



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 12:20 PM UTC

PDB ID : 7LPO / pdb_00007lpo
Title : Crystal structure of Cryptococcus neoformans sterylglucosidase 1 with tris
Authors : Pereira de Sa, N.; Del Poeta, M.; Airola, M.V.
Deposited on : 2021-02-12
Resolution : 2.13 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

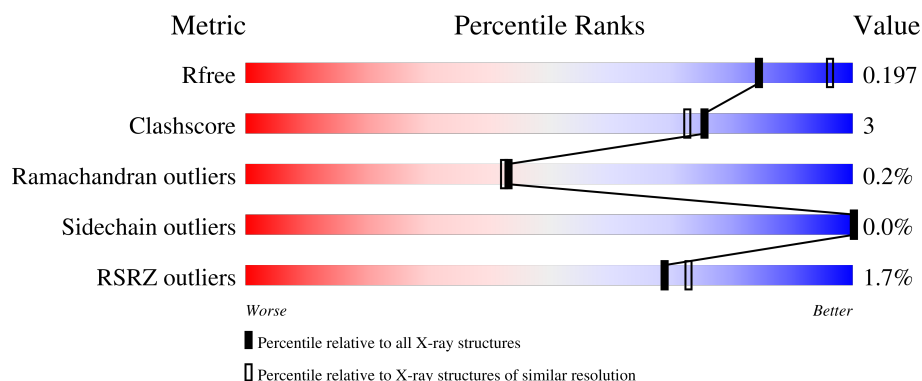
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.13 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	3689 (2.16-2.12)
Clashscore	190562	3812 (2.16-2.12)
Ramachandran outliers	187476	3773 (2.16-2.12)
Sidechain outliers	187428	3772 (2.16-2.12)
RSRZ outliers	180081	3691 (2.16-2.12)

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	797	2% 86% 5% 9%
1	B	797	% 88% 5% 8%
1	C	797	% 82% 9% 9%
1	D	797	2% 84% 7% 9%

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	B	901	-	X	-	-

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 47454 atoms, of which 22138 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 Cytoplasmic protein.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	724	Total	C	H	N	O	S	0	2	0
			11267	3689	5507	988	1060	23			
1	B	735	Total	C	H	N	O	S	0	2	0
			11427	3742	5584	999	1079	23			
1	C	723	Total	C	H	N	O	S	0	1	0
			11210	3672	5474	978	1062	24			
1	D	726	Total	C	H	N	O	S	0	2	0
			11298	3699	5525	987	1064	23			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	0	SER	-	expression tag	UNP J9W473
B	0	SER	-	expression tag	UNP J9W473
C	0	SER	-	expression tag	UNP J9W473
D	0	SER	-	expression tag	UNP J9W473

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



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	H	N	O	0	0
			20	4	12	1	3		
2	B	1	Total	C	H	N	O	0	0
			20	4	12	1	3		
2	C	1	Total	C	H	N	O	0	0
			20	4	12	1	3		
2	D	1	Total	C	H	N	O	0	0
			20	4	12	1	3		

- Molecule 3 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	B	1	Total	Mg	0	0
			1	1		

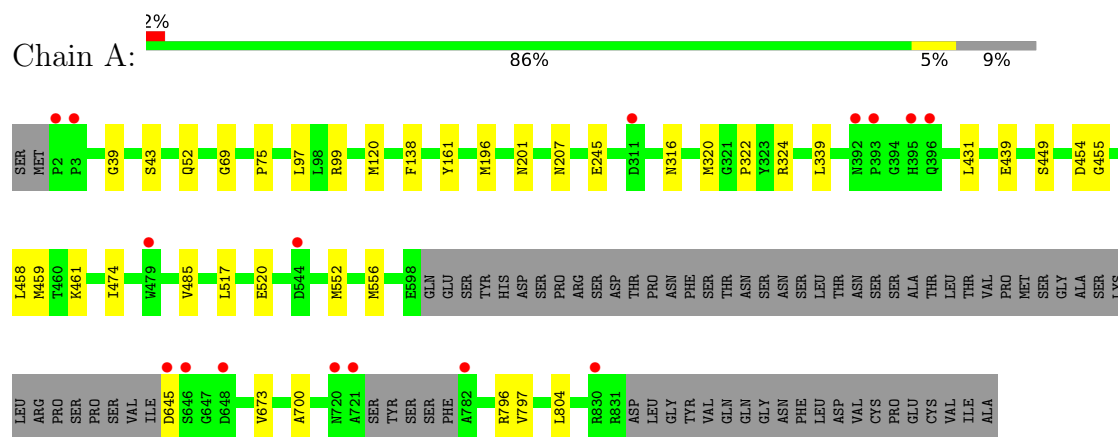
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	628	Total	O	0	0
			628	628		
4	B	611	Total	O	0	0
			611	611		
4	C	521	Total	O	0	0
			521	521		
4	D	411	Total	O	0	0
			411	411		

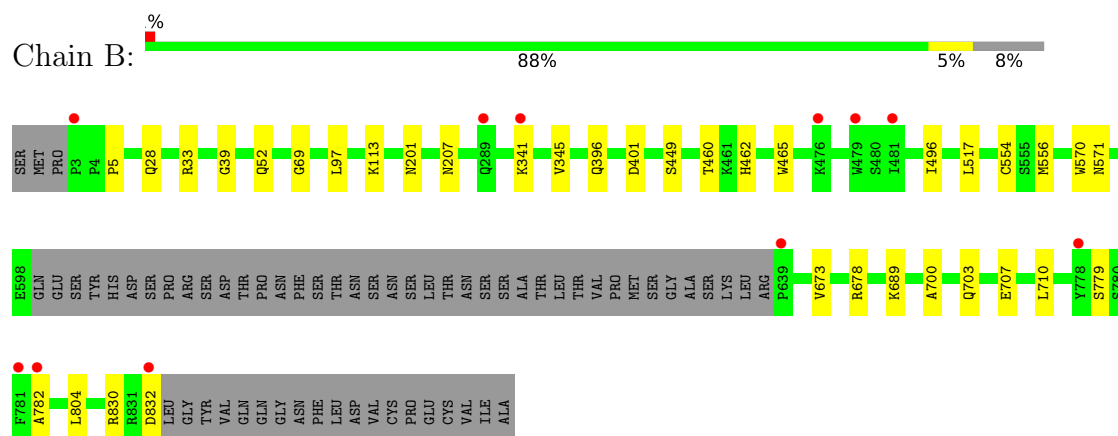
3 Residue-property plots [i](#)

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.

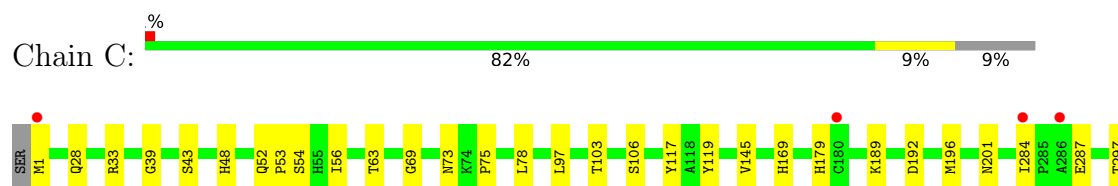
• Molecule 1: Cytoplasmic protein

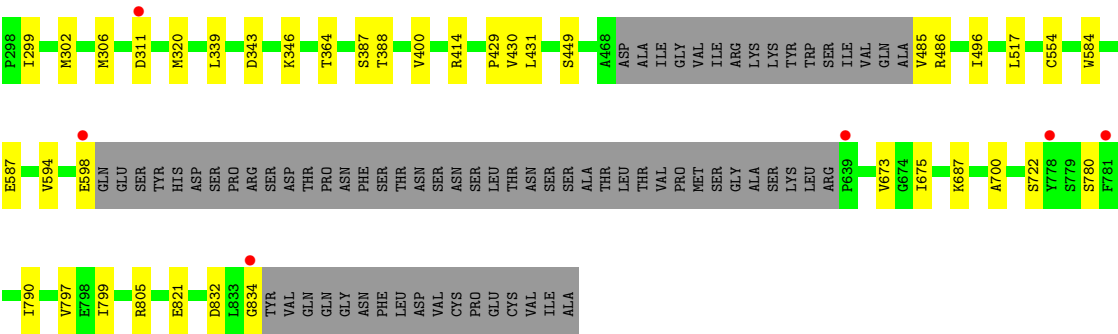


• Molecule 1: Cytoplasmic protein

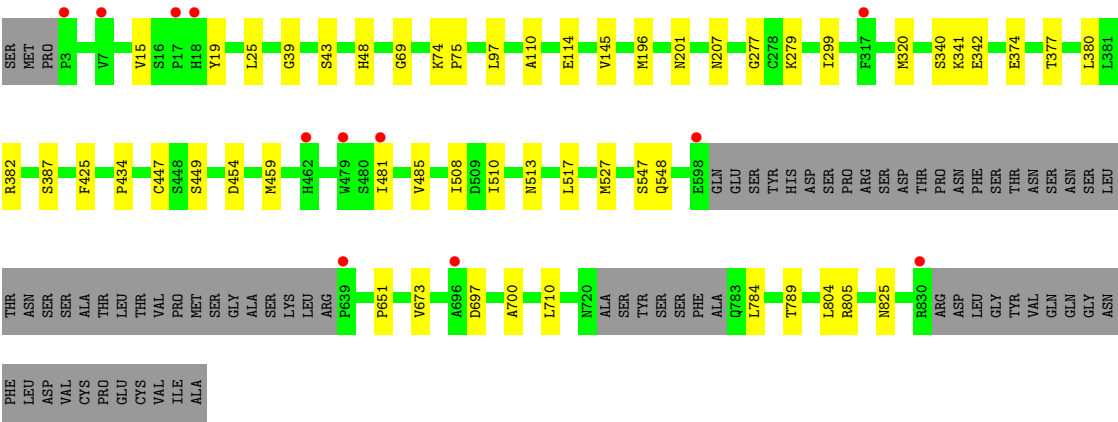
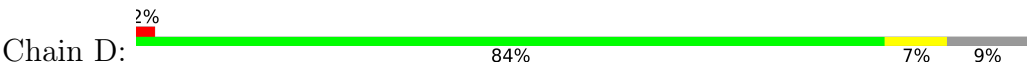


• Molecule 1: Cytoplasmic protein





● Molecule 1: Cytoplasmic protein



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	98.60Å 126.61Å 126.66Å 90.00° 95.46° 90.00°	Depositor
Resolution (Å)	47.28 – 2.13 47.28 – 2.13	Depositor EDS
% Data completeness (in resolution range)	96.5 (47.28-2.13) 96.4 (47.28-2.13)	Depositor EDS
R_{merge}	0.11	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.81 (at 2.14Å)	Xtriage
Refinement program	PHENIX 1.17.1-3660	Depositor
R, R_{free}	0.157 , 0.198 0.157 , 0.197	Depositor DCC
R_{free} test set	8287 reflections (4.66%)	wwPDB-VP
Wilson B-factor (Å ²)	22.9	Xtriage
Anisotropy	0.579	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.40 , 45.3	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	0.96	EDS
Total number of atoms	47454	wwPDB-VP
Average B, all atoms (Å ²)	30.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 7.04% 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, MG

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.29	0/5959	0.45	0/8124
1	B	0.27	0/6046	0.44	0/8244
1	C	0.28	0/5922	0.45	0/8075
1	D	0.25	0/5973	0.42	0/8144
All	All	0.27	0/23900	0.44	0/32587

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [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	5760	5507	5496	23	0
1	B	5843	5584	5572	30	1
1	C	5736	5474	5475	44	0
1	D	5773	5525	5511	39	1
2	A	8	12	12	1	0
2	B	8	12	12	0	0
2	C	8	12	12	0	0
2	D	8	12	12	0	0
3	B	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	A	628	0	0	5	2
4	B	611	0	0	9	1
4	C	521	0	0	8	2
4	D	411	0	0	4	1
All	All	25316	22138	22102	135	4

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 3.

All (135) 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:D:342:GLU:OE2	4:D:1001:HOH:O	1.79	0.98
1:D:341:LYS:NZ	4:D:1002:HOH:O	1.96	0.97
1:B:396:GLN:NE2	4:B:1001:HOH:O	1.99	0.93
1:C:311:ASP:OD1	4:C:1001:HOH:O	1.87	0.92
1:A:324:ARG:NH1	4:A:1001:HOH:O	2.09	0.85
1:B:689:LYS:NZ	4:B:1002:HOH:O	2.13	0.81
1:A:320:MET:HE1	1:A:485:VAL:HG21	1.66	0.77
1:C:722:SER:O	1:C:780:SER:OG	2.05	0.75
1:D:341:LYS:H	1:D:341:LYS:HE2	1.53	0.74
1:C:790:ILE:HD11	1:C:799:ILE:HD11	1.70	0.74
1:B:341:LYS:NZ	1:B:345:VAL:HG23	2.04	0.72
1:C:103:THR:O	1:C:106:SER:OG	2.09	0.70
1:C:1:MET:HE2	1:C:675:ILE:HD12	1.76	0.68
1:B:460:THR:O	1:B:462[B]:HIS:ND1	2.27	0.67
1:D:651:PRO:HG3	1:D:784:LEU:HD21	1.77	0.66
1:B:832:ASP:OD2	4:B:1003:HOH:O	2.14	0.66
1:C:169:HIS:NE2	4:C:1005:HOH:O	2.28	0.65
1:D:196:MET:HE2	1:D:459:MET:HE1	1.80	0.64
1:D:320:MET:HE1	1:D:485:VAL:HG21	1.78	0.64
1:B:707:GLU:OE1	4:B:1004:HOH:O	2.16	0.63
1:C:1:MET:HE2	1:C:675:ILE:CD1	2.28	0.63
1:A:120:MET:HE1	1:A:245:GLU:HB3	1.83	0.60
1:C:299:ILE:HA	1:C:302:MET:HE3	1.84	0.59
1:D:340:SER:HB2	4:D:1002:HOH:O	2.03	0.59
1:A:797:VAL:HB	1:A:804:LEU:HD11	1.84	0.59
1:D:277:GLY:O	1:D:279:LYS:HD3	2.03	0.58
1:D:341:LYS:H	1:D:341:LYS:CE	2.16	0.57
1:A:520:GLU:OE1	2:A:901:TRS:N	2.36	0.57
1:D:382:ARG:HH11	1:D:382:ARG:HG2	1.70	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:25:LEU:HD21	1:D:508:ILE:HD13	1.85	0.56
1:C:346:LYS:NZ	4:C:1014:HOH:O	2.38	0.56
1:A:196:MET:HE2	1:A:458:LEU:HG	1.88	0.55
1:B:341:LYS:HZ2	1:B:345:VAL:HG23	1.71	0.55
1:C:486:ARG:NH1	4:C:1009:HOH:O	2.34	0.54
1:D:145:VAL:HG11	1:D:201:ASN:HB2	1.88	0.54
1:C:306:MET:HE1	1:C:364:THR:HA	1.90	0.54
1:D:481:ILE:H	1:D:481:ILE:HD12	1.73	0.53
1:B:52:GLN:HG3	4:B:1007:HOH:O	2.08	0.53
1:D:196:MET:CE	1:D:459:MET:HE1	2.39	0.53
1:D:374:GLU:HG2	1:D:377:THR:HG22	1.91	0.53
1:A:431:LEU:HD22	1:A:474:ILE:HD13	1.91	0.53
1:C:189:LYS:HE2	1:C:192:ASP:OD2	2.09	0.52
1:A:552:MET:CE	1:A:556:MET:HE3	2.39	0.52
1:D:299:ILE:HD13	1:D:380:LEU:HD13	1.92	0.51
1:C:196:MET:HE1	1:C:587:GLU:OE2	2.11	0.51
1:C:449:SER:HA	1:C:517:LEU:O	2.11	0.51
1:B:678:ARG:HD3	4:B:1002:HOH:O	2.11	0.51
1:C:496:ILE:HD12	1:C:554:CYS:SG	2.51	0.50
1:D:110:ALA:HB3	1:D:114:GLU:HB3	1.93	0.50
1:B:449:SER:HA	1:B:517:LEU:O	2.11	0.50
1:D:43:SER:HB3	1:D:75:PRO:HB3	1.94	0.50
1:D:201:ASN:O	1:D:207:ASN:HB2	2.11	0.50
1:B:710:LEU:HD11	1:B:804:LEU:HD12	1.95	0.49
1:B:556:MET:HA	1:B:556:MET:HE2	1.95	0.49
1:C:594:VAL:HG22	4:C:1067:HOH:O	2.13	0.49
1:C:52[B]:GLN:HE22	1:C:63:THR:HG21	1.76	0.48
1:B:341:LYS:HZ1	1:B:345:VAL:HG23	1.75	0.48
1:C:287:GLU:H	1:C:287:GLU:CD	2.21	0.48
1:A:161:TYR:HD1	1:A:339:LEU:HD11	1.78	0.48
1:A:439:GLU:OE1	4:A:1002:HOH:O	2.19	0.48
1:A:449:SER:HA	1:A:517:LEU:O	2.13	0.48
1:B:517:LEU:C	1:B:517:LEU:HD23	2.39	0.48
1:D:697:ASP:OD1	1:D:697:ASP:N	2.46	0.48
1:D:804:LEU:C	1:D:804:LEU:HD23	2.39	0.48
1:C:673:VAL:HG11	1:C:700:ALA:HB2	1.96	0.47
1:D:517:LEU:C	1:D:517:LEU:HD23	2.39	0.47
1:B:341:LYS:C	1:B:341:LYS:HD3	2.39	0.47
1:D:710:LEU:HD11	1:D:804:LEU:HD12	1.95	0.47
1:D:341:LYS:CE	4:D:1001:HOH:O	2.61	0.47
1:B:201:ASN:O	1:B:207:ASN:HB2	2.15	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:796:ARG:NH1	4:A:1008:HOH:O	2.38	0.47
1:C:485:VAL:N	4:C:1030:HOH:O	2.48	0.47
1:D:39:GLY:HA3	1:D:97:LEU:O	2.16	0.46
1:C:387:SER:OG	1:C:388:THR:HG23	2.15	0.46
1:D:434:PRO:O	1:D:510:ILE:HG21	2.15	0.46
1:C:106:SER:HB2	1:C:119:TYR:CE2	2.51	0.46
1:B:28:GLN:HA	1:B:33:ARG:O	2.16	0.45
1:B:401:ASP:OD2	4:B:1005:HOH:O	2.21	0.45
1:D:508:ILE:HD11	1:D:513:ASN:OD1	2.16	0.45
1:D:449:SER:HA	1:D:517:LEU:O	2.14	0.45
1:D:481:ILE:HD12	1:D:481:ILE:N	2.31	0.45
1:B:5:PRO:HG3	4:B:1421:HOH:O	2.17	0.45
1:B:804:LEU:C	1:B:804:LEU:HD23	2.41	0.45
1:D:527:MET:HE2	1:D:548:GLN:HG3	1.99	0.45
1:A:120:MET:HE1	1:A:245:GLU:CB	2.46	0.45
1:C:832:ASP:OD1	1:C:834:GLY:N	2.50	0.45
1:B:570:TRP:CD2	1:B:571:ASN:HB3	2.52	0.45
1:C:43:SER:HB3	1:C:75:PRO:HB3	1.98	0.44
1:C:145:VAL:HG11	1:C:201:ASN:HB2	1.99	0.44
1:C:414:ARG:NH1	4:C:1025:HOH:O	2.46	0.44
1:C:790:ILE:HD11	1:C:799:ILE:CD1	2.43	0.44
1:A:43:SER:HB3	1:A:75:PRO:HB3	1.97	0.44
1:D:341:LYS:H	1:D:341:LYS:CD	2.31	0.44
1:D:527:MET:HE1	1:D:547:SER:HB3	2.00	0.44
1:C:339:LEU:HD22	1:C:343:ASP:HB3	2.00	0.44
1:A:39:GLY:HA3	1:A:97:LEU:O	2.18	0.44
1:C:598:GLU:HA	1:C:598:GLU:OE2	2.18	0.44
1:C:52[B]:GLN:HE22	1:C:63:THR:CG2	2.31	0.43
1:C:54:SER:HB3	1:C:584:TRP:HA	2.00	0.43
1:C:400:VAL:HG22	1:C:429:PRO:HG2	2.00	0.43
1:C:73:ASN:ND2	1:C:78:LEU:H	2.17	0.43
1:B:673:VAL:HG11	1:B:700:ALA:HB2	1.99	0.43
1:A:517:LEU:C	1:A:517:LEU:HD23	2.44	0.42
1:C:39:GLY:HA3	1:C:97:LEU:O	2.19	0.42
1:A:201:ASN:O	1:A:207:ASN:HB2	2.20	0.42
1:A:461:LYS:HE2	4:A:1253:HOH:O	2.19	0.42
1:B:345:VAL:HG13	1:C:117:TYR:CD2	2.55	0.42
1:C:797:VAL:HA	1:C:805:ARG:O	2.20	0.42
1:C:430:VAL:HG12	1:C:431:LEU:HG	2.01	0.42
1:D:425:PHE:HA	1:D:447:CYS:O	2.19	0.42
1:B:39:GLY:HA3	1:B:97:LEU:O	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:113:LYS:NZ	4:B:1041:HOH:O	2.53	0.41
1:A:52:GLN:NE2	4:A:1020:HOH:O	2.46	0.41
1:A:455:GLY:O	1:A:459:MET:HG2	2.20	0.41
1:B:570:TRP:HA	1:B:571:ASN:HB3	2.02	0.41
1:B:830:ARG:HA	1:B:830:ARG:HD3	1.95	0.41
1:A:673:VAL:HG11	1:A:700:ALA:HB2	2.02	0.41
1:D:15:VAL:HB	1:D:19:TYR:CG	2.55	0.41
1:C:48:HIS:HE1	4:C:1097:HOH:O	2.03	0.41
1:C:284:ILE:HG12	1:C:297:THR:HG22	2.01	0.41
1:C:320:MET:HE3	1:C:320:MET:HA	2.02	0.41
1:B:779:SER:HA	1:B:782:ALA:O	2.20	0.41
1:C:53:PRO:HG2	1:C:56:ILE:HD12	2.03	0.41
1:A:316:ASN:O	1:A:322:PRO:HA	2.21	0.41
1:C:28:GLN:HA	1:C:33:ARG:O	2.20	0.41
1:C:687:LYS:HE2	1:C:821:GLU:HB3	2.02	0.41
1:C:54:SER:HG	1:C:179:HIS:CE1	2.38	0.41
1:D:48:HIS:O	1:D:74:LYS:NZ	2.50	0.41
1:A:99:ARG:HD2	1:A:138:PHE:CZ	2.56	0.40
1:D:673:VAL:HG11	1:D:700:ALA:HB2	2.02	0.40
1:D:789:THR:OG1	1:D:825:ASN:OD1	2.36	0.40
1:D:279:LYS:HA	1:D:387:SER:OG	2.21	0.40
1:B:465:TRP:CD1	1:B:465:TRP:H	2.40	0.40
1:B:496:ILE:HD12	1:B:554:CYS:SG	2.61	0.40
1:D:804:LEU:HD23	1:D:805:ARG:N	2.36	0.40

All (4) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:C:1489:HOH:O	4:D:1410:HOH:O[2_544]	1.95	0.25
1:B:703:GLN:OE1	4:A:1610:HOH:O[2_555]	2.07	0.13
4:A:1624:HOH:O	4:C:1311:HOH:O[2_544]	2.12	0.08
1:D:114:GLU:OE2	4:B:1581:HOH:O[1_554]	2.15	0.05

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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	720/797 (90%)	697 (97%)	21 (3%)	2 (0%)	36	33
1	B	733/797 (92%)	709 (97%)	23 (3%)	1 (0%)	48	49
1	C	718/797 (90%)	691 (96%)	26 (4%)	1 (0%)	48	49
1	D	722/797 (91%)	696 (96%)	24 (3%)	2 (0%)	36	33
All	All	2893/3188 (91%)	2793 (96%)	94 (3%)	6 (0%)	43	42

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	454	ASP
1	A	454	ASP
1	D	69	GLY
1	C	69	GLY
1	A	69	GLY
1	B	69	GLY

5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	605/670 (90%)	604 (100%)	1 (0%)	87	91
1	B	616/670 (92%)	616 (100%)	0	100	100
1	C	605/670 (90%)	605 (100%)	0	100	100
1	D	609/670 (91%)	609 (100%)	0	100	100
All	All	2435/2680 (91%)	2434 (100%)	1 (0%)	100	100

All (1) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	645	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (18) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	50	ASN
1	A	204	HIS
1	A	328	GLN
1	A	549	GLN
1	B	28	GLN
1	B	51	ASN
1	B	497	GLN
1	B	583	ASN
1	C	18	HIS
1	C	26	HIS
1	C	48	HIS
1	C	73	ASN
1	C	369	HIS
1	C	505	GLN
1	C	513	ASN
1	C	549	GLN
1	D	13	ASN
1	D	823	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 5 ligands modelled in this entry, 1 is monoatomic - leaving 4 for Mogul analysis.

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	901	-	7,7,7	1.78	1 (14%)	9,9,9	2.53	4 (44%)
2	TRS	A	901	-	7,7,7	1.82	1 (14%)	9,9,9	2.48	5 (55%)
2	TRS	D	901	-	7,7,7	1.83	1 (14%)	9,9,9	2.34	5 (55%)
2	TRS	B	901	-	7,7,7	1.79	1 (14%)	9,9,9	2.42	4 (44%)

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	901	-	-	4/9/9/9	-
2	TRS	A	901	-	-	1/9/9/9	-
2	TRS	D	901	-	-	0/9/9/9	-
2	TRS	B	901	-	-	5/9/9/9	-

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	901	TRS	C-N	4.12	1.62	1.49
2	C	901	TRS	C-N	4.07	1.62	1.49
2	A	901	TRS	C-N	4.06	1.62	1.49
2	B	901	TRS	C-N	4.00	1.62	1.49

All (18) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	901	TRS	C2-C-N	5.38	121.89	108.17
2	A	901	TRS	C3-C-N	5.08	121.13	108.17
2	B	901	TRS	C2-C-N	5.08	121.13	108.17
2	D	901	TRS	C3-C-N	4.38	119.34	108.17
2	B	901	TRS	C2-C-C1	-3.49	101.36	110.66
2	C	901	TRS	C2-C-C1	-3.46	101.43	110.66

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	901	TRS	C3-C-C1	-3.25	102.01	110.66
2	D	901	TRS	C3-C-C1	-3.09	102.43	110.66
2	D	901	TRS	C2-C-N	2.86	115.47	108.17
2	A	901	TRS	C2-C-N	2.43	114.38	108.17
2	C	901	TRS	C3-C-C1	-2.29	104.56	110.66
2	D	901	TRS	C2-C-C1	-2.23	104.72	110.66
2	A	901	TRS	C2-C-C1	-2.22	104.73	110.66
2	C	901	TRS	C1-C-N	2.17	113.71	108.17
2	B	901	TRS	C3-C-C1	-2.16	104.89	110.66
2	B	901	TRS	O3-C3-C	2.15	116.86	110.88
2	A	901	TRS	C3-C-C2	-2.10	105.06	110.66
2	D	901	TRS	C3-C-C2	-2.06	105.18	110.66

There are no chirality outliers.

All (10) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	B	901	TRS	N-C-C3-O3
2	C	901	TRS	N-C-C1-O1
2	B	901	TRS	C2-C-C1-O1
2	B	901	TRS	C3-C-C1-O1
2	B	901	TRS	C1-C-C3-O3
2	C	901	TRS	C3-C-C1-O1
2	B	901	TRS	N-C-C1-O1
2	C	901	TRS	C1-C-C2-O2
2	A	901	TRS	C2-C-C3-O3
2	C	901	TRS	N-C-C2-O2

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	901	TRS	1	0

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

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	724/797 (90%)	-0.42	16 (2%) 62 66	12, 24, 50, 115	1 (0%)
1	B	735/797 (92%)	-0.42	11 (1%) 72 76	13, 24, 51, 106	1 (0%)
1	C	723/797 (90%)	-0.32	10 (1%) 73 77	16, 27, 53, 102	1 (0%)
1	D	726/797 (91%)	-0.14	12 (1%) 69 73	13, 34, 57, 112	1 (0%)
All	All	2908/3188 (91%)	-0.33	49 (1%) 69 73	12, 27, 54, 115	4 (0%)

All (49) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	544	ASP	7.2
1	D	639	PRO	5.4
1	B	781	PHE	4.6
1	B	3	PRO	4.3
1	D	479	TRP	4.3
1	C	639	PRO	4.0
1	B	778	TYR	3.9
1	A	2	PRO	3.8
1	C	781	PHE	3.7
1	B	639	PRO	3.7
1	A	782	ALA	3.7
1	A	395	HIS	3.3
1	B	289	GLN	3.3
1	D	17	PRO	3.3
1	A	645	ASP	3.2
1	A	721	ALA	3.2
1	A	3	PRO	3.1
1	C	311	ASP	3.1
1	B	479	TRP	3.0
1	A	479	TRP	3.0
1	C	1	MET	2.8

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Mol	Chain	Res	Type	RSRZ
1	D	3	PRO	2.6
1	B	481	ILE	2.6
1	C	834	GLY	2.6
1	A	648	ASP	2.6
1	A	646	SER	2.6
1	D	317	PHE	2.6
1	C	284	ILE	2.6
1	D	462[A]	HIS	2.5
1	B	476	LYS	2.5
1	C	180	CYS	2.4
1	C	286	ALA	2.4
1	A	830	ARG	2.3
1	C	598	GLU	2.3
1	D	598	GLU	2.2
1	D	830	ARG	2.2
1	D	481	ILE	2.2
1	A	311	ASP	2.2
1	B	832	ASP	2.2
1	C	778	TYR	2.1
1	A	393	PRO	2.1
1	B	782	ALA	2.1
1	D	696	ALA	2.1
1	B	341	LYS	2.0
1	D	7	VAL	2.0
1	A	392	ASN	2.0
1	A	720	ASN	2.0
1	A	396	GLN	2.0
1	D	18	HIS	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	D	901	8/8	0.88	0.09	30,36,40,40	0
2	TRS	B	901	8/8	0.90	0.10	25,31,37,40	0
2	TRS	C	901	8/8	0.90	0.10	30,36,43,44	0
2	TRS	A	901	8/8	0.90	0.09	23,28,33,35	0
3	MG	B	902	1/1	0.96	0.04	24,24,24,24	0

6.5 Other polymers [i](#)

There are no such residues in this entry.