



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 20, 2026 – 04:28 PM UTC

PDB ID : 7ESH / pdb_00007esh
Title : Crystal structure of amylosucrase from *Calidithermus timidus*
Authors : Tian, Y.; Hou, X.; Ni, D.; Xu, W.; Guang, C.; Zhang, W.; Rao, Y.; Mu, W.
Deposited on : 2021-05-10
Resolution : 2.29 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

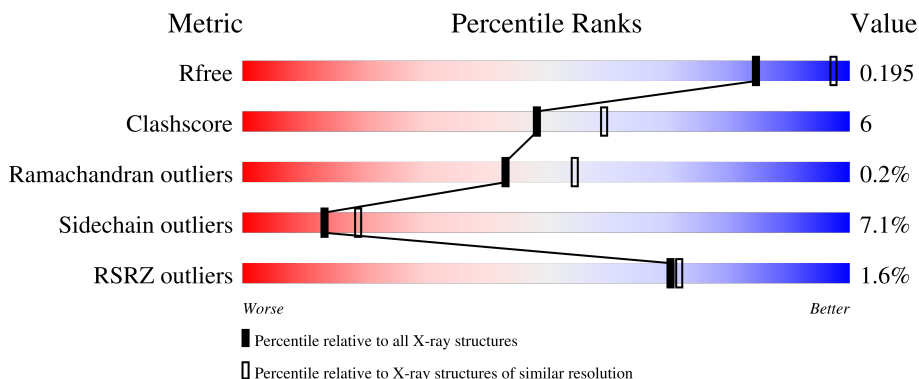
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION


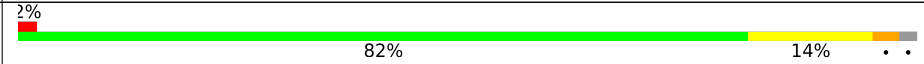
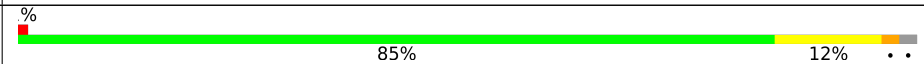

The reported resolution of this entry is 2.29 Å.

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	6319 (2.30-2.30)
Clashscore	190562	6919 (2.30-2.30)
Ramachandran outliers	187476	6854 (2.30-2.30)
Sidechain outliers	187428	6854 (2.30-2.30)
RSRZ outliers	180081	6325 (2.30-2.30)

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	656	 2% 85% 12% ..
1	B	656	 2% 82% 14% ..
1	C	656	 2% 85% 12% ..
1	D	656	 2% 82% 14% ..

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	TRS	A	701	-	X	-	-

2 Entry composition [i](#)

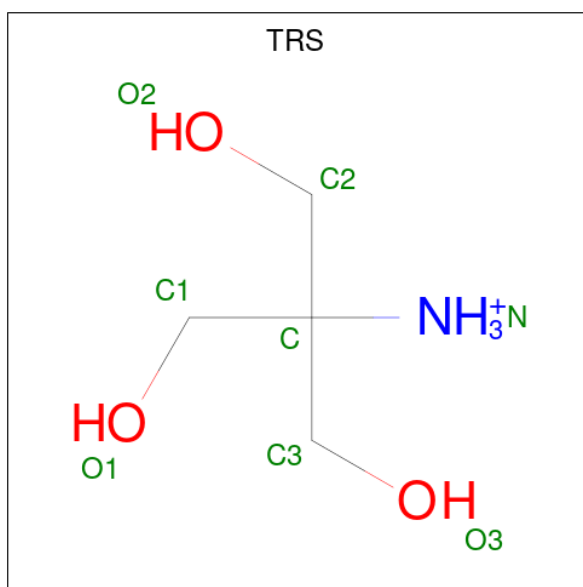
There are 3 unique types of molecules in this entry. The entry contains 21669 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 amylosucrase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	646	Total 5251	C 3362	N 943	O 930	S 16	0	2	0
1	B	646	Total 5244	C 3356	N 942	O 930	S 16	0	1	0
1	C	646	Total 5252	C 3362	N 943	O 931	S 16	0	2	0
1	D	646	Total 5251	C 3361	N 943	O 931	S 16	0	2	0

- Molecule 2 is 2-AMINO-2-HYDROXYMETHYL-PROPANE-1,3-DIOL (CCD ID: TRS) (formula: C₄H₁₂NO₃).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	N	O		
2	A	1	Total 8	C 4	N 1	O 3	0	0
2	B	1	Total 8	C 4	N 1	O 3	0	0

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	C	1	Total	C	N	O	0	0
			8	4	1	3		
2	D	1	Total	C	N	O	0	0
			8	4	1	3		

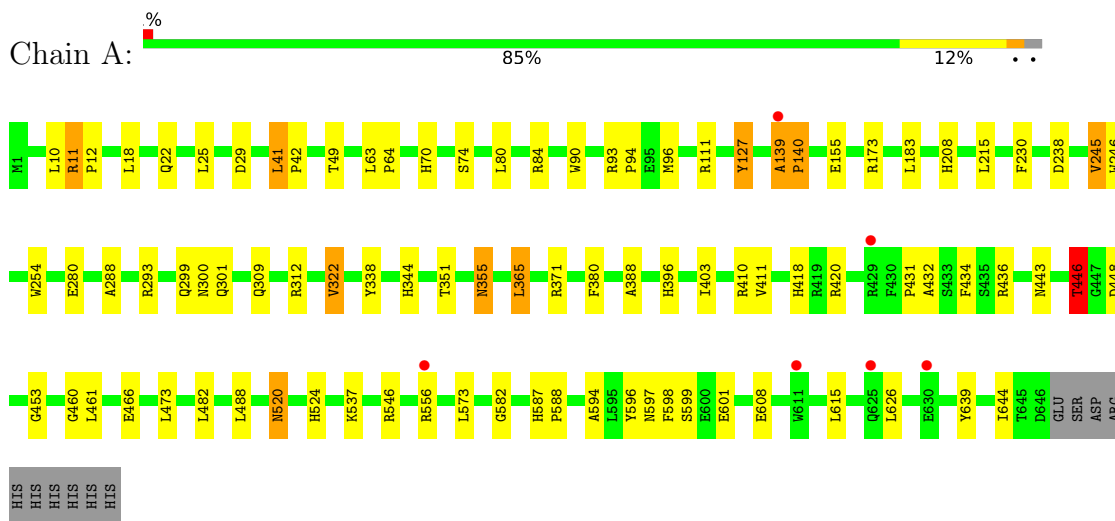
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	188	Total	O	0	0
			188	188		
3	B	169	Total	O	0	0
			169	169		
3	C	162	Total	O	0	0
			162	162		
3	D	120	Total	O	0	0
			120	120		

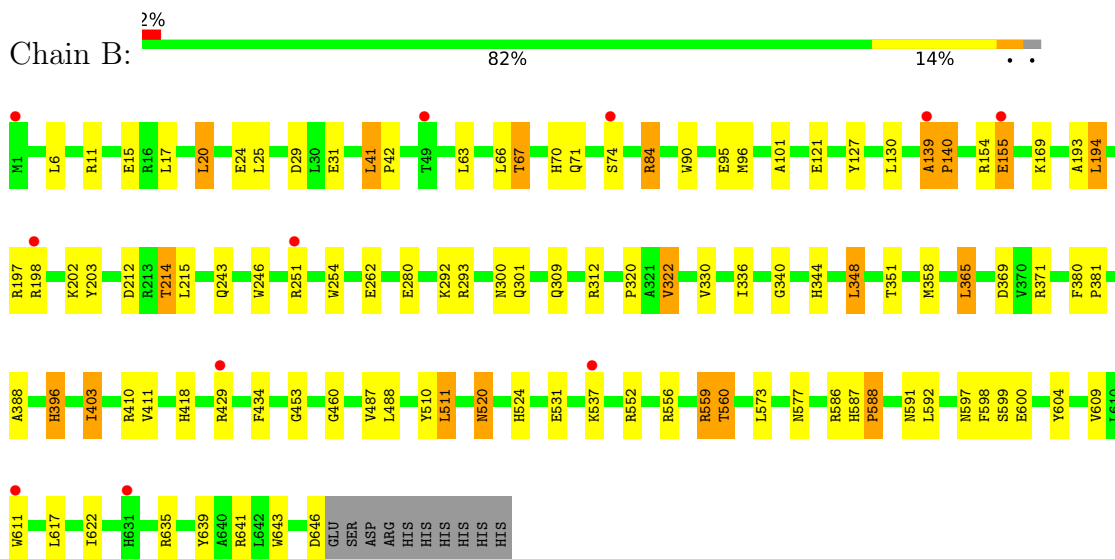
3 Residue-property plots [i](#)

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.

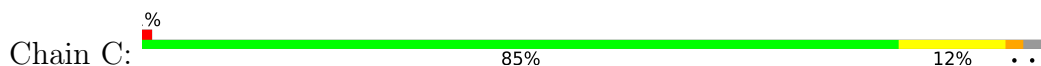
- Molecule 1: amylосуcrase

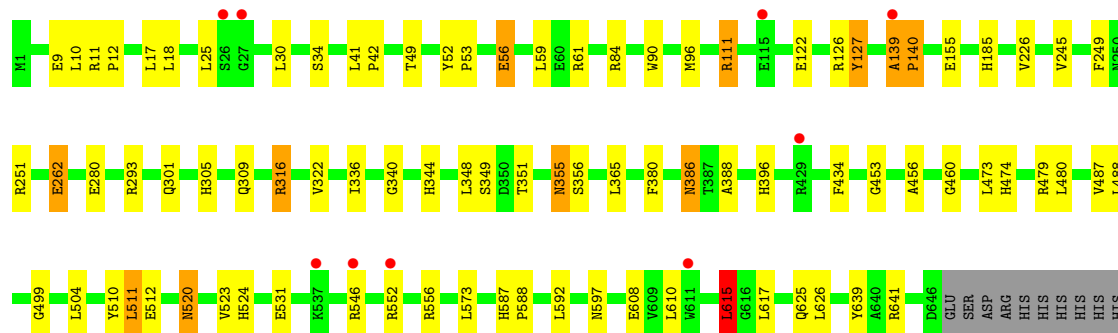


- Molecule 1: amylосуcrase

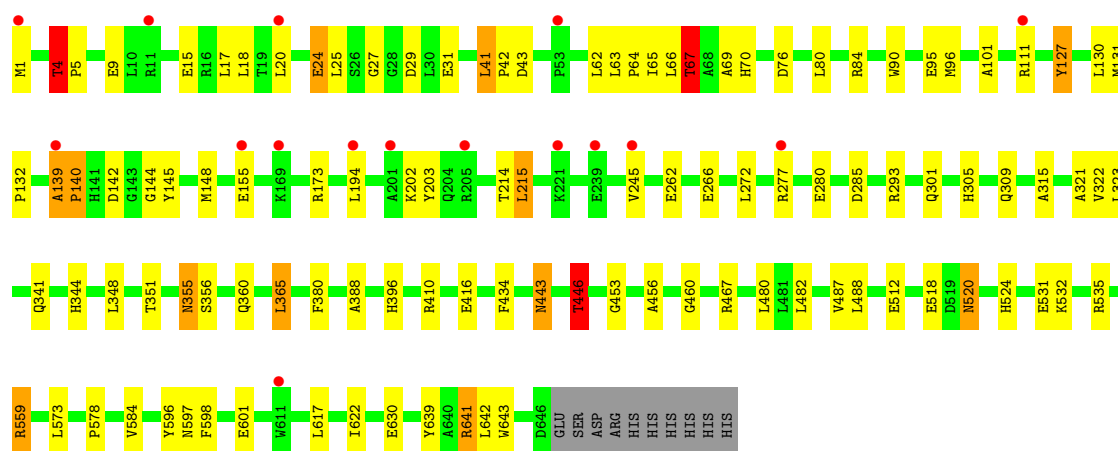
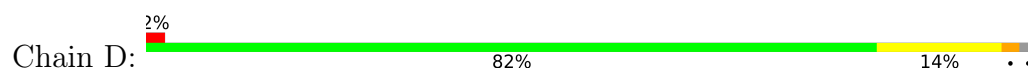


- Molecule 1: amylосуcrase





• Molecule 1: amylsucrase



4 Data and refinement statistics

Property	Value	Source
Space group	P 2 21 21	Depositor
Cell constants a, b, c, α , β , γ	105.75Å 126.66Å 294.73Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	48.07 – 2.29 48.07 – 2.29	Depositor EDS
% Data completeness (in resolution range)	96.6 (48.07-2.29) 96.9 (48.07-2.29)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.68 (at 2.29Å)	Xtrriage
Refinement program	REFMAC 5.8.0238	Depositor
R, R_{free}	0.192 , 0.228 (Not available) , 0.195	Depositor DCC
R_{free} test set	8633 reflections (4.83%)	wwPDB-VP
Wilson B-factor (Å ²)	31.7	Xtrriage
Anisotropy	0.026	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 20.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	21669	wwPDB-VP
Average B, all atoms (Å ²)	32.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.02% 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: TRS

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	1.07	1/5403 (0.0%)	1.36	8/7355 (0.1%)
1	B	1.11	4/5396 (0.1%)	1.36	5/7346 (0.1%)
1	C	1.07	2/5404 (0.0%)	1.37	4/7357 (0.1%)
1	D	1.08	1/5403 (0.0%)	1.38	8/7355 (0.1%)
All	All	1.08	8/21606 (0.0%)	1.37	25/29413 (0.1%)

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	140	PRO	C-O	-7.34	1.16	1.23
1	C	185	HIS	CE1-NE2	6.13	1.38	1.32
1	B	588	PRO	C-O	-5.48	1.17	1.24
1	B	140	PRO	C-O	-5.40	1.17	1.23
1	B	381	PRO	C-O	-5.33	1.17	1.23
1	B	396	HIS	CE1-NE2	5.25	1.37	1.32
1	D	140	PRO	C-O	-5.24	1.17	1.23
1	C	140	PRO	C-O	-5.21	1.17	1.23

All (25) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	446	THR	CB-CA-C	6.34	119.30	109.03
1	D	4	THR	CB-CA-C	6.19	119.41	109.51
1	D	443	ASN	CB-CA-C	5.84	115.95	110.17
1	C	615	LEU	CA-C-N	5.72	126.17	119.94
1	C	615	LEU	C-N-CA	5.72	126.17	119.94
1	A	238	ASP	CA-C-N	5.60	127.72	120.44
1	A	238	ASP	C-N-CA	5.60	127.72	120.44
1	A	230	PHE	CA-CB-CG	5.50	119.31	113.80
1	D	148	MET	N-CA-C	-5.50	106.70	113.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	420	ARG	N-CA-C	-5.49	105.38	111.36
1	D	27	GLY	CA-C-N	5.46	126.97	120.14
1	D	27	GLY	C-N-CA	5.46	126.97	120.14
1	A	420	ARG	CB-CA-C	5.33	119.92	110.85
1	D	67	THR	CB-CA-C	5.28	119.17	110.88
1	C	111	ARG	CA-C-N	5.26	125.92	120.03
1	C	111	ARG	C-N-CA	5.26	125.92	120.03
1	B	537	LYS	CB-CA-C	5.23	119.17	110.90
1	D	76	ASP	CA-CB-CG	5.21	117.81	112.60
1	A	74	SER	CA-C-N	5.18	127.48	120.38
1	A	74	SER	C-N-CA	5.18	127.48	120.38
1	B	66	LEU	CA-C-N	5.15	127.45	120.65
1	B	66	LEU	C-N-CA	5.15	127.45	120.65
1	B	154	ARG	CA-C-N	5.11	127.43	120.54
1	B	154	ARG	C-N-CA	5.11	127.43	120.54
1	A	446	THR	CB-CA-C	5.09	118.21	109.15

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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	5251	0	5121	55	0
1	B	5244	0	5112	66	0
1	C	5252	0	5122	49	0
1	D	5251	0	5118	60	0
2	A	8	0	12	0	0
2	B	8	0	12	0	0
2	C	8	0	12	0	0
2	D	8	0	12	3	0
3	A	188	0	0	6	0
3	B	169	0	0	3	0
3	C	162	0	0	4	0
3	D	120	0	0	2	0
All	All	21669	0	20521	229	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 6.

All (229) 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:A:446:THR:HG21	3:A:978:HOH:O	1.39	1.21
1:A:139:ALA:CB	1:A:140:PRO:HD3	1.67	1.21
1:D:139:ALA:HB1	1:D:140:PRO:HD3	1.30	1.12
1:A:139:ALA:CB	1:A:140:PRO:CD	2.23	1.11
1:C:139:ALA:CB	1:C:140:PRO:CD	2.31	1.08
1:B:139:ALA:CB	1:B:140:PRO:CD	2.32	1.07
1:D:139:ALA:CB	1:D:140:PRO:CD	2.30	1.07
1:B:139:ALA:HB3	1:B:140:PRO:HD2	1.37	1.06
1:C:139:ALA:HB3	1:C:140:PRO:HD2	1.38	1.06
1:C:139:ALA:HB1	1:C:140:PRO:CD	1.88	1.04
1:C:608:GLU:HG2	3:C:924:HOH:O	1.58	1.03
1:B:139:ALA:HB1	1:B:140:PRO:HD3	1.41	1.03
1:C:139:ALA:CB	1:C:140:PRO:HD2	1.90	1.00
1:A:139:ALA:HB1	1:A:140:PRO:CD	1.86	0.99
1:A:139:ALA:HB1	1:A:140:PRO:HD3	1.01	0.99
1:D:139:ALA:HB3	1:D:140:PRO:HD2	1.42	0.98
1:C:139:ALA:HB1	1:C:140:PRO:HD3	1.43	0.95
1:D:4:THR:HG21	1:D:43:ASP:OD1	1.64	0.95
1:D:139:ALA:CB	1:D:140:PRO:HD3	1.96	0.94
1:A:139:ALA:HB3	1:A:140:PRO:CD	1.98	0.93
1:B:139:ALA:HB1	1:B:140:PRO:CD	1.97	0.92
1:D:139:ALA:HB3	1:D:140:PRO:CD	1.98	0.86
1:B:139:ALA:CB	1:B:140:PRO:HD2	1.99	0.86
1:A:556:ARG:HD3	3:A:808:HOH:O	1.76	0.84
1:B:293:ARG:HH11	1:B:301:GLN:HE21	1.22	0.83
1:B:560:THR:CG2	3:B:958:HOH:O	2.27	0.82
1:A:139:ALA:HB3	1:A:140:PRO:HD2	1.64	0.80
1:C:520:ASN:C	1:C:520:ASN:HD22	1.91	0.79
1:D:4:THR:CG2	1:D:43:ASP:OD1	2.30	0.79
1:C:293:ARG:HH11	1:C:301:GLN:HE21	1.31	0.78
1:C:96:MET:HE1	1:C:127:TYR:HB2	1.66	0.77
1:A:293:ARG:HH11	1:A:301:GLN:HE21	1.28	0.77
1:D:520:ASN:C	1:D:520:ASN:HD22	1.93	0.76
1:C:84:ARG:HD3	1:C:90:TRP:CE2	2.22	0.75
1:C:84:ARG:HD3	1:C:90:TRP:NE1	2.04	0.72
1:B:520:ASN:C	1:B:520:ASN:HD22	1.97	0.72
1:B:340:GLY:HA2	1:B:348:LEU:HD22	1.71	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:293:ARG:HH11	1:D:301:GLN:HE21	1.35	0.71
1:B:20:LEU:HB3	1:B:63:LEU:HD13	1.73	0.70
1:B:84:ARG:HD2	1:B:90:TRP:NE1	2.06	0.69
1:A:371:ARG:NH1	1:A:411:VAL:O	2.26	0.69
1:B:155:GLU:CD	1:B:155:GLU:H	2.00	0.69
1:A:453:GLY:H	1:A:524:HIS:HD2	1.39	0.68
1:C:453:GLY:H	1:C:524:HIS:HD2	1.41	0.68
1:C:453:GLY:H	1:C:524:HIS:CD2	2.11	0.68
1:D:24:GLU:HG2	1:D:67:THR:CG2	2.24	0.68
1:D:155:GLU:H	1:D:155:GLU:CD	2.02	0.67
1:A:93:ARG:HB3	3:A:970:HOH:O	1.93	0.67
1:A:94:PRO:HD2	3:A:970:HOH:O	1.93	0.67
1:A:453:GLY:H	1:A:524:HIS:CD2	2.13	0.66
1:A:96:MET:HE1	1:A:127:TYR:HB2	1.76	0.65
1:D:96:MET:HE1	1:D:127:TYR:HB2	1.79	0.65
1:B:300:ASN:HD21	1:B:330:VAL:HG11	1.62	0.65
1:A:520:ASN:C	1:A:520:ASN:HD22	2.05	0.64
1:B:351:THR:HA	1:B:388:ALA:O	1.98	0.64
1:B:309:GLN:OE1	1:B:344:HIS:HD2	1.81	0.63
1:B:453:GLY:H	1:B:524:HIS:HD2	1.44	0.63
1:A:443:ASN:HB3	1:A:446:THR:HG22	1.79	0.63
1:B:560:THR:HG23	3:B:958:HOH:O	1.93	0.62
1:D:1:MET:HE3	3:D:908:HOH:O	1.99	0.62
1:B:24:GLU:HG3	1:B:67:THR:HG21	1.82	0.62
1:D:443:ASN:HB3	1:D:446:THR:HG22	1.82	0.60
1:B:396:HIS:O	1:B:524:HIS:HE1	1.85	0.60
1:B:84:ARG:HD2	1:B:90:TRP:CD1	2.37	0.60
1:B:17:LEU:O	1:B:63:LEU:HD11	2.02	0.60
1:C:456:ALA:HA	1:C:480:LEU:HD11	1.83	0.60
1:C:386:ASN:HD22	1:C:386:ASN:H	1.47	0.59
1:B:96:MET:HE1	1:B:127:TYR:HB2	1.83	0.59
1:D:559:ARG:CG	1:D:559:ARG:HH21	2.16	0.59
1:D:305:HIS:HB3	1:D:348[A]:LEU:HD21	1.84	0.58
1:B:453:GLY:H	1:B:524:HIS:CD2	2.20	0.58
1:B:17:LEU:HA	1:B:63:LEU:HD11	1.86	0.58
1:B:212:ASP:OD1	1:B:214:THR:OG1	2.20	0.57
1:B:434:PHE:O	1:B:460:GLY:HA2	2.05	0.57
1:D:453:GLY:H	1:D:524:HIS:HD2	1.52	0.56
1:C:316:ARG:HD2	3:C:938:HOH:O	2.06	0.56
1:C:30:LEU:O	1:C:34:SER:HB2	2.04	0.56
1:C:434:PHE:O	1:C:460:GLY:HA2	2.06	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:597:ASN:O	1:C:639:TYR:HA	2.05	0.56
1:D:453:GLY:H	1:D:524:HIS:CD2	2.24	0.56
1:A:351:THR:HA	1:A:388:ALA:O	2.06	0.55
1:B:17:LEU:CA	1:B:63:LEU:HD11	2.36	0.55
1:C:355:ASN:HD22	1:C:355:ASN:H	1.54	0.55
1:A:280:GLU:O	1:A:322:VAL:HA	2.06	0.55
1:A:482:LEU:HD11	1:A:596:TYR:HB3	1.89	0.55
1:C:41:LEU:N	1:C:42:PRO:CD	2.70	0.54
1:C:510:TYR:CZ	1:C:511:LEU:HD13	2.42	0.54
1:B:84:ARG:HD2	1:B:90:TRP:CE2	2.42	0.54
1:D:285:ASP:OD1	2:D:701:TRS:N	2.38	0.54
1:A:293:ARG:HH11	1:A:301:GLN:NE2	2.01	0.53
1:D:559:ARG:HH21	1:D:559:ARG:HG3	1.72	0.53
1:A:309:GLN:OE1	1:A:344:HIS:HD2	1.92	0.52
1:B:20:LEU:CB	1:B:63:LEU:HD13	2.37	0.52
1:A:597:ASN:O	1:A:639:TYR:HA	2.09	0.52
1:D:482:LEU:HD11	1:D:596:TYR:HB3	1.91	0.52
1:A:355:ASN:HD22	1:A:355:ASN:H	1.57	0.51
1:A:84:ARG:NH1	1:A:280:GLU:OE1	2.43	0.51
1:B:293:ARG:NH1	1:B:301:GLN:HE21	2.00	0.51
1:B:510:TYR:CZ	1:B:511:LEU:HD13	2.46	0.51
1:A:371:ARG:NH2	3:A:806:HOH:O	2.43	0.51
1:D:597:ASN:O	1:D:639:TYR:HA	2.11	0.51
1:B:24:GLU:CG	1:B:67:THR:HG21	2.42	0.50
1:D:355:ASN:H	1:D:355:ASN:HD22	1.57	0.50
1:A:396:HIS:O	1:A:524:HIS:HE1	1.95	0.50
1:B:193:ALA:O	1:B:197:ARG:HG2	2.12	0.50
1:D:641:ARG:C	1:D:642:LEU:HD23	2.36	0.50
1:C:309:GLN:OE1	1:C:344:HIS:HD2	1.94	0.50
1:C:280:GLU:O	1:C:322:VAL:HA	2.11	0.50
1:B:587:HIS:CG	1:B:588:PRO:HD2	2.47	0.49
1:D:142:ASP:OD2	2:D:701:TRS:H21	2.12	0.49
1:A:80:LEU:O	1:A:84:ARG:HG2	2.13	0.49
1:D:63:LEU:HD13	1:D:63:LEU:C	2.37	0.49
1:B:95:GLU:HG2	3:B:956:HOH:O	2.12	0.49
1:B:403:ILE:HD12	1:B:418:HIS:HD2	1.78	0.49
1:B:600:GLU:HG3	1:B:639:TYR:OH	2.13	0.49
1:D:396:HIS:O	1:D:524:HIS:HE1	1.96	0.49
1:C:344:HIS:HB3	1:C:348[A]:LEU:CD1	2.42	0.48
1:A:11:ARG:HB2	1:A:12:PRO:HD3	1.95	0.48
1:B:592:LEU:C	1:B:592:LEU:HD23	2.39	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:351:THR:HA	1:D:388:ALA:O	2.14	0.48
1:D:24:GLU:HG2	1:D:67:THR:HG21	1.94	0.48
1:D:80:LEU:O	1:D:84:ARG:HG2	2.14	0.48
1:B:24:GLU:O	1:B:71:GLN:NE2	2.47	0.48
1:D:434:PHE:O	1:D:460:GLY:HA2	2.14	0.48
1:A:626:LEU:H	1:A:626:LEU:HD22	1.78	0.48
1:C:396:HIS:O	1:C:524:HIS:HE1	1.97	0.48
1:C:587:HIS:CG	1:C:588:PRO:HD2	2.49	0.48
1:D:41:LEU:N	1:D:42:PRO:CD	2.77	0.48
1:D:84:ARG:HG3	1:D:321:ALA:HA	1.96	0.47
1:D:520:ASN:C	1:D:520:ASN:ND2	2.66	0.47
1:D:365:LEU:HD13	1:D:598:PHE:CD2	2.48	0.47
1:B:369:ASP:OD2	1:B:371:ARG:HD3	2.14	0.47
1:D:309:GLN:OE1	1:D:344:HIS:HD2	1.98	0.47
1:C:139:ALA:HB3	1:C:140:PRO:CD	2.13	0.47
1:B:29:ASP:OD1	1:B:70:HIS:HE1	1.97	0.47
1:B:622:ILE:HD11	1:B:643:TRP:CD2	2.50	0.47
1:A:41:LEU:N	1:A:42:PRO:CD	2.77	0.47
1:B:197:ARG:HD3	1:B:254:TRP:CH2	2.49	0.47
1:B:246:TRP:CE2	1:B:292:LYS:HE3	2.50	0.47
1:C:305:HIS:HB3	1:C:348[A]:LEU:HD21	1.97	0.47
1:B:280:GLU:O	1:B:322:VAL:HA	2.14	0.46
1:A:434:PHE:O	1:A:460:GLY:HA2	2.16	0.46
1:B:17:LEU:HA	1:B:63:LEU:CD1	2.45	0.46
1:B:510:TYR:CE2	1:B:511:LEU:HD13	2.50	0.46
1:D:262:GLU:O	1:D:266:GLU:HG2	2.16	0.46
1:B:597:ASN:OD1	1:B:599:SER:HB3	2.16	0.46
1:C:344:HIS:HB3	1:C:348[A]:LEU:HD13	1.98	0.46
1:B:340:GLY:CA	1:B:348:LEU:HD22	2.42	0.46
1:D:62:LEU:O	1:D:65:ILE:HB	2.16	0.46
1:D:95:GLU:HA	1:D:559:ARG:HG2	1.98	0.46
1:A:587:HIS:CG	1:A:588:PRO:HD2	2.51	0.45
1:A:608:GLU:HG2	3:A:837:HOH:O	2.16	0.45
1:D:29:ASP:OD1	1:D:70:HIS:HE1	1.98	0.45
1:C:293:ARG:HH11	1:C:301:GLN:NE2	2.08	0.45
1:C:340:GLY:HA2	1:C:348[B]:LEU:HD12	1.98	0.45
1:C:351:THR:HA	1:C:388:ALA:O	2.15	0.45
1:B:597:ASN:O	1:B:639:TYR:HA	2.16	0.45
1:B:202:LYS:HE3	1:B:203:TYR:CZ	2.52	0.45
1:A:461:LEU:HD11	1:A:473:LEU:HD13	1.99	0.45
1:B:17:LEU:HD22	1:B:63:LEU:HG	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:453:GLY:N	1:C:524:HIS:HD2	2.10	0.45
1:C:355:ASN:HD22	1:C:355:ASN:N	2.14	0.45
1:C:56:GLU:CD	1:C:56:GLU:H	2.26	0.44
1:D:456:ALA:HA	1:D:480:LEU:HD11	2.00	0.44
1:A:453:GLY:N	1:A:524:HIS:HD2	2.11	0.44
1:C:61:ARG:HH12	1:C:262:GLU:CD	2.25	0.44
1:B:520:ASN:C	1:B:520:ASN:ND2	2.69	0.44
1:A:582:GLY:HA2	1:A:594:ALA:O	2.17	0.44
1:B:41:LEU:N	1:B:42:PRO:CD	2.80	0.44
1:A:312:ARG:HA	1:A:312:ARG:HD2	1.86	0.44
1:A:288:ALA:O	1:A:299:GLN:HA	2.17	0.44
1:C:592:LEU:C	1:C:592:LEU:HD23	2.42	0.44
1:A:371:ARG:CZ	1:D:578:PRO:HD3	2.48	0.43
1:C:226:VAL:HG11	1:C:249[B]:PHE:CE1	2.53	0.43
1:D:84:ARG:NH1	1:D:280:GLU:OE1	2.51	0.43
1:D:559:ARG:HH21	1:D:559:ARG:CB	2.31	0.43
1:B:84:ARG:NH1	1:B:280:GLU:OE1	2.51	0.43
1:B:396:HIS:O	1:B:524:HIS:CE1	2.70	0.43
1:A:245:VAL:HG21	1:A:254:TRP:CD2	2.53	0.43
1:A:300:ASN:ND2	1:A:338:TYR:OH	2.47	0.43
1:A:446:THR:HG22	1:A:448:ASP:H	1.84	0.43
1:D:69:ALA:HB1	1:D:272:LEU:HB3	1.99	0.43
1:D:202:LYS:HE3	1:D:203:TYR:CZ	2.53	0.43
1:B:577:ASN:C	1:B:577:ASN:OD1	2.61	0.43
1:D:344:HIS:HB3	1:D:348[A]:LEU:HD13	2.00	0.43
1:A:84:ARG:HD2	1:A:90:TRP:CD1	2.54	0.43
1:B:194:LEU:O	1:B:198:ARG:HG3	2.19	0.42
1:D:70:HIS:CD2	3:D:884:HOH:O	2.72	0.42
1:D:622:ILE:HD11	1:D:643:TRP:CD2	2.54	0.42
1:D:4:THR:HA	1:D:5:PRO:HD3	1.84	0.42
1:D:132:PRO:HB2	1:D:144:GLY:HA3	2.00	0.42
1:B:371:ARG:NH1	1:B:411:VAL:O	2.52	0.42
1:D:215:LEU:HD12	1:D:215:LEU:HA	1.88	0.42
1:A:615:LEU:HD23	1:A:644:ILE:HG22	2.01	0.42
1:C:11:ARG:N	1:C:12:PRO:CD	2.82	0.42
1:C:474:HIS:HD2	1:C:546:ARG:NH2	2.18	0.42
1:B:556:ARG:HA	1:B:559:ARG:HD3	2.02	0.42
1:A:403:ILE:HD13	1:A:418:HIS:HD2	1.85	0.42
1:B:586:ARG:HA	1:B:591:ASN:HD22	1.83	0.42
1:C:84:ARG:CD	1:C:90:TRP:CE2	2.99	0.42
1:A:29:ASP:OD1	1:A:70:HIS:HE1	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:183:LEU:HD23	1:A:183:LEU:H	1.85	0.42
1:B:358:MET:HE3	1:B:358:MET:HB3	1.98	0.42
1:C:349:SER:HB2	3:C:811:HOH:O	2.19	0.42
1:D:315:ALA:HB1	1:D:322:VAL:CG2	2.50	0.42
1:D:559:ARG:HG3	1:D:559:ARG:NH2	2.33	0.41
1:A:63:LEU:HB3	1:A:64:PRO:HD3	2.02	0.41
1:B:155:GLU:CD	1:B:155:GLU:N	2.72	0.41
1:D:101:ALA:O	1:D:130:LEU:HA	2.20	0.41
1:D:145:TYR:HB3	2:D:701:TRS:O1	2.20	0.41
1:C:520:ASN:O	1:C:523:VAL:HG12	2.21	0.41
1:D:356:SER:O	1:D:360:GLN:HG2	2.21	0.41
1:A:208:HIS:HB2	1:A:246:TRP:HB2	2.02	0.41
1:A:436:ARG:NH2	1:A:466:GLU:OE1	2.53	0.41
1:B:365:LEU:HD13	1:B:598:PHE:CD2	2.55	0.41
1:C:349:SER:CB	3:C:811:HOH:O	2.68	0.41
1:C:499:GLY:HA3	1:C:504:LEU:HD12	2.03	0.41
1:C:610:LEU:O	1:C:615:LEU:HB2	2.21	0.41
1:C:52:TYR:HA	1:C:53:PRO:HD3	1.90	0.41
1:C:479:ARG:HD3	1:C:639:TYR:CZ	2.56	0.41
1:D:84:ARG:HD2	1:D:90:TRP:CD1	2.56	0.41
1:A:63:LEU:C	1:A:63:LEU:HD13	2.46	0.40
1:D:131:MET:HB3	1:D:132:PRO:HD2	2.04	0.40
1:B:604:TYR:CE1	1:B:635:ARG:HG3	2.56	0.40
1:A:431:PRO:O	1:A:432:ALA:HB3	2.22	0.40
1:A:365:LEU:HD13	1:A:598:PHE:CD2	2.57	0.40
1:A:520:ASN:C	1:A:520:ASN:ND2	2.77	0.40
1:B:101:ALA:O	1:B:130:LEU:HA	2.22	0.40
1:D:63:LEU:HB3	1:D:64:PRO:HD3	2.03	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	646/656 (98%)	628 (97%)	17 (3%)	1 (0%)	43	55
1	B	645/656 (98%)	629 (98%)	15 (2%)	1 (0%)	43	55
1	C	646/656 (98%)	627 (97%)	18 (3%)	1 (0%)	43	55
1	D	646/656 (98%)	616 (95%)	29 (4%)	1 (0%)	43	55
All	All	2583/2624 (98%)	2500 (97%)	79 (3%)	4 (0%)	43	55

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	139	ALA
1	B	139	ALA
1	C	139	ALA
1	D	139	ALA

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	537/548 (98%)	511 (95%)	26 (5%)	23	35
1	B	536/548 (98%)	493 (92%)	43 (8%)	11	15
1	C	537/548 (98%)	499 (93%)	38 (7%)	13	19
1	D	537/548 (98%)	493 (92%)	44 (8%)	10	14
All	All	2147/2192 (98%)	1996 (93%)	151 (7%)	13	19

All (151) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	10	LEU
1	A	11	ARG
1	A	18	LEU
1	A	22	GLN
1	A	25	LEU
1	A	41	LEU
1	A	49	THR

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Mol	Chain	Res	Type
1	A	111	ARG
1	A	127	TYR
1	A	155	GLU
1	A	173	ARG
1	A	215	LEU
1	A	245	VAL
1	A	322	VAL
1	A	355	ASN
1	A	365	LEU
1	A	380	PHE
1	A	410	ARG
1	A	446	THR
1	A	488	LEU
1	A	520	ASN
1	A	537	LYS
1	A	546	ARG
1	A	573	LEU
1	A	599	SER
1	A	601	GLU
1	B	6	LEU
1	B	11	ARG
1	B	15	GLU
1	B	20	LEU
1	B	25	LEU
1	B	31	GLU
1	B	41	LEU
1	B	67	THR
1	B	74	SER
1	B	84	ARG
1	B	121	GLU
1	B	155	GLU
1	B	169	LYS
1	B	194	LEU
1	B	214	THR
1	B	215	LEU
1	B	243	GLN
1	B	251	ARG
1	B	262	GLU
1	B	312	ARG
1	B	320	PRO
1	B	322	VAL
1	B	336	ILE

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Mol	Chain	Res	Type
1	B	348	LEU
1	B	365	LEU
1	B	380	PHE
1	B	403	ILE
1	B	410	ARG
1	B	429	ARG
1	B	487	VAL
1	B	488	LEU
1	B	511	LEU
1	B	520	ASN
1	B	531	GLU
1	B	552	ARG
1	B	559	ARG
1	B	560	THR
1	B	573	LEU
1	B	609	VAL
1	B	611	TRP
1	B	617	LEU
1	B	641	ARG
1	B	646	ASP
1	C	9	GLU
1	C	10	LEU
1	C	17	LEU
1	C	18	LEU
1	C	25	LEU
1	C	49	THR
1	C	56	GLU
1	C	59	LEU
1	C	111	ARG
1	C	122	GLU
1	C	126	ARG
1	C	127	TYR
1	C	155	GLU
1	C	245	VAL
1	C	251	ARG
1	C	262	GLU
1	C	316	ARG
1	C	336	ILE
1	C	355	ASN
1	C	356	SER
1	C	365	LEU
1	C	380	PHE

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Mol	Chain	Res	Type
1	C	386	ASN
1	C	473	LEU
1	C	487	VAL
1	C	488	LEU
1	C	511	LEU
1	C	512	GLU
1	C	520	ASN
1	C	531	GLU
1	C	552	ARG
1	C	556	ARG
1	C	573	LEU
1	C	615	LEU
1	C	617	LEU
1	C	625	GLN
1	C	626	LEU
1	C	641	ARG
1	D	4	THR
1	D	9	GLU
1	D	15	GLU
1	D	17	LEU
1	D	18	LEU
1	D	20	LEU
1	D	24	GLU
1	D	25	LEU
1	D	31	GLU
1	D	41	LEU
1	D	66	LEU
1	D	67	THR
1	D	111	ARG
1	D	127	TYR
1	D	173	ARG
1	D	194	LEU
1	D	214	THR
1	D	215	LEU
1	D	245	VAL
1	D	277	ARG
1	D	323	LEU
1	D	341	GLN
1	D	355	ASN
1	D	365	LEU
1	D	380	PHE
1	D	410	ARG

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Mol	Chain	Res	Type
1	D	416	GLU
1	D	446	THR
1	D	467	ARG
1	D	487	VAL
1	D	488	LEU
1	D	512	GLU
1	D	518	GLU
1	D	520	ASN
1	D	531	GLU
1	D	532	LYS
1	D	535	ARG
1	D	559	ARG
1	D	573	LEU
1	D	584	VAL
1	D	601	GLU
1	D	617	LEU
1	D	630	GLU
1	D	641	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (56) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	45	HIS
1	A	70	HIS
1	A	204	GLN
1	A	243	GLN
1	A	250	ASN
1	A	299	GLN
1	A	300	ASN
1	A	301	GLN
1	A	344	HIS
1	A	355	ASN
1	A	463	GLN
1	A	471	HIS
1	A	520	ASN
1	A	524	HIS
1	A	612	GLN
1	B	70	HIS
1	B	204	GLN
1	B	250	ASN
1	B	300	ASN
1	B	301	GLN

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Mol	Chain	Res	Type
1	B	344	HIS
1	B	463	GLN
1	B	520	ASN
1	B	524	HIS
1	B	591	ASN
1	B	612	GLN
1	C	22	GLN
1	C	204	GLN
1	C	243	GLN
1	C	250	ASN
1	C	299	GLN
1	C	301	GLN
1	C	337	HIS
1	C	344	HIS
1	C	355	ASN
1	C	386	ASN
1	C	463	GLN
1	C	474	HIS
1	C	520	ASN
1	C	524	HIS
1	C	549	HIS
1	D	70	HIS
1	D	188	GLN
1	D	204	GLN
1	D	243	GLN
1	D	250	ASN
1	D	299	GLN
1	D	301	GLN
1	D	344	HIS
1	D	355	ASN
1	D	474	HIS
1	D	520	ASN
1	D	524	HIS
1	D	549	HIS
1	D	612	GLN
1	D	632	HIS

5.3.3 RNA

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

4 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	TRS	C	701	-	7,7,7	0.15	0	9,9,9	0.38	0
2	TRS	B	701	-	7,7,7	0.19	0	9,9,9	0.59	0
2	TRS	A	701	-	7,7,7	0.24	0	9,9,9	1.01	1 (11%)
2	TRS	D	701	-	7,7,7	0.19	0	9,9,9	0.67	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	TRS	C	701	-	-	0/9/9/9	-
2	TRS	B	701	-	-	6/9/9/9	-
2	TRS	A	701	-	-	9/9/9/9	-
2	TRS	D	701	-	-	4/9/9/9	-

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
2	A	701	TRS	C1-C-N	2.13	113.61	108.17

There are no chirality outliers.

All (19) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	701	TRS	C2-C-C1-O1
2	A	701	TRS	C3-C-C1-O1
2	D	701	TRS	C3-C-C2-O2
2	A	701	TRS	C3-C-C2-O2
2	A	701	TRS	N-C-C2-O2
2	A	701	TRS	C2-C-C3-O3
2	B	701	TRS	C3-C-C2-O2
2	B	701	TRS	N-C-C2-O2
2	B	701	TRS	C1-C-C3-O3
2	D	701	TRS	N-C-C2-O2
2	A	701	TRS	C1-C-C2-O2
2	B	701	TRS	C1-C-C2-O2
2	B	701	TRS	C2-C-C3-O3
2	D	701	TRS	C1-C-C2-O2
2	A	701	TRS	N-C-C1-O1
2	B	701	TRS	N-C-C3-O3
2	D	701	TRS	C3-C-C1-O1
2	A	701	TRS	C1-C-C3-O3
2	A	701	TRS	N-C-C3-O3

There are no ring outliers.

1 monomer is involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	D	701	TRS	3	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	646/656 (98%)	-0.29	6 (0%) 81 82	11, 28, 49, 79	2 (0%)
1	B	646/656 (98%)	-0.19	11 (1%) 69 70	12, 30, 50, 78	1 (0%)
1	C	646/656 (98%)	-0.25	9 (1%) 73 75	11, 29, 49, 68	2 (0%)
1	D	646/656 (98%)	-0.01	16 (2%) 58 60	13, 34, 58, 79	2 (0%)
All	All	2584/2624 (98%)	-0.19	42 (1%) 70 72	11, 30, 52, 79	7 (0%)

All (42) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	611	TRP	6.8
1	D	139	ALA	6.1
1	B	611	TRP	5.3
1	C	139	ALA	5.0
1	C	611	TRP	4.6
1	D	611	TRP	4.4
1	C	537	LYS	4.2
1	A	139	ALA	4.0
1	B	139	ALA	3.9
1	D	194	LEU	3.6
1	B	537	LYS	3.3
1	D	205	ARG	3.1
1	D	155	GLU	3.0
1	C	552	ARG	3.0
1	D	277	ARG	3.0
1	D	1	MET	2.8
1	D	111	ARG	2.7
1	D	11	ARG	2.7
1	B	198	ARG	2.6
1	D	53	PRO	2.6
1	D	20	LEU	2.6

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Mol	Chain	Res	Type	RSRZ
1	C	429	ARG	2.6
1	B	1	MET	2.5
1	A	429	ARG	2.5
1	C	26	SER	2.5
1	D	245	VAL	2.4
1	D	221	LYS	2.4
1	B	155	GLU	2.4
1	A	556	ARG	2.3
1	C	115	GLU	2.3
1	D	201	ALA	2.3
1	B	74	SER	2.3
1	D	239	GLU	2.2
1	A	630	GLU	2.2
1	B	49	THR	2.2
1	B	429	ARG	2.1
1	C	27	GLY	2.1
1	C	546	ARG	2.1
1	A	625	GLN	2.1
1	B	251	ARG	2.1
1	B	631	HIS	2.1
1	D	169	LYS	2.0

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

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

6.3 Carbohydrates [i](#)

There are no 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
2	TRS	A	701	8/8	0.93	0.10	24,28,33,36	0
2	TRS	D	701	8/8	0.93	0.10	32,35,39,43	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
2	TRS	C	701	8/8	0.96	0.07	25,27,27,29	0
2	TRS	B	701	8/8	0.97	0.06	22,24,25,25	0

6.5 Other polymers [i](#)

There are no such residues in this entry.