA:O	1:C:193:LEU:HG	2.04	0.58
1:C:234:GLN:HG2	5:C:681:HOH:O	2.04	0.58
1:C:268:HIS:HD2	1:C:377:VAL:O	1.89	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:326:ARG:HG3	1:A:326:ARG:NH1	2.21	0.56
1:A:354:THR:OG1	1:A:355:HIS:HD2	1.89	0.56
1:B:47:GLN:NE2	1:B:51:GLY:H	2.03	0.56
1:D:122:VAL:O	1:D:126:THR:HB	2.06	0.55
1:A:321:PHE:HB2	1:A:370:ASP:HB3	1.88	0.55
1:C:350:PRO:O	1:C:355:HIS:N	2.37	0.55
1:B:95:VAL:HA	1:B:235:MET:HE1	1.88	0.55
1:B:137:THR:HG22	1:B:165:LEU:O	2.07	0.55
1:C:350:PRO:HA	1:C:354:THR:OG1	2.08	0.54
1:B:360:VAL:HG23	1:B:363:ARG:NH1	2.24	0.53
1:B:47:GLN:HE22	1:B:51:GLY:H	1.57	0.53
1:B:59:SER:HA	1:B:62:HIS:O	2.08	0.53
1:C:268:HIS:HE1	5:C:538:HOH:O	1.91	0.53
1:B:147:ARG:C	1:B:149:ASP:H	2.15	0.53
1:B:386:ARG:O	1:B:390:GLU:HG3	2.09	0.53
1:A:168:ILE:H	1:A:305:GLN:NE2	2.05	0.52
1:B:188:PHE:CD2	1:B:188:PHE:C	2.88	0.52
1:C:150:THR:CG2	1:C:180:LEU:CD1	2.76	0.52
1:D:104:HIS:HB3	1:D:149:ASP:HB3	1.91	0.52
1:D:123:ARG:HD3	1:D:126:THR:HG22	1.92	0.52
1:B:268:HIS:HD2	1:B:377:VAL:O	1.92	0.52
1:D:137:THR:HG22	1:D:165:LEU:O	2.10	0.52
1:A:14:ALA:N	5:A:543:HOH:O	2.43	0.51
1:B:120:GLU:OE1	1:B:124:ARG:HD2	2.11	0.51
1:B:98:LEU:CG	1:B:235:MET:HE2	2.40	0.51
1:B:350:PRO:HD2	5:B:578:HOH:O	2.11	0.50
1:D:167:ASP:OD2	1:D:304:ARG:NH2	2.43	0.50
1:A:116:PHE:CZ	1:A:120:GLU:HG3	2.47	0.50
1:B:358:ILE:N	1:B:358:ILE:CD1	2.75	0.50
1:B:372:LEU:C	1:B:372:LEU:HD23	2.37	0.50
1:C:47:GLN:HE22	1:C:51:GLY:H	1.60	0.49
1:C:126:THR:CG2	1:D:97:GLU:OE1	2.47	0.49
1:B:220:GLY:HA3	1:B:246:GLN:NE2	2.22	0.49
1:D:120:GLU:HA	1:D:124:ARG:HG3	1.95	0.49
1:D:372:LEU:C	1:D:372:LEU:HD23	2.38	0.49
1:D:268:HIS:HE1	5:D:563:HOH:O	1.95	0.48
1:B:147:ARG:NH1	1:B:149:ASP:OD2	2.46	0.48
1:A:358:ILE:O	1:A:363:ARG:NH2	2.46	0.48
1:C:122:VAL:O	1:C:126:THR:HB	2.14	0.48
1:B:246:GLN:NE2	5:B:551:HOH:O	2.47	0.48
1:A:249:PHE:CD1	5:A:737:HOH:O	2.53	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:170:ALA:O	1:C:174:ILE:HD12	2.14	0.47
1:C:350:PRO:CA	1:C:354:THR:OG1	2.62	0.47
1:D:170:ALA:O	1:D:173:VAL:HG22	2.14	0.47
1:B:360:VAL:O	1:B:364:GLU:HG2	2.13	0.47
1:B:364:GLU:HA	1:B:364:GLU:OE1	2.14	0.47
1:C:350:PRO:CB	1:C:354:THR:OG1	2.62	0.47
1:D:154:TRP:CZ3	1:D:183:VAL:HG11	2.49	0.47
1:A:92:THR:O	1:A:96:MET:HG2	2.15	0.47
1:B:189:ALA:HB1	1:B:193:LEU:HB2	1.96	0.47
1:B:279:LEU:HD13	1:B:315:ILE:HG21	1.96	0.47
1:C:255:LEU:C	1:C:255:LEU:HD13	2.40	0.47
1:B:137:THR:O	1:B:139:PRO:HD3	2.15	0.46
1:C:33:GLY:O	1:C:34:ALA:C	2.58	0.46
1:A:300:VAL:HG22	5:A:662:HOH:O	2.15	0.46
1:B:16[B]:SER:OG	5:B:634:HOH:O	2.01	0.46
1:D:130:ASP:OD2	1:D:147:ARG:NH2	2.46	0.46
1:A:49:SER:O	1:A:50:PRO:C	2.58	0.46
1:A:164:LYS:HD2	5:A:507:HOH:O	2.14	0.46
1:C:143:LYS:HG3	1:C:174:ILE:HG21	1.99	0.45
1:D:230:GLU:HB3	5:D:594:HOH:O	2.14	0.45
1:C:49:SER:HB3	1:C:52:GLU:HG3	1.99	0.45
1:A:300:VAL:HG23	5:A:643:HOH:O	2.16	0.45
1:B:278:TRP:CZ2	1:B:390:GLU:HG2	2.51	0.45
1:A:59:SER:HA	1:A:62:HIS:O	2.17	0.45
1:B:92:THR:HG23	1:B:154:TRP:CH2	2.52	0.45
1:B:211:TYR:CE1	1:B:341:GLY:HA2	2.52	0.45
1:C:47:GLN:NE2	1:C:51:GLY:H	2.15	0.45
1:C:92:THR:HG23	1:C:154:TRP:CH2	2.52	0.45
1:D:108:MET:O	1:D:111:LEU:HD22	2.17	0.45
1:B:308:GLY:HA3	3:B:401:BME:S2	2.57	0.45
1:C:97:GLU:OE1	1:D:126:THR:CG2	2.52	0.45
1:C:102:GLY:HA2	1:C:128:GLY:O	2.17	0.45
1:D:59:SER:HA	1:D:62:HIS:O	2.17	0.45
1:D:176:ARG:NH1	1:D:200:GLY:O	2.39	0.45
1:B:110:ASP:OD2	1:B:164:LYS:HE3	2.18	0.44
1:D:169:ALA:HA	1:D:199:LEU:O	2.16	0.44
1:B:110:ASP:OD1	1:B:110:ASP:C	2.60	0.44
1:D:355:HIS:O	1:D:359:PRO:HD2	2.17	0.44
1:C:266:ARG:HA	3:C:401:BME:H12	2.00	0.44
1:A:176:ARG:NH1	1:A:200:GLY:O	2.36	0.44
1:A:111:LEU:O	1:A:355:HIS:HE1	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:73:VAL:HG11	1:A:222:ILE:HG21	2.00	0.44
1:A:326:ARG:HH11	1:A:326:ARG:CG	2.28	0.44
1:B:203:LEU:HD21	1:B:235:MET:HE3	1.97	0.44
1:C:330:LYS:HB3	1:C:330:LYS:HE2	1.76	0.44
1:D:334:PHE:CD2	1:D:345:SER:HB3	2.53	0.44
5:C:513:HOH:O	1:D:126:THR:HG23	2.17	0.44
1:A:176:ARG:HE	1:A:176:ARG:HB2	1.31	0.43
1:C:175:ALA:HB1	1:C:180:LEU:HB2	2.00	0.43
1:C:178:HIS:C	1:C:180:LEU:HD23	2.43	0.43
1:D:111:LEU:HA	1:D:111:LEU:HD12	1.39	0.43
1:B:83:PHE:HE2	1:B:225:VAL:HG13	1.84	0.43
1:D:107:ALA:O	1:D:108:MET:C	2.62	0.43
1:C:209:THR:HG21	1:D:58:TYR:OH	2.18	0.43
1:A:39:ILE:HB	1:C:39:ILE:HB	2.00	0.43
1:D:120:GLU:OE1	1:D:124:ARG:NH1	2.45	0.43
1:A:334:PHE:CD2	1:A:345:SER:HB3	2.54	0.43
1:A:193:LEU:CD2	3:A:402:BME:S2	3.06	0.43
1:C:137:THR:HG22	1:C:165:LEU:O	2.19	0.42
1:D:143:LYS:HE3	1:D:143:LYS:HB3	1.84	0.42
1:B:268:HIS:HE1	5:B:555:HOH:O	2.01	0.42
1:C:123:ARG:HD3	1:C:126:THR:HG22	2.01	0.42
1:D:61:THR:OG1	1:D:240:ASN:ND2	2.52	0.42
1:B:147:ARG:C	1:B:149:ASP:N	2.78	0.42
1:A:278:TRP:CD1	1:A:386:ARG:NH1	2.88	0.42
1:C:211:TYR:CE1	1:C:341:GLY:HA2	2.55	0.42
1:C:308:GLY:HA3	3:C:401:BME:S2	2.59	0.42
1:C:326:ARG:NH2	5:C:633:HOH:O	2.52	0.42
1:C:47:GLN:HG2	1:C:53:HIS:HB3	2.02	0.42
1:C:160:ASN:HB2	1:C:188:PHE:CZ	2.54	0.42
1:B:36:MET:HE1	1:B:259:LYS:HE2	2.02	0.41
1:C:246:GLN:NE2	5:C:557:HOH:O	2.53	0.41
1:A:40:TYR:CE2	1:C:38:PRO:HG3	2.55	0.41
1:B:210:LLP:O3	1:B:210:LLP:NZ	2.53	0.41
1:B:372:LEU:HD23	1:B:373:VAL:N	2.36	0.41
1:C:327:PHE:CE2	1:C:373:VAL:HG21	2.55	0.41
1:B:157:THR:HA	1:B:158:PRO:C	2.45	0.41
1:D:155:ILE:HB	1:D:184:VAL:HG22	2.03	0.41
1:A:102:GLY:HA2	1:A:128:GLY:O	2.21	0.41
1:B:256:ARG:HA	5:B:542:HOH:O	2.20	0.41
1:A:154:TRP:CZ3	1:A:183:VAL:HG11	2.56	0.41
1:B:304:ARG:NE	5:B:694:HOH:O	2.09	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:157:THR:HA	1:D:158:PRO:C	2.45	0.41
1:B:77:GLU:OE2	1:B:206:HIS:NE2	2.46	0.41
1:A:106:VAL:HG22	1:A:153:VAL:HG23	2.02	0.41
1:D:157:THR:HB	1:D:166:VAL:HG13	2.02	0.41
1:C:386:ARG:NE	5:C:673:HOH:O	2.54	0.40
1:B:189:ALA:O	1:B:190:SER:CB	2.68	0.40
1:B:163:LEU:HD22	1:B:188:PHE:CZ	2.56	0.40
1:B:362:ARG:HE	1:B:366:LEU:HD11	1.86	0.40
1:C:206:HIS:HB2	1:C:222:ILE:HB	2.03	0.40
1:D:120:GLU:OE1	1:D:124:ARG:HD2	2.21	0.40
1:B:393:LEU:O	1:B:394:VAL:C	2.62	0.40
1:D:104:HIS:NE2	1:D:132:SER:OG	2.47	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	379/397 (96%)	369 (97%)	10 (3%)	0	100	100
1	B	380/397 (96%)	372 (98%)	7 (2%)	1 (0%)	36	30
1	C	374/397 (94%)	361 (96%)	12 (3%)	1 (0%)	36	30
1	D	375/397 (94%)	361 (96%)	14 (4%)	0	100	100
All	All	1508/1588 (95%)	1463 (97%)	43 (3%)	2 (0%)	48	44

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	339	SER
1	B	339	SER

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	298/312 (96%)	284 (95%)	14 (5%)	23	16
1	B	299/312 (96%)	284 (95%)	15 (5%)	22	14
1	C	294/312 (94%)	284 (97%)	10 (3%)	32	27
1	D	294/312 (94%)	287 (98%)	7 (2%)	43	40
All	All	1185/1248 (95%)	1139 (96%)	46 (4%)	29	23

All (46) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	16[A]	SER
1	A	16[B]	SER
1	A	106	VAL
1	A	166	VAL
1	A	176	ARG
1	A	177	LYS
1	A	195	ARG
1	A	234	GLN
1	A	325	LYS
1	A	326	ARG
1	A	340	LEU
1	A	364	GLU
1	A	373	VAL
1	A	386	ARG
1	B	59	SER
1	B	111	LEU
1	B	132	SER
1	B	166	VAL
1	B	176	ARG
1	B	177	LYS
1	B	188	PHE
1	B	193	LEU
1	B	225	VAL
1	B	234	GLN

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Mol	Chain	Res	Type
1	B	255	LEU
1	B	326	ARG
1	B	344	GLU
1	B	358	ILE
1	B	369	SER
1	C	117	ARG
1	C	126	THR
1	C	177	LYS
1	C	180	LEU
1	C	193	LEU
1	C	195	ARG
1	C	255	LEU
1	C	340	LEU
1	C	373	VAL
1	C	386	ARG
1	D	105	VAL
1	D	111	LEU
1	D	126	THR
1	D	166	VAL
1	D	176	ARG
1	D	193	LEU
1	D	300	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (30) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	47	GLN
1	A	54	GLN
1	A	178	HIS
1	A	194	GLN
1	A	234	GLN
1	A	246	GLN
1	A	268	HIS
1	A	271	ASN
1	A	305	GLN
1	A	349	HIS
1	A	355	HIS
1	B	47	GLN
1	B	246	GLN
1	B	268	HIS
1	B	271	ASN
1	B	355	HIS

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Mol	Chain	Res	Type
1	C	47	GLN
1	C	234	GLN
1	C	246	GLN
1	C	268	HIS
1	C	271	ASN
1	D	47	GLN
1	D	178	HIS
1	D	194	GLN
1	D	240	ASN
1	D	246	GLN
1	D	268	HIS
1	D	271	ASN
1	D	348	ASN
1	D	355	HIS

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

4 non-standard protein/DNA/RNA residues 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	$\# Z > 2$
1	LLP	D	210	1	23,24,25	2.46	6 (26%)	25,32,34	2.00	8 (32%)
1	LLP	A	210	1	23,24,25	2.87	7 (30%)	25,32,34	2.14	9 (36%)
1	LLP	C	210	1	23,24,25	2.34	9 (39%)	25,32,34	1.91	6 (24%)
1	LLP	B	210	1	23,24,25	2.73	8 (34%)	25,32,34	1.74	8 (32%)

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
1	LLP	D	210	1	-	5/16/17/19	0/1/1/1
1	LLP	A	210	1	-	4/16/17/19	0/1/1/1
1	LLP	C	210	1	-	4/16/17/19	0/1/1/1
1	LLP	B	210	1	-	3/16/17/19	0/1/1/1

All (30) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	210	LLP	C3-C2	8.20	1.49	1.41
1	D	210	LLP	C3-C2	7.06	1.48	1.41
1	B	210	LLP	C3-C2	7.04	1.48	1.41
1	C	210	LLP	C3-C2	5.29	1.46	1.41
1	A	210	LLP	C4-C5	4.95	1.48	1.42
1	D	210	LLP	C4-C5	4.93	1.48	1.42
1	B	210	LLP	C4-C3	4.92	1.49	1.41
1	B	210	LLP	C4-C5	4.85	1.48	1.42
1	A	210	LLP	CB-CA	4.76	1.60	1.53
1	C	210	LLP	P-OP2	-4.54	1.37	1.54
1	B	210	LLP	P-OP2	-4.50	1.38	1.54
1	C	210	LLP	C4-C5	4.46	1.48	1.42
1	A	210	LLP	C4-C3	4.42	1.48	1.41
1	A	210	LLP	P-OP3	-4.17	1.39	1.54
1	D	210	LLP	P-OP1	-3.51	1.39	1.50
1	B	210	LLP	P-OP3	-3.51	1.41	1.54
1	C	210	LLP	C4-C3	3.45	1.46	1.41
1	D	210	LLP	P-OP2	-3.34	1.42	1.54
1	A	210	LLP	P-OP2	-3.27	1.42	1.54
1	D	210	LLP	P-OP3	-3.24	1.42	1.54
1	D	210	LLP	C4-C3	3.01	1.46	1.41
1	B	210	LLP	P-OP4	-2.80	1.51	1.60
1	B	210	LLP	CB-CA	2.65	1.57	1.53
1	C	210	LLP	P-OP1	-2.56	1.42	1.50
1	C	210	LLP	P-OP4	-2.44	1.52	1.60
1	C	210	LLP	P-OP3	-2.41	1.45	1.54
1	C	210	LLP	CB-CA	-2.24	1.50	1.53
1	A	210	LLP	P-OP1	-2.16	1.43	1.50
1	B	210	LLP	CD-CE	2.09	1.58	1.51
1	C	210	LLP	OP4-C5'	-2.09	1.37	1.44

All (31) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	210	LLP	OP4-C5'-C5	5.31	119.30	109.36
1	A	210	LLP	OP4-C5'-C5	5.09	118.90	109.36
1	D	210	LLP	C2'-C2-C3	-4.11	115.98	120.80
1	D	210	LLP	C2'-C2-N1	3.94	125.07	117.64
1	A	210	LLP	C2'-C2-C3	-3.78	116.38	120.80
1	C	210	LLP	CE-NZ-C4'	3.67	130.47	118.72
1	A	210	LLP	C3-C4-C5	-3.67	115.33	118.28
1	A	210	LLP	C2'-C2-N1	3.57	124.36	117.64
1	D	210	LLP	C3-C4-C5	-3.57	115.41	118.28
1	B	210	LLP	CD-CG-CB	3.56	127.04	113.62
1	B	210	LLP	C6-N1-C2	3.27	125.13	119.20
1	D	210	LLP	OP2-P-OP4	-2.93	99.03	106.67
1	D	210	LLP	CE-NZ-C4'	2.87	127.90	118.72
1	C	210	LLP	OP3-P-OP4	-2.84	99.26	106.67
1	A	210	LLP	CE-NZ-C4'	2.77	127.59	118.72
1	C	210	LLP	C6-N1-C2	2.70	124.09	119.20
1	B	210	LLP	CE-NZ-C4'	2.66	127.23	118.72
1	B	210	LLP	C3-C2-N1	-2.66	117.61	120.96
1	A	210	LLP	CG-CD-CE	2.64	122.56	113.38
1	D	210	LLP	C5'-C5-C6	-2.57	115.17	119.36
1	B	210	LLP	OP4-C5'-C5	2.55	114.13	109.36
1	D	210	LLP	C5-C4-C4'	2.54	125.40	121.47
1	A	210	LLP	C5-C4-C4'	2.29	125.00	121.47
1	B	210	LLP	C4-C4'-NZ	-2.25	113.64	124.04
1	C	210	LLP	C3-C2-N1	-2.19	118.20	120.96
1	D	210	LLP	OP2-P-OP1	2.17	119.30	110.83
1	A	210	LLP	O3-C3-C2	2.13	122.00	117.58
1	B	210	LLP	C2'-C2-N1	2.11	121.62	117.64
1	A	210	LLP	CD-CE-NZ	-2.03	105.46	110.83
1	C	210	LLP	C5-C4-C4'	2.03	124.60	121.47
1	B	210	LLP	C3-C4-C5	-2.02	116.66	118.28

There are no chirality outliers.

All (16) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	A	210	LLP	O-C-CA-CB
1	B	210	LLP	O-C-CA-CB
1	C	210	LLP	O-C-CA-CB
1	D	210	LLP	O-C-CA-CB
1	A	210	LLP	CG-CD-CE-NZ
1	C	210	LLP	CA-CB-CG-CD
1	D	210	LLP	CG-CD-CE-NZ

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Mol	Chain	Res	Type	Atoms
1	B	210	LLP	CA-CB-CG-CD
1	C	210	LLP	C-CA-CB-CG
1	A	210	LLP	C3-C4-C4'-NZ
1	C	210	LLP	C3-C4-C4'-NZ
1	D	210	LLP	CD-CE-NZ-C4'
1	D	210	LLP	C3-C4-C4'-NZ
1	B	210	LLP	C-CA-CB-CG
1	A	210	LLP	N-CA-CB-CG
1	D	210	LLP	N-CA-CB-CG

There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	D	210	LLP	1	0
1	B	210	LLP	1	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

5 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	$\# Z > 2$
3	BME	B	401	1	3,3,3	0.12	0	2,2,2	1.88	1 (50%)
2	BCT	A	401	-	3,3,3	1.03	0	2,3,3	2.40	2 (100%)
3	BME	A	402	1	3,3,3	0.24	0	2,2,2	0.61	0
3	BME	C	401	1	3,3,3	0.24	0	2,2,2	1.41	0
4	GOL	D	401	-	5,5,5	0.38	0	5,5,5	0.52	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	BME	B	401	1	-	1/1/1/1	-
4	GOL	D	401	-	-	0/4/4/4	-
3	BME	A	402	1	-	0/1/1/1	-
3	BME	C	401	1	-	0/1/1/1	-

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	401	BCT	O3-C-O1	2.58	126.27	119.68
2	A	401	BCT	O2-C-O1	-2.22	114.00	119.68
3	B	401	BME	O1-C1-C2	-2.01	102.98	110.82

There are no chirality outliers.

All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	B	401	BME	O1-C1-C2-S2

There are no ring outliers.

4 monomers are involved in 9 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	401	BME	2	0
2	A	401	BCT	2	0
3	A	402	BME	3	0
3	C	401	BME	2	0

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	380/397 (95%)	-0.09	2 (0%)	87 89	10, 19, 33, 44	1 (0%)
1	B	380/397 (95%)	-0.19	3 (0%)	82 84	9, 19, 35, 47	2 (0%)
1	C	377/397 (94%)	0.03	12 (3%)	50 50	10, 22, 43, 61	1 (0%)
1	D	377/397 (94%)	0.07	9 (2%)	59 61	10, 23, 44, 62	2 (0%)
All	All	1514/1588 (95%)	-0.05	26 (1%)	69 71	9, 20, 40, 62	6 (0%)

All (26) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	351	ALA	4.0
1	D	360	VAL	3.9
1	C	361	ALA	3.8
1	C	359	PRO	3.8
1	C	360	VAL	3.6
1	D	359	PRO	3.3
1	D	361	ALA	3.2
1	D	356	ALA	3.2
1	C	362	ARG	2.9
1	C	370	ASP	2.7
1	D	362	ARG	2.6
1	C	173	VAL	2.5
1	C	354	THR	2.5
1	A	321	PHE	2.5
1	A	394	VAL	2.5
1	B	149	ASP	2.4
1	C	368	ILE	2.3
1	C	121	ARG	2.2
1	C	394	VAL	2.2
1	B	321	PHE	2.2
1	D	148	ALA	2.2

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Mol	Chain	Res	Type	RSRZ
1	B	227	ASP	2.2
1	D	176	ARG	2.1
1	D	364	GLU	2.1
1	C	149	ASP	2.1
1	C	175	ALA	2.1

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

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
1	LLP	C	210	24/25	0.93	0.10	13,19,27,29	0
1	LLP	D	210	24/25	0.94	0.09	14,19,23,26	0
1	LLP	A	210	24/25	0.95	0.08	10,17,22,26	0
1	LLP	B	210	24/25	0.95	0.09	11,16,21,22	0

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(Å ²)	Q<0.9
3	BME	B	401	4/4	0.85	0.15	43,47,47,48	0
3	BME	A	402	4/4	0.91	0.13	49,53,53,53	0
3	BME	C	401	4/4	0.92	0.14	43,43,46,47	0
2	BCT	A	401	4/4	0.93	0.10	18,22,24,30	0
4	GOL	D	401	6/6	0.95	0.07	18,22,24,27	0

6.5 Other polymers [i](#)

There are no such residues in this entry.