



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 05:37 PM GMT

PDB ID : 4IXZ
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
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467
Mogul : 1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix) : 1.9-1692
EDS : rb-20026688
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac : 5.8.0135
CCP4 : 6.5.0
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : trunk26865

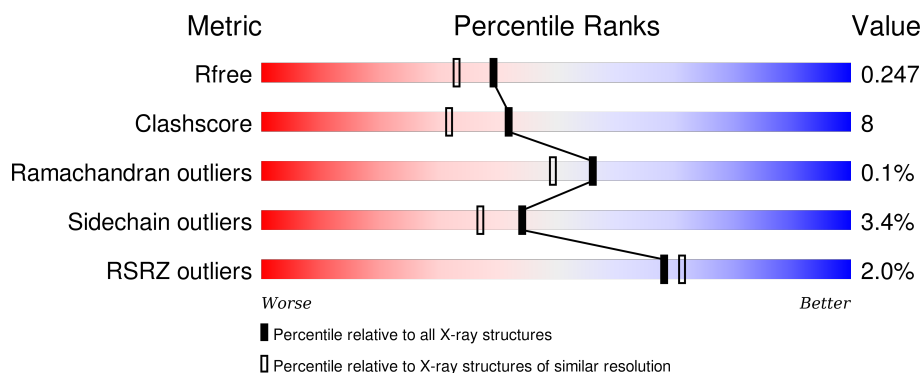
1 Overall quality at a glance

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}	91344	1799 (2.08-2.04)
Clashscore	102246	1910 (2.08-2.04)
Ramachandran outliers	100387	1893 (2.08-2.04)
Sidechain outliers	100360	1893 (2.08-2.04)
RSRZ outliers	91569	1802 (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 on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. 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	<div> <div>80%</div> <div>14%</div> <div>• •</div> </div>
1	B	397	<div> <div>77%</div> <div>17%</div> <div>• •</div> </div>
1	C	397	<div> <div>3%</div> <div>78%</div> <div>15%</div> <div>• 5%</div> </div>
1	D	397	<div> <div>4%</div> <div>79%</div> <div>14%</div> <div>• 5%</div> </div>

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	-
3	BME	B	401	-	-	-	X

2 Entry composition [i](#)

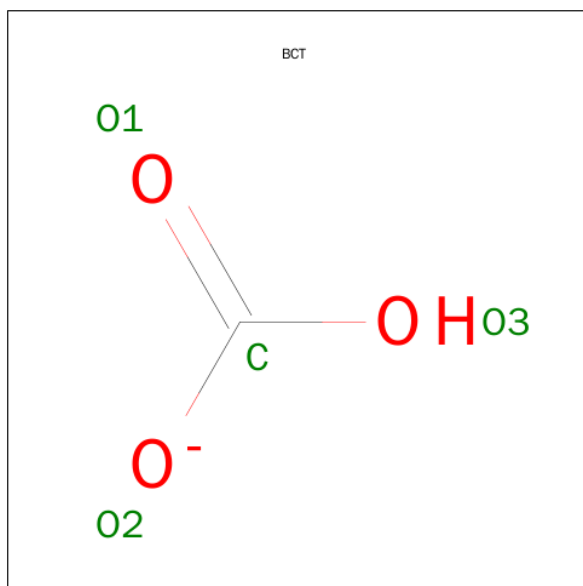
There are 5 unique types of molecules in this entry. The entry contains 12425 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 (three-letter code: 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 (three-letter code: 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 (three-letter code: GOL) (formula: $C_3H_8O_3$).



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

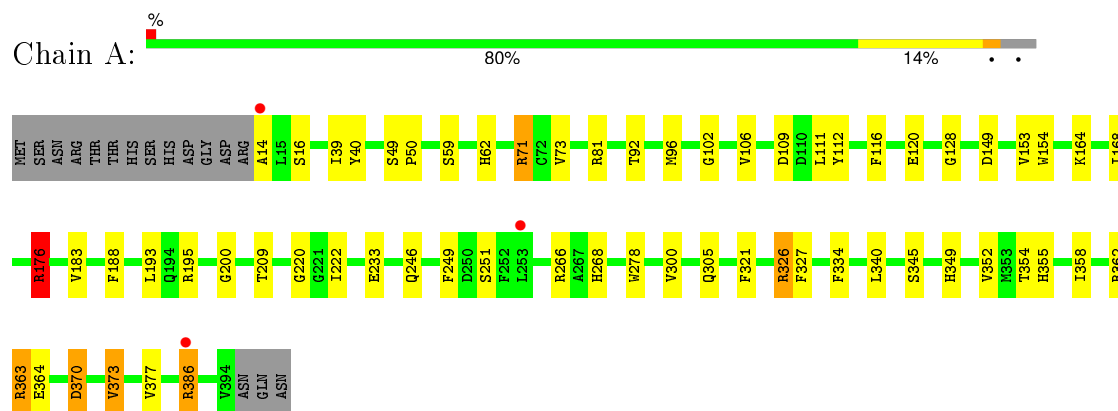
- Molecule 5 is water.

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

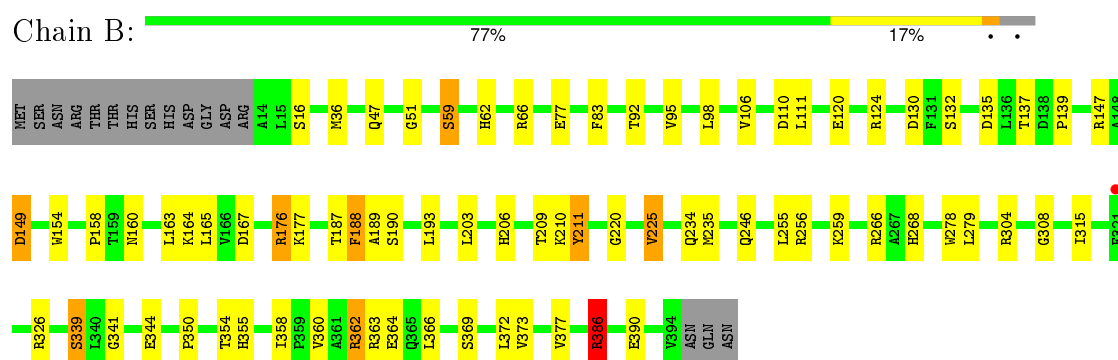
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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.

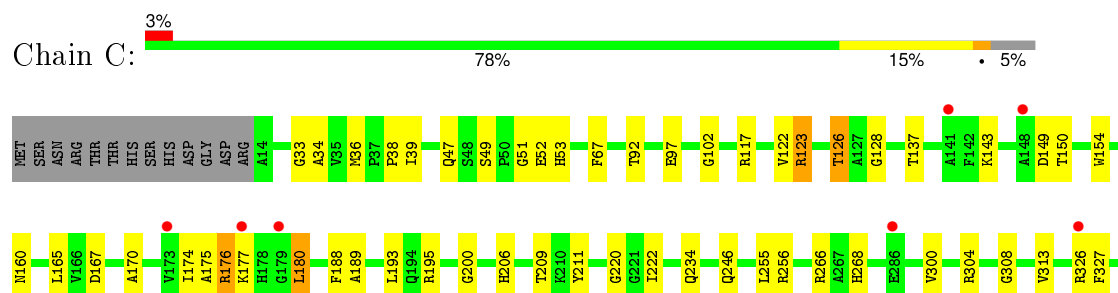
- Molecule 1: Cystathionine gamma-lyase-like protein

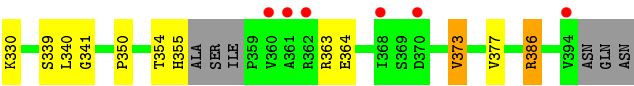


- Molecule 1: Cystathionine gamma-lyase-like protein

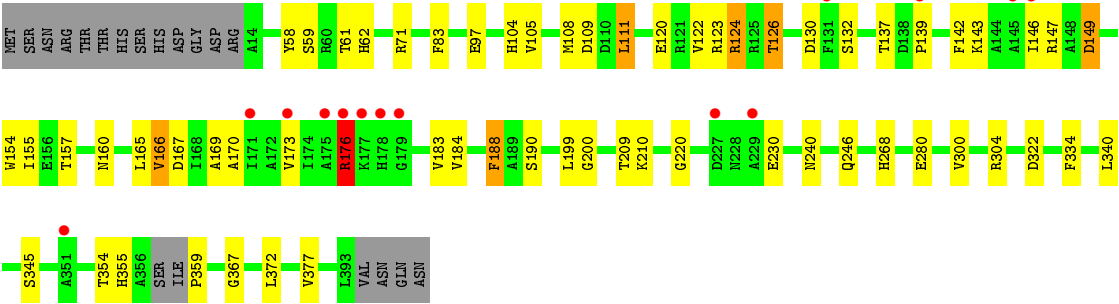
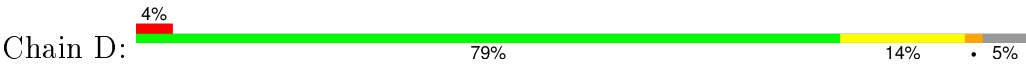


- Molecule 1: Cystathionine gamma-lyase-like protein





● 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	4700 reflections (5.31%)	DCC
Wilson B-factor (Å ²)	21.4	Xtriage
Anisotropy	0.199	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 49.8	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Outliers	0 of 93396 reflections	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, 0.375 respectively for untwinned datasets, and 0.333, 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: BCT, GOL, IT1, 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	1.13	4/2917 (0.1%)	1.06	10/3958 (0.3%)
1	B	1.14	3/2928 (0.1%)	1.00	9/3973 (0.2%)
1	C	1.03	2/2888 (0.1%)	0.96	4/3916 (0.1%)
1	D	1.11	4/2898 (0.1%)	0.95	5/3930 (0.1%)
All	All	1.11	13/11631 (0.1%)	0.99	28/15777 (0.2%)

All (13) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	209	THR	C-O	9.41	1.41	1.23
1	A	209	THR	C-O	6.94	1.36	1.23
1	B	211	TYR	CE1-CZ	6.11	1.46	1.38
1	B	209	THR	C-O	6.00	1.34	1.23
1	A	251	SER	CB-OG	5.96	1.50	1.42
1	C	67	PHE	CE2-CZ	5.38	1.47	1.37
1	D	188	PHE	CG-CD1	5.33	1.46	1.38
1	C	313	VAL	CB-CG1	5.29	1.64	1.52
1	A	188	PHE	CE1-CZ	5.19	1.47	1.37
1	A	233	GLU	CG-CD	5.05	1.59	1.51
1	D	83	PHE	CE1-CZ	5.04	1.47	1.37
1	D	105	VAL	CA-CB	5.02	1.65	1.54
1	B	106	VAL	CB-CG2	5.01	1.63	1.52

All (28) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	71	ARG	NE-CZ-NH2	-14.17	113.22	120.30
1	A	176	ARG	NE-CZ-NH1	-11.72	114.44	120.30
1	A	71	ARG	NE-CZ-NH1	11.58	126.09	120.30
1	A	176	ARG	NE-CZ-NH2	9.57	125.08	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	149	ASP	CB-CG-OD1	-9.55	109.71	118.30
1	A	363	ARG	NE-CZ-NH2	7.37	123.98	120.30
1	C	123	ARG	NE-CZ-NH1	7.08	123.84	120.30
1	B	167	ASP	CB-CG-OD2	-6.99	112.01	118.30
1	B	167	ASP	CB-CG-OD1	6.85	124.47	118.30
1	A	109	ASP	CB-CG-OD1	6.55	124.20	118.30
1	D	176	ARG	NE-CZ-NH1	-6.51	117.04	120.30
1	A	362	ARG	NE-CZ-NH2	-6.40	117.10	120.30
1	D	71	ARG	NE-CZ-NH2	-6.39	117.11	120.30
1	D	176	ARG	NE-CZ-NH2	6.31	123.45	120.30
1	A	81	ARG	NE-CZ-NH1	6.27	123.44	120.30
1	B	66	ARG	NE-CZ-NH1	6.03	123.31	120.30
1	B	386	ARG	NE-CZ-NH1	6.01	123.30	120.30
1	B	176	ARG	NE-CZ-NH1	5.95	123.28	120.30
1	C	176	ARG	NE-CZ-NH2	5.71	123.16	120.30
1	B	362	ARG	NE-CZ-NH2	5.67	123.14	120.30
1	D	71	ARG	NE-CZ-NH1	5.62	123.11	120.30
1	D	109	ASP	CB-CG-OD1	5.59	123.33	118.30
1	C	123	ARG	NE-CZ-NH2	-5.49	117.56	120.30
1	B	225	VAL	CG1-CB-CG2	5.39	119.52	110.90
1	A	362	ARG	NE-CZ-NH1	5.37	122.98	120.30
1	C	256	ARG	NE-CZ-NH2	-5.31	117.64	120.30
1	A	149	ASP	CB-CG-OD2	5.20	122.98	118.30
1	B	135	ASP	CB-CG-OD1	5.17	122.95	118.30

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	2880	40	0
1	B	2889	0	2893	58	0
1	C	2855	0	2848	57	0
1	D	2860	0	2851	44	0
2	A	4	0	0	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
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	11495	193	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 8.

All (193) 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	1.22	1.09
1:C:150:THR:HG22	1:C:180:LEU:CD1	1.89	1.03
1:C:126:THR:HG21	1:D:97:GLU:OE1	1.62	1.00
1:C:180:LEU:N	1:C:180:LEU:CD2	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:H	1:C:180:LEU:HD23	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:B:98:LEU:CD1	1:B:235:MET:CE	2.59	0.80
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:IT1:HDA	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
1:A:112:TYR:HE1	2:A:401:BCT:O2	1.72	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:B:98:LEU:HD11	1:B:235:MET:HE1	1.75	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
5:B:708:HOH:O	1:C:36:MET:SD	2.51	0.67
1:A:326:ARG:HG3	1:A:326:ARG:HH11	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:98:LEU:CD1	1:B:235:MET:HE1	2.25	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:D:367:GLY:O	5:D:683:HOH:O	2.16	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:C:176:ARG:NH1	1:C:200:GLY:O	2.27	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: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:B:160:ASN:CG	5:B:668:HOH:O	2.38	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:B:95:VAL:HG22	1:B:235:MET:HE3	1.86	0.58
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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:36:MET:HE3	5:C:659:HOH:O	2.01	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:C:268:HIS:HE1	5:C:538:HOH:O	1.91	0.53
1:B:59:SER:HA	1:B:62:HIS:O	2.08	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:98:LEU:CD1	1:B:235:MET:HE2	2.15	0.52
1:C:150:THR:CG2	1:C:180:LEU:CD1	2.76	0.52
1:D:123:ARG:HD3	1:D:126:THR:HG22	1.92	0.52
1:D:104:HIS:HB3	1:D:149:ASP:HB3	1.91	0.52
1:D:137:THR:HG22	1:D:165:LEU:O	2.10	0.52
1:B:268:HIS:HD2	1:B:377:VAL:O	1.92	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: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:B:203:LEU:HD22	1:B:235:MET:HE3	1.93	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:C:126:THR:CG2	1:D:97:GLU:OE1	2.47	0.49
1:C:47:GLN:HE22	1:C:51:GLY:H	1.60	0.49
1:B:220:GLY:HA3	1:B:246:GLN:NE2	2.22	0.49
1:B:147:ARG:C	1:B:149:ASP:H	2.15	0.49
1:D:120:GLU:HA	1:D:124:ARG:HG3	1.95	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:B:188:PHE:CD2	1:B:188:PHE:C	2.88	0.48
1:A:249:PHE:CD1	5:A:737:HOH:O	2.53	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:C:170:ALA:O	1:C:174:ILE:HD12	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:364:GLU:OE1	1:B:364:GLU:HA	2.14	0.47
1:B:360:VAL:O	1:B:364:GLU:HG2	2.13	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:279:LEU:HD13	1:B:315:ILE:HG21	1.96	0.47
1:B:189:ALA:HB1	1:B:193:LEU:HB2	1.96	0.47
1:B:137:THR:O	1:B:139:PRO:HD3	2.15	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:104:HIS:NE2	1:D:132:SER:OG	2.47	0.46
1:D:130:ASP:OD2	1:D:147:ARG:NH2	2.46	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:B:278:TRP:CZ2	1:B:390:GLU:HG2	2.51	0.45
1:A:300:VAL:HG23	5:A:643:HOH:O	2.16	0.45
1:B:372:LEU:HD23	1:B:372:LEU:C	2.37	0.45
1:B:92:THR:HG23	1:B:154:TRP:CH2	2.52	0.45
1:A:59:SER:HA	1:A:62:HIS:O	2.17	0.45
1:C:47:GLN:NE2	1:C:51:GLY:H	2.15	0.45
1:D:108:MET:O	1:D:111:LEU:HD22	2.17	0.45
1:B:211:TYR:CE1	1:B:341:GLY:HA2	2.52	0.45
1:C:92:THR:HG23	1:C:154:TRP:CH2	2.52	0.45
1:C:97:GLU:OE1	1:D:126:THR:CG2	2.52	0.45
1:B:308:GLY:HA3	3:B:401:BME:S2	2.57	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:D:169:ALA:HA	1:D:199:LEU:O	2.16	0.44
1:B:110:ASP:OD2	1:B:164:LYS:HE3	2.18	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:D:372:LEU:C	1:D:372:LEU:HD23	2.38	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
1:A:326:ARG:CG	1:A:326:ARG:HH11	2.28	0.44
1:C:330:LYS:HB3	1:C:330:LYS:HE2	1.76	0.44
1:A:73:VAL:HG11	1:A:222:ILE:HG21	2.00	0.44
1:D:334:PHE:CD2	1:D:345:SER:HB3	2.53	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:C:513:HOH:O	1:D:126:THR:HG23	2.17	0.44
1:A:176:ARG:HB2	1:A:176:ARG:HE	1.31	0.43
1:C:175:ALA:HB1	1:C:180:LEU:HB2	2.00	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:C:209:THR:HG21	1:D:58:TYR:OH	2.18	0.43
1:D:120:GLU:OE1	1:D:124:ARG:NH1	2.45	0.43
1:A:39:ILE:HB	1:C:39:ILE:HB	2.00	0.43
1:B:187:THR:HB	1:B:210:IT1:H2AB	2.01	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:C:123:ARG:HD3	1:C:126:THR:HG22	2.01	0.42
1:B:268:HIS:HE1	5:B:555:HOH:O	2.01	0.42
1:D:61:THR:OG1	1:D:240:ASN:ND2	2.52	0.42
1:C:255:LEU:HD13	1:C:255:LEU:C	2.40	0.42
1:C:211:TYR:CE1	1:C:341:GLY:HA2	2.55	0.42
1:A:278:TRP:CD1	1:A:386:ARG:NH1	2.88	0.42
1:B:36:MET:HE1	1:B:259:LYS:HE2	2.01	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:33:GLY:O	1:C:34:ALA:C	2.58	0.42
1:C:160:ASN:HB2	1:C:188:PHE:CZ	2.54	0.42
1:C:246:GLN:NE2	5:C:557:HOH:O	2.53	0.41
1:B:372:LEU:HD23	1:B:373:VAL:N	2.36	0.41
1:B:210:IT1:O3	1:B:210:IT1:NZ	2.53	0.41
1:C:327:PHE:CE2	1:C:373:VAL:HG21	2.55	0.41
1:A:40:TYR:CE2	1:C:38:PRO:HG3	2.55	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:B:304:ARG:NE	5:B:694:HOH:O	2.09	0.41
1:A:154:TRP:CZ3	1:A:183:VAL:HG11	2.56	0.41
1:A:49:SER:O	1:A:50:PRO:C	2.58	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:163:LEU:HD22	1:B:188:PHE:CZ	2.56	0.40
1:D:120:GLU:OE1	1:D:124:ARG:HD2	2.21	0.40
1:C:206:HIS:HB2	1:C:222:ILE:HB	2.03	0.40
1:B:362:ARG:HE	1:B:366:LEU:HD11	1.86	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%)	46	36
1	C	374/397 (94%)	361 (96%)	12 (3%)	1 (0%)	46	36
1	D	375/397 (94%)	361 (96%)	14 (4%)	0	100	100
All	All	1508/1588 (95%)	1463 (97%)	43 (3%)	2 (0%)	56	49

All (2) Ramachandran outliers are listed below:

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

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	298/312 (96%)	288 (97%)	10 (3%)	44	37
1	B	299/312 (96%)	286 (96%)	13 (4%)	35	27
1	C	294/312 (94%)	285 (97%)	9 (3%)	47	41
1	D	294/312 (94%)	285 (97%)	9 (3%)	47	41
All	All	1185/1248 (95%)	1144 (96%)	41 (4%)	44	35

All (41) 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	176	ARG
1	A	195	ARG
1	A	326	ARG
1	A	340	LEU
1	A	364	GLU
1	A	370	ASP
1	A	373	VAL
1	A	386	ARG
1	B	59	SER
1	B	111	LEU
1	B	132	SER
1	B	176	ARG
1	B	177	LYS
1	B	188	PHE
1	B	234	GLN
1	B	255	LEU
1	B	326	ARG
1	B	339	SER
1	B	344	GLU
1	B	369	SER
1	B	386	ARG
1	C	117	ARG
1	C	126	THR
1	C	149	ASP
1	C	177	LYS
1	C	180	LEU
1	C	195	ARG
1	C	340	LEU
1	C	373	VAL
1	C	386	ARG
1	D	111	LEU

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Mol	Chain	Res	Type
1	D	124	ARG
1	D	126	THR
1	D	149	ASP
1	D	166	VAL
1	D	176	ARG
1	D	190	SER
1	D	300	VAL
1	D	322	ASP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (29) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	47	GLN
1	A	240	ASN
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	240	ASN
1	B	246	GLN
1	B	268	HIS
1	B	271	ASN
1	B	348	ASN
1	B	355	HIS
1	C	47	GLN
1	C	234	GLN
1	C	240	ASN
1	C	246	GLN
1	C	268	HIS
1	C	271	ASN
1	C	348	ASN
1	D	47	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	IT1	A	210	1	23,24,25	3.79	7 (30%)	28,32,34	2.26	11 (39%)
1	IT1	B	210	1	23,24,25	3.43	8 (34%)	28,32,34	1.70	7 (25%)
1	IT1	C	210	1	23,24,25	2.83	8 (34%)	28,32,34	2.10	9 (32%)
1	IT1	D	210	1	23,24,25	3.07	6 (26%)	28,32,34	1.97	11 (39%)

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	IT1	A	210	1	-	0/15/17/19	0/1/1/1
1	IT1	B	210	1	-	0/15/17/19	0/1/1/1
1	IT1	C	210	1	-	0/15/17/19	0/1/1/1
1	IT1	D	210	1	-	0/15/17/19	0/1/1/1

All (29) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	210	IT1	P-OP2	-4.67	1.37	1.54
1	B	210	IT1	P-OP2	-4.62	1.38	1.54
1	A	210	IT1	P-OP3	-4.28	1.39	1.54
1	C	210	IT1	CB-CA	-3.69	1.50	1.53
1	B	210	IT1	P-OP3	-3.60	1.41	1.54
1	D	210	IT1	P-OP1	-3.53	1.39	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	210	IT1	P-OP2	-3.43	1.42	1.54
1	A	210	IT1	P-OP2	-3.36	1.42	1.54
1	D	210	IT1	P-OP3	-3.33	1.42	1.54
1	C	210	IT1	P-OP1	-2.64	1.42	1.51
1	B	210	IT1	P-OP4	-2.62	1.51	1.60
1	C	210	IT1	P-OP3	-2.47	1.45	1.54
1	C	210	IT1	P-OP4	-2.29	1.52	1.60
1	A	210	IT1	P-OP1	-2.25	1.43	1.51
1	B	210	IT1	CD-CE	2.27	1.58	1.51
1	B	210	IT1	CB-CA	4.00	1.57	1.53
1	D	210	IT1	C4-C3	4.22	1.46	1.40
1	C	210	IT1	C4-C5	4.60	1.48	1.42
1	C	210	IT1	C4-C3	4.80	1.46	1.40
1	B	210	IT1	C4-C5	5.00	1.48	1.42
1	D	210	IT1	C4-C5	5.08	1.48	1.42
1	A	210	IT1	C4-C5	5.09	1.48	1.42
1	A	210	IT1	C4-C3	6.06	1.48	1.40
1	B	210	IT1	C4-C3	6.72	1.49	1.40
1	A	210	IT1	CB-CA	7.33	1.60	1.53
1	C	210	IT1	C3-C2	8.22	1.46	1.40
1	B	210	IT1	C3-C2	10.86	1.48	1.40
1	D	210	IT1	C3-C2	10.88	1.48	1.40
1	A	210	IT1	C3-C2	12.59	1.49	1.40

All (38) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	210	IT1	C2A-C2-C3	-4.19	115.98	121.04
1	A	210	IT1	C2A-C2-C3	-3.86	116.38	121.04
1	A	210	IT1	C3-C4-C5	-3.70	115.33	118.11
1	D	210	IT1	C3-C4-C5	-3.59	115.41	118.11
1	A	210	IT1	CD-CE-NZ	-3.37	105.46	110.98
1	C	210	IT1	CB-CA-N	-3.04	101.89	110.52
1	D	210	IT1	OP2-P-OP4	-2.62	99.03	106.56
1	C	210	IT1	OP3-P-OP4	-2.54	99.26	106.56
1	C	210	IT1	CD-CE-NZ	-2.37	107.10	110.98
1	D	210	IT1	O-C-CA	-2.34	119.38	125.49
1	D	210	IT1	C5A-C5-C6	-2.17	115.17	119.28
1	B	210	IT1	C3-C2-N1	-2.17	117.61	120.61
1	B	210	IT1	CD-CE-NZ	-2.08	107.56	110.98
1	B	210	IT1	C4-C4A-NZ	-2.05	113.64	125.06
1	A	210	IT1	CG-CD-CE	2.10	122.56	113.97

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	210	IT1	C5-C4-C4A	2.14	124.60	121.52
1	C	210	IT1	C5A-C5-C4	2.20	125.16	121.47
1	A	210	IT1	OP2-P-OP1	2.24	117.80	110.58
1	D	210	IT1	OP4-C5A-C5	2.33	112.84	108.99
1	C	210	IT1	C6-N1-C2	2.36	124.09	119.28
1	C	210	IT1	OP2-P-OP1	2.41	118.33	110.58
1	A	210	IT1	C5-C4-C4A	2.42	125.00	121.52
1	A	210	IT1	O3-C3-C2	2.50	122.00	117.66
1	D	210	IT1	C5A-C5-C4	2.61	125.86	121.47
1	D	210	IT1	C5-C4-C4A	2.70	125.40	121.52
1	D	210	IT1	OP2-P-OP1	2.71	119.30	110.58
1	B	210	IT1	CE-NZ-C4A	2.86	127.23	118.97
1	B	210	IT1	C6-N1-C2	2.87	125.13	119.28
1	A	210	IT1	C2A-C2-N1	2.89	124.36	117.95
1	A	210	IT1	CB-CA-N	2.96	118.92	110.52
1	A	210	IT1	CE-NZ-C4A	2.99	127.59	118.97
1	D	210	IT1	CE-NZ-C4A	3.09	127.90	118.97
1	B	210	IT1	OP4-C5A-C5	3.11	114.13	108.99
1	D	210	IT1	C2A-C2-N1	3.21	125.07	117.95
1	B	210	IT1	CD-CG-CB	3.77	127.04	113.66
1	C	210	IT1	CE-NZ-C4A	3.98	130.47	118.97
1	A	210	IT1	OP4-C5A-C5	5.99	118.90	108.99
1	C	210	IT1	OP4-C5A-C5	6.24	119.30	108.99

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	B	210	IT1	2	0
1	D	210	IT1	1	0

5.5 Carbohydrates [i](#)

There are no carbohydrates 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
2	BCT	A	401	-	0,3,3	0.00	-	0,3,3	0.00	-
3	BME	A	402	1	3,3,3	0.23	0	2,2,2	0.84	0
3	BME	B	401	1	3,3,3	0.19	0	2,2,2	2.15	1 (50%)
3	BME	C	401	1	3,3,3	0.27	0	2,2,2	1.34	0
4	GOL	D	401	-	5,5,5	0.30	0	5,5,5	0.46	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
2	BCT	A	401	-	-	0/0/0/0	0/0/0/0
3	BME	A	402	1	-	0/1/1/1	0/0/0/0
3	BME	B	401	1	-	0/1/1/1	0/0/0/0
3	BME	C	401	1	-	0/1/1/1	0/0/0/0
4	GOL	D	401	-	-	0/4/4/4	0/0/0/0

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	401	BME	C1-C2-S2	-2.46	99.20	112.58

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

4 monomers are involved in 9 short contacts:

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

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	401	BME	2	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%)	-0.20	3 (0%) 87 89	10, 19, 33, 44	0
1	B	380/397 (95%)	-0.34	1 (0%) 94 95	9, 19, 35, 47	0
1	C	377/397 (94%)	-0.13	13 (3%) 49 54	10, 22, 43, 61	0
1	D	377/397 (94%)	-0.04	14 (3%) 45 50	10, 23, 44, 62	0
All	All	1514/1588 (95%)	-0.18	31 (2%) 68 71	9, 21, 40, 62	0

All (31) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	394	VAL	4.5
1	C	361	ALA	4.4
1	D	178	HIS	4.2
1	D	351	ALA	3.7
1	C	360	VAL	3.7
1	C	326	ARG	2.9
1	C	370	ASP	2.8
1	D	146	ILE	2.8
1	D	139	PRO	2.7
1	D	177	LYS	2.6
1	D	173	VAL	2.5
1	D	229	ALA	2.5
1	D	131	PHE	2.5
1	C	368	ILE	2.5
1	C	173	VAL	2.5
1	C	177	LYS	2.5
1	D	145	ALA	2.3
1	D	175	ALA	2.3
1	D	176	ARG	2.3
1	D	227	ASP	2.2
1	C	362	ARG	2.2

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Mol	Chain	Res	Type	RSRZ
1	D	179	GLY	2.2
1	A	253	LEU	2.2
1	A	386	ARG	2.1
1	C	148	ALA	2.1
1	C	286	GLU	2.1
1	D	171	ILE	2.1
1	C	141	ALA	2.1
1	C	179	GLY	2.1
1	B	321	PHE	2.1
1	A	14	ALA	2.0

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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. 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	LLDF	B-factors(Å ²)	Q<0.9
1	IT1	B	210	24/25	0.95	0.12	-	11,16,21,22	0
1	IT1	C	210	24/25	0.94	0.13	-	13,19,27,29	0
1	IT1	A	210	24/25	0.95	0.13	-	10,17,22,26	0
1	IT1	D	210	24/25	0.95	0.10	-	14,19,23,26	0

6.3 Carbohydrates [i](#)

There are no carbohydrates 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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. 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	LLDF	B-factors(Å ²)	Q<0.9
3	BME	B	401	4/4	0.88	0.15	3.37	43,47,47,48	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
3	BME	C	401	4/4	0.94	0.13	1.72	43,43,46,47	0
2	BCT	A	401	4/4	0.95	0.12	1.43	18,22,24,30	0
3	BME	A	402	4/4	0.94	0.11	-0.02	49,53,53,53	0
4	GOL	D	401	6/6	0.95	0.08	-1.16	18,22,24,27	0

6.5 Other polymers [i](#)

There are no such residues in this entry.