



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 01:59 AM UTC

PDB ID : 4FJ6 / pdb_00004fj6
Title : Crystal structure of a glycoside hydrolase family 33, candidate sialidase (BDI_2946) from Parabacteroides distasonis ATCC 8503 at 1.90 Å resolution
Authors : Joint Center for Structural Genomics (JCSG)
Deposited on : 2012-06-11
Resolution : 1.90 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

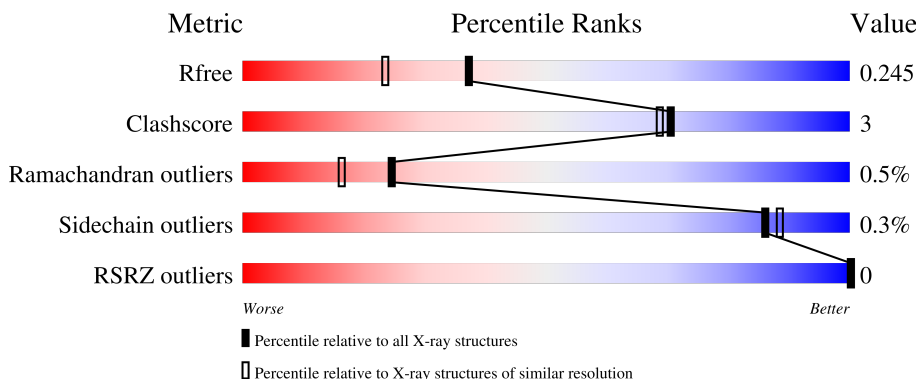
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

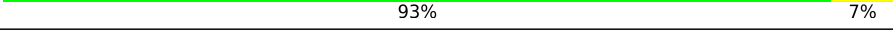
The reported resolution of this entry is 1.90 Å.

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	7789 (1.90-1.90)
Clashscore	190562	8410 (1.90-1.90)
Ramachandran outliers	187476	8333 (1.90-1.90)
Sidechain outliers	187428	8333 (1.90-1.90)
RSRZ outliers	180081	7790 (1.90-1.90)

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	523	
1	B	523	
1	C	523	
1	D	523	

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 18571 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 glycoside hydrolase family 33, candidate sialidase.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	519	Total	C	N	O	S	Se	0	13	0
			4107	2593	711	783	2	18			
1	B	520	Total	C	N	O	S	Se	0	8	0
			4091	2573	710	787	2	19			
1	C	519	Total	C	N	O	S	Se	0	9	0
			4078	2572	707	779	2	18			
1	D	521	Total	C	N	O	S	Se	0	10	0
			4100	2585	710	785	2	18			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	0	GLY	-	expression tag	UNP A6LG40
B	0	GLY	-	expression tag	UNP A6LG40
C	0	GLY	-	expression tag	UNP A6LG40
D	0	GLY	-	expression tag	UNP A6LG40

- Molecule 2 is GLYCEROL (CCD ID: GOL) (formula: C₃H₈O₃).



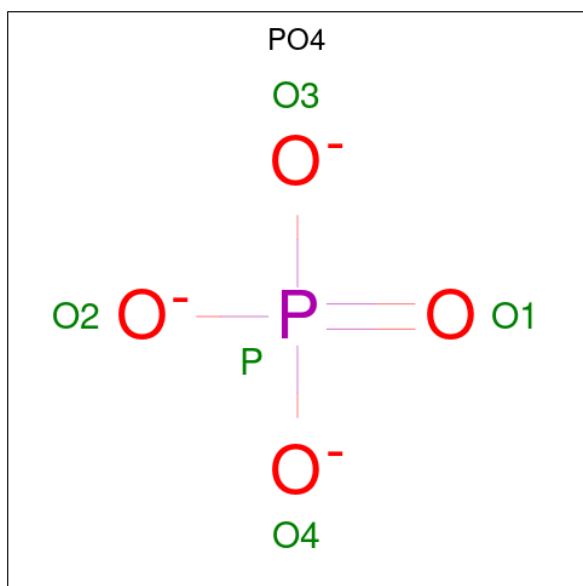
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	C	O	0	0
			6	3	3		
2	A	1	Total	C	O	0	0
			6	3	3		
2	A	1	Total	C	O	0	0
			6	3	3		
2	A	1	Total	C	O	0	0
			6	3	3		
2	B	1	Total	C	O	0	0
			6	3	3		
2	B	1	Total	C	O	0	0
			6	3	3		
2	B	1	Total	C	O	0	1
			12	6	6		
2	C	1	Total	C	O	0	0
			6	3	3		
2	C	1	Total	C	O	0	0
			6	3	3		
2	C	1	Total	C	O	0	0
			6	3	3		
2	D	1	Total	C	O	0	0
			6	3	3		
2	D	1	Total	C	O	0	0
			6	3	3		
2	D	1	Total	C	O	0	0
			6	3	3		
2	D	1	Total	C	O	0	0
			6	3	3		

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

- Molecule 3 is PHOSPHATE ION (CCD ID: PO4) (formula: O₄P).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	O	P	0	0
			5	4	1		
3	A	1	Total	O	P	0	0
			5	4	1		
3	A	1	Total	O	P	0	0
			5	4	1		
3	A	1	Total	O	P	0	0
			5	4	1		
3	A	1	Total	O	P	0	0
			5	4	1		
3	B	1	Total	O	P	0	0
			5	4	1		
3	B	1	Total	O	P	0	0
			5	4	1		
3	B	1	Total	O	P	0	0
			5	4	1		
3	C	1	Total	O	P	0	0
			5	4	1		
3	C	1	Total	O	P	0	0
			5	4	1		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	C	1	Total	O	P	0	0
			5	4	1		
3	C	1	Total	O	P	0	0
			5	4	1		
3	C	1	Total	O	P	0	0
			5	4	1		
3	D	1	Total	O	P	0	0
			5	4	1		
3	D	1	Total	O	P	0	0
			5	4	1		
3	D	1	Total	O	P	0	0
			5	4	1		
3	D	1	Total	O	P	0	0
			5	4	1		

- Molecule 4 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	B	2	Total	Cl	0	0
			2	2		
4	D	1	Total	Cl	0	0
			1	1		

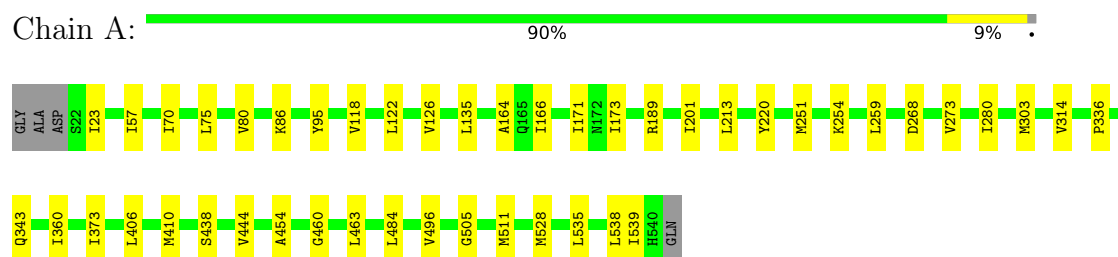
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	500	Total	O	0	4
			504	504		
5	B	475	Total	O	0	3
			478	478		
5	C	496	Total	O	0	1
			497	497		
5	D	529	Total	O	0	3
			532	532		

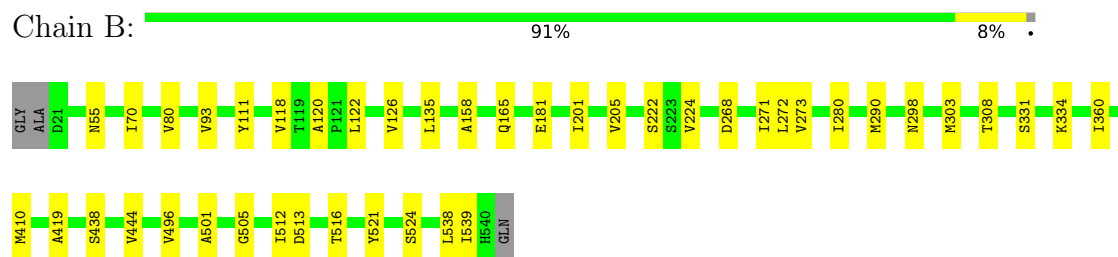
3 Residue-property plots

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

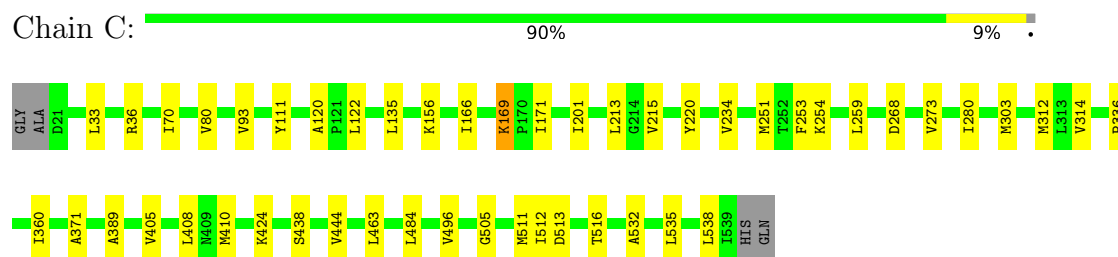
- Molecule 1: glycoside hydrolase family 33, candidate sialidase



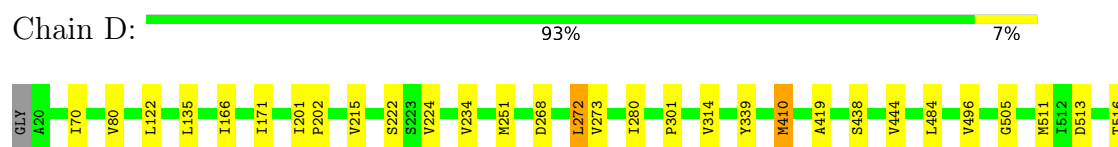
- Molecule 1: glycoside hydrolase family 33, candidate sialidase



- Molecule 1: glycoside hydrolase family 33, candidate sialidase



- Molecule 1: glycoside hydrolase family 33, candidate sialidase



W528
K534
L535
L538
I539
H540
GLN

4 Data and refinement statistics

Property	Value	Source
Space group	H 3	Depositor
Cell constants a, b, c, α , β , γ	171.74Å 171.74Å 243.79Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	29.77 – 1.90 29.77 – 1.90	Depositor EDS
% Data completeness (in resolution range)	99.1 (29.77-1.90) 99.1 (29.77-1.90)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.07 (at 1.91Å)	Xtriage
Refinement program	REFMAC 5.6.0117	Depositor
R, R_{free}	0.207 , 0.243 0.212 , 0.245	Depositor DCC
R_{free} test set	10525 reflections (4.98%)	wwPDB-VP
Wilson B-factor (Å ²)	19.6	Xtriage
Anisotropy	0.164	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.40 , 36.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.45$, $\langle L^2 \rangle = 0.27$	Xtriage
Estimated twinning fraction	0.048 for h,-h-k,-l	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	18571	wwPDB-VP
Average B, all atoms (Å ²)	27.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 45.13 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 1.3813e-04.*

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: CL, PO4, GOL

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	0.52	0/4213	0.79	4/5692 (0.1%)
1	B	0.52	0/4184	0.78	2/5657 (0.0%)
1	C	0.53	0/4173	0.80	2/5643 (0.0%)
1	D	0.52	0/4198	0.80	2/5677 (0.0%)
All	All	0.52	0/16768	0.79	10/22669 (0.0%)

There are no bond length outliers.

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	505	GLY	N-CA-C	6.33	122.61	115.08
1	A	505	GLY	N-CA-C	6.04	122.27	115.08
1	B	505	GLY	N-CA-C	5.61	121.37	114.69
1	A	220	TYR	N-CA-C	5.60	117.38	111.28
1	D	505	GLY	N-CA-C	5.57	121.71	115.08
1	A	410	MSE	N-CA-C	5.32	118.06	109.40
1	C	220	TYR	N-CA-C	5.21	116.96	111.28
1	A	95	TYR	N-CA-C	5.17	117.00	111.36
1	D	410	MSE	N-CA-C	5.11	117.73	109.40
1	B	521	TYR	N-CA-C	5.00	116.68	109.07

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	4107	0	4126	28	0
1	B	4091	0	4062	25	0
1	C	4078	0	4069	35	0
1	D	4100	0	4099	27	0
2	A	24	0	32	0	0
2	B	24	0	32	0	0
2	C	18	0	24	0	0
2	D	30	0	40	0	0
3	A	25	0	0	0	0
3	B	15	0	0	0	0
3	C	25	0	0	0	0
3	D	20	0	0	0	0
4	B	2	0	0	0	0
4	D	1	0	0	0	0
5	A	504	0	0	0	0
5	B	478	0	0	0	0
5	C	497	0	0	0	0
5	D	532	0	0	1	0
All	All	18571	0	16484	112	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 3.

All (112) 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:C:371:ALA:HB3	1:C:410[B]:MSE:HE2	1.13	1.08
1:D:528[B]:MSE:CE	1:D:528[B]:MSE:HA	1.99	0.93
1:C:215[B]:VAL:HG12	1:C:234:VAL:HG22	1.47	0.92
1:C:371:ALA:HB3	1:C:410[B]:MSE:CE	2.02	0.87
1:C:273:VAL:HG22	1:C:280[A]:ILE:HD12	1.57	0.87
1:C:371:ALA:CB	1:C:410[B]:MSE:HE2	2.05	0.82
1:D:528[B]:MSE:HA	1:D:528[B]:MSE:HE3	1.60	0.81
1:C:213:LEU:HD11	1:C:280[B]:ILE:HD13	1.65	0.79
1:A:213:LEU:HD11	1:A:280[B]:ILE:HD13	1.65	0.78
1:C:166:ILE:HD12	1:C:171:ILE:HD12	1.65	0.77
1:C:389:ALA:HB3	1:C:410[B]:MSE:HE1	1.66	0.77
1:B:303[A]:MSE:HE1	1:B:334:LYS:O	1.85	0.77
1:C:389:ALA:HB3	1:C:410[B]:MSE:CE	2.17	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:512:ILE:HB	1:B:516[B]:THR:HG23	1.72	0.71
1:D:202:PRO:HB3	1:D:528[B]:MSE:HE1	1.74	0.70
1:C:408:LEU:HD23	1:C:410[B]:MSE:HE3	1.76	0.68
1:A:80:VAL:HG11	1:A:135:LEU:HB2	1.77	0.67
1:D:511:MSE:HE1	1:D:535[B]:LEU:HD11	1.76	0.67
1:A:213:LEU:CD1	1:A:280[B]:ILE:HD13	2.26	0.66
1:B:70:ILE:HG21	1:B:122:LEU:HD22	1.78	0.65
1:D:215[B]:VAL:HG12	1:D:234:VAL:HG22	1.80	0.64
1:A:496:VAL:HG23	1:A:538:LEU:HD23	1.80	0.64
1:C:496:VAL:HG23	1:C:538:LEU:HD23	1.79	0.64
1:B:512:ILE:HD12	1:B:516[A]:THR:HG22	1.81	0.63
1:B:273:VAL:HG22	1:B:280:ILE:HD12	1.79	0.63
1:A:273:VAL:HG22	1:A:280[A]:ILE:HD12	1.80	0.62
1:C:213:LEU:CD1	1:C:280[B]:ILE:HD13	2.30	0.62
1:B:201:ILE:HG21	1:B:268:ASP:HA	1.82	0.62
1:D:528[B]:MSE:HA	1:D:528[B]:MSE:HE2	1.80	0.61
1:D:496:VAL:HG23	1:D:538:LEU:HD23	1.84	0.60
1:B:513:ASP:OD1	1:B:516[B]:THR:HG22	2.02	0.59
1:A:201:ILE:HG21	1:A:268:ASP:HA	1.84	0.59
1:C:80:VAL:HG11	1:C:135:LEU:HB2	1.85	0.58
1:D:70:ILE:HG21	1:D:122:LEU:HD22	1.87	0.57
1:B:118:VAL:HG21	1:B:126:VAL:HG13	1.85	0.57
1:A:463:LEU:HD23	1:A:484:LEU:HD23	1.86	0.57
1:C:303:MSE:HE1	1:C:336:PRO:CD	2.36	0.56
1:A:70:ILE:HG21	1:A:122:LEU:HD22	1.88	0.55
1:C:408:LEU:CD2	1:C:410[B]:MSE:HE3	2.38	0.54
1:D:80:VAL:HG11	1:D:135:LEU:HB2	1.89	0.54
1:B:158:ALA:HB2	1:B:181[B]:GLU:HG2	1.88	0.54
1:D:410:MSE:HE3	1:D:419:ALA:CB	2.38	0.53
1:B:55:ASN:HD21	1:B:165[B]:GLN:NE2	2.07	0.53
1:C:201:ILE:HG21	1:C:268:ASP:HA	1.91	0.53
1:C:70:ILE:HG21	1:C:122:LEU:HD22	1.91	0.52
1:C:93:VAL:HG21	1:C:111:TYR:CG	2.45	0.52
1:C:251:MSE:HE2	1:C:314:VAL:HG22	1.92	0.51
1:A:360:ILE:HD12	1:A:360:ILE:C	2.36	0.51
1:C:463:LEU:HD23	1:C:484:LEU:HD23	1.93	0.50
1:D:201:ILE:HG21	1:D:268:ASP:HA	1.93	0.50
1:B:80:VAL:HG11	1:B:135:LEU:HB2	1.93	0.50
1:A:511:MSE:HE1	1:A:535[B]:LEU:HD11	1.93	0.49
1:B:303[A]:MSE:HE3	1:B:331:SER:HA	1.93	0.49
1:A:303[A]:MSE:HE1	1:A:336:PRO:HD3	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:273[A]:VAL:HG22	1:D:280:ILE:HD12	1.94	0.49
1:C:253:PHE:CE1	1:C:312:MSE:HE2	2.49	0.48
1:C:303:MSE:HE1	1:C:336:PRO:CG	2.44	0.48
1:B:70:ILE:CG2	1:B:122:LEU:HD22	2.43	0.47
1:D:166:ILE:HD12	1:D:171:ILE:HD12	1.97	0.47
1:C:120:ALA:HA	1:C:122:LEU:HD12	1.97	0.46
1:C:360:ILE:C	1:C:360:ILE:HD12	2.40	0.46
1:A:118:VAL:HG21	1:A:126:VAL:CG1	2.45	0.46
1:D:166:ILE:HB	1:D:171:ILE:HD11	1.97	0.46
1:C:303:MSE:HE1	1:C:336:PRO:HD3	1.97	0.46
1:B:512:ILE:HD12	1:B:516[A]:THR:CG2	2.47	0.45
1:B:360:ILE:C	1:B:360:ILE:HD12	2.42	0.45
1:D:511:MSE:CE	1:D:535[B]:LEU:HD11	2.45	0.44
1:A:251:MSE:HE2	1:A:314:VAL:HG22	1.98	0.44
1:D:410:MSE:HE3	1:D:419:ALA:HB3	1.99	0.44
1:D:251:MSE:HE2	1:D:314:VAL:HG22	2.00	0.44
1:A:189:ARG:HB2	1:A:528:MSE:HB2	2.00	0.44
1:B:501:ALA:HB3	1:B:524:SER:CB	2.48	0.44
1:C:511:MSE:HE3	1:C:513:ASP:O	2.18	0.43
1:C:259:LEU:HD11	1:D:135:LEU:HD11	2.00	0.43
1:A:166:ILE:HD12	1:A:171:ILE:HD13	2.01	0.43
1:A:303[A]:MSE:HE1	1:A:336:PRO:CD	2.47	0.43
1:D:540:HIS:N	5:D:914:HOH:O	2.50	0.43
1:D:70:ILE:CG2	1:D:122:LEU:HD22	2.48	0.43
1:C:33:LEU:HD12	1:C:36:ARG:HD2	2.00	0.43
1:B:222:SER:OG	1:B:224:VAL:HG22	2.18	0.43
1:D:484:LEU:HD21	1:D:539:ILE:HD13	2.00	0.43
1:B:496:VAL:HG23	1:B:538:LEU:HD23	2.00	0.43
1:D:516[B]:THR:HG22	1:D:534:LYS:HA	2.01	0.42
1:C:169[B]:LYS:HB3	1:C:169[B]:LYS:HE2	1.71	0.42
1:A:539:ILE:HD12	1:A:539:ILE:N	2.34	0.42
1:D:301:PRO:HD3	1:D:339:TYR:CD2	2.54	0.42
1:B:539:ILE:HD12	1:B:539:ILE:N	2.34	0.42
1:D:511:MSE:HE3	1:D:513:ASP:O	2.20	0.42
1:A:57:ILE:HD11	1:A:75:LEU:HD13	2.00	0.42
1:A:118:VAL:HG21	1:A:126:VAL:HG13	2.02	0.42
1:B:120:ALA:HA	1:B:122:LEU:HD12	2.00	0.42
1:D:272:LEU:C	1:D:272:LEU:HD12	2.44	0.42
1:A:511:MSE:CE	1:A:535[B]:LEU:HD11	2.50	0.41
1:C:512:ILE:HD12	1:C:516:THR:HG22	2.02	0.41
1:A:23:ILE:HD11	1:A:166:ILE:HD11	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:164:ALA:HB2	1:A:173:ILE:HD11	2.03	0.41
1:A:373[A]:ILE:HD12	1:A:406:LEU:HD13	2.01	0.41
1:B:205:VAL:HG13	1:B:271:ILE:HG23	2.02	0.41
1:C:511:MSE:HE1	1:C:535:LEU:HD11	2.01	0.41
1:C:516:THR:HG21	1:C:532:ALA:HB1	2.01	0.41
1:D:222:SER:OG	1:D:224[A]:VAL:HG22	2.20	0.41
1:A:343:GLN:H	1:A:343:GLN:CD	2.29	0.41
1:B:93:VAL:HG21	1:B:111:TYR:CG	2.55	0.41
1:B:290[B]:MSE:HE3	1:B:298:ASN:C	2.46	0.41
1:B:410:MSE:HE3	1:B:419:ALA:C	2.46	0.41
1:C:405:VAL:HG22	1:C:424:LYS:HG2	2.03	0.41
1:C:259:LEU:HD11	1:D:135:LEU:CD1	2.50	0.41
1:A:273:VAL:HG22	1:A:280[A]:ILE:CD1	2.49	0.40
1:A:454:ALA:HB1	1:A:460:GLY:O	2.21	0.40
1:A:86[A]:LYS:HE2	1:A:86[A]:LYS:HB3	1.86	0.40
1:C:389:ALA:HB3	1:C:410[B]:MSE:HE3	2.01	0.40
1:A:259:LEU:HD11	1:B:135:LEU:CD1	2.51	0.40

There are no symmetry-related clashes.

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	530/523 (101%)	510 (96%)	17 (3%)	3 (1%)	21	13
1	B	526/523 (101%)	502 (95%)	22 (4%)	2 (0%)	30	22
1	C	526/523 (101%)	507 (96%)	16 (3%)	3 (1%)	21	13
1	D	529/523 (101%)	511 (97%)	16 (3%)	2 (0%)	30	22
All	All	2111/2092 (101%)	2030 (96%)	71 (3%)	10 (0%)	24	16

All (10) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	438	SER
1	C	254	LYS
1	C	438	SER
1	A	254	LYS
1	A	438	SER
1	A	444	VAL
1	B	438	SER
1	C	444	VAL
1	D	444	VAL
1	B	444	VAL

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	458/433 (106%)	458 (100%)	0	100	100
1	B	454/433 (105%)	452 (100%)	2 (0%)	84	87
1	C	451/433 (104%)	448 (99%)	3 (1%)	76	78
1	D	456/433 (105%)	455 (100%)	1 (0%)	87	90
All	All	1819/1732 (105%)	1813 (100%)	6 (0%)	86	88

All (6) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	272	LEU
1	B	308	THR
1	C	156	LYS
1	C	169[A]	LYS
1	C	169[B]	LYS
1	D	272	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (7) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	165	GLN

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Mol	Chain	Res	Type
1	A	441	GLN
1	B	49	GLN
1	C	352	GLN
1	D	71	GLN
1	D	221	ASN
1	D	255	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 36 ligands modelled in this entry, 3 are monoatomic - leaving 33 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	GOL	C	603	-	5,5,5	0.34	0	5,5,5	0.42	0
2	GOL	B	605[A]	-	5,5,5	0.27	0	5,5,5	0.36	0
2	GOL	D	606	-	5,5,5	0.36	0	5,5,5	0.10	0
2	GOL	A	601	-	5,5,5	0.44	0	5,5,5	0.67	0
3	PO4	A	607	-	4,4,4	0.88	0	6,6,6	0.93	0
2	GOL	D	603	-	5,5,5	0.37	0	5,5,5	0.48	0
2	GOL	B	603	-	5,5,5	0.20	0	5,5,5	0.26	0
3	PO4	A	609	-	4,4,4	0.99	0	6,6,6	0.47	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	PO4	C	608	-	4,4,4	0.96	0	6,6,6	0.44	0
3	PO4	D	607	-	4,4,4	0.89	0	6,6,6	0.56	0
2	GOL	C	601	-	5,5,5	0.35	0	5,5,5	0.18	0
3	PO4	C	607	-	4,4,4	0.92	0	6,6,6	0.51	0
2	GOL	B	604	-	5,5,5	0.42	0	5,5,5	0.45	0
3	PO4	B	606	-	4,4,4	0.84	0	6,6,6	0.39	0
3	PO4	A	605	-	4,4,4	0.97	0	6,6,6	0.44	0
3	PO4	A	606	-	4,4,4	0.98	0	6,6,6	0.34	0
3	PO4	D	609	-	4,4,4	1.16	0	6,6,6	0.56	0
2	GOL	A	602	-	5,5,5	0.37	0	5,5,5	0.30	0
3	PO4	B	608	-	4,4,4	0.94	0	6,6,6	0.51	0
2	GOL	C	602	-	5,5,5	0.37	0	5,5,5	0.66	0
2	GOL	B	605[B]	-	5,5,5	0.24	0	5,5,5	0.31	0
3	PO4	A	608	-	4,4,4	0.95	0	6,6,6	0.49	0
2	GOL	D	604	-	5,5,5	0.29	0	5,5,5	0.65	0
3	PO4	C	606	-	4,4,4	0.93	0	6,6,6	0.66	0
3	PO4	D	608	-	4,4,4	1.07	0	6,6,6	0.48	0
2	GOL	A	604	-	5,5,5	0.36	0	5,5,5	0.48	0
2	GOL	A	603	-	5,5,5	0.23	0	5,5,5	0.37	0
3	PO4	D	610	-	4,4,4	0.88	0	6,6,6	0.50	0
3	PO4	C	604	-	4,4,4	0.84	0	6,6,6	0.74	0
2	GOL	D	605	-	5,5,5	0.20	0	5,5,5	0.61	0
3	PO4	B	607	-	4,4,4	1.12	0	6,6,6	0.64	0
3	PO4	C	605	-	4,4,4	0.97	0	6,6,6	0.79	0
2	GOL	D	602	-	5,5,5	0.27	0	5,5,5	0.25	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	GOL	C	603	-	-	1/4/4/4	-
2	GOL	A	601	-	-	4/4/4/4	-
2	GOL	A	602	-	-	2/4/4/4	-
2	GOL	D	603	-	-	0/4/4/4	-
2	GOL	B	603	-	-	2/4/4/4	-
2	GOL	B	605[B]	-	-	0/4/4/4	-
2	GOL	C	602	-	-	2/4/4/4	-
2	GOL	D	602	-	-	0/4/4/4	-
2	GOL	A	603	-	-	0/4/4/4	-
2	GOL	D	605	-	-	2/4/4/4	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	GOL	D	604	-	-	0/4/4/4	-
2	GOL	D	606	-	-	2/4/4/4	-
2	GOL	C	601	-	-	2/4/4/4	-
2	GOL	B	605[A]	-	-	0/4/4/4	-
2	GOL	B	604	-	-	2/4/4/4	-
2	GOL	A	604	-	-	1/4/4/4	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (20) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	601	GOL	O1-C1-C2-C3
2	B	603	GOL	C1-C2-C3-O3
2	B	604	GOL	C1-C2-C3-O3
2	C	601	GOL	O1-C1-C2-C3
2	C	602	GOL	O1-C1-C2-C3
2	D	605	GOL	O1-C1-C2-O2
2	D	605	GOL	O1-C1-C2-C3
2	D	606	GOL	O1-C1-C2-C3
2	A	601	GOL	O1-C1-C2-O2
2	C	601	GOL	O1-C1-C2-O2
2	A	601	GOL	C1-C2-C3-O3
2	A	602	GOL	C1-C2-C3-O3
2	C	602	GOL	O1-C1-C2-O2
2	D	606	GOL	O1-C1-C2-O2
2	A	601	GOL	O2-C2-C3-O3
2	A	602	GOL	O2-C2-C3-O3
2	B	604	GOL	O2-C2-C3-O3
2	B	603	GOL	O2-C2-C3-O3
2	C	603	GOL	O1-C1-C2-O2
2	A	604	GOL	C1-C2-C3-O3

There are no ring outliers.

No monomer is involved in short contacts.

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 [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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	502/523 (95%)	-1.36	0 100 100	12, 24, 37, 57	12 (2%)
1	B	503/523 (96%)	-1.31	0 100 100	15, 25, 39, 69	6 (1%)
1	C	502/523 (95%)	-1.32	0 100 100	14, 26, 41, 61	8 (1%)
1	D	504/523 (96%)	-1.35	0 100 100	11, 23, 36, 64	9 (1%)
All	All	2011/2092 (96%)	-1.33	0 100 100	11, 24, 38, 69	35 (1%)

There are no RSRZ outliers to report.

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
3	PO4	A	608	5/5	0.98	0.05	77,81,85,85	0
3	PO4	C	607	5/5	0.98	0.07	70,72,77,78	0
3	PO4	C	608	5/5	0.98	0.04	61,62,73,74	0
3	PO4	D	610	5/5	0.98	0.04	53,53,58,61	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	GOL	B	604	6/6	0.99	0.04	35,38,39,43	0
2	GOL	B	605[A]	6/6	0.99	0.03	25,27,30,30	6
2	GOL	B	605[B]	6/6	0.99	0.03	51,53,54,55	6
2	GOL	C	601	6/6	0.99	0.04	27,35,38,44	0
2	GOL	C	602	6/6	0.99	0.03	23,28,31,33	0
2	GOL	C	603	6/6	0.99	0.04	31,35,40,47	0
2	GOL	D	602	6/6	0.99	0.04	21,21,24,28	0
2	GOL	D	603	6/6	0.99	0.03	26,29,29,30	0
2	GOL	D	604	6/6	0.99	0.04	38,39,41,46	0
2	GOL	D	605	6/6	0.99	0.05	19,29,34,36	0
2	GOL	D	606	6/6	0.99	0.04	30,36,38,48	0
3	PO4	A	605	5/5	0.99	0.04	37,50,57,59	0
3	PO4	A	606	5/5	0.99	0.03	30,32,35,37	0
3	PO4	A	607	5/5	0.99	0.04	24,26,36,40	0
2	GOL	A	601	6/6	0.99	0.05	32,37,40,42	0
3	PO4	A	609	5/5	0.99	0.03	61,63,71,77	0
3	PO4	B	606	5/5	0.99	0.05	27,32,38,45	0
3	PO4	B	608	5/5	0.99	0.04	55,55,62,64	0
3	PO4	C	604	5/5	0.99	0.04	37,40,46,50	0
3	PO4	C	606	5/5	0.99	0.04	30,31,32,32	0
2	GOL	A	602	6/6	0.99	0.03	31,34,37,38	0
2	GOL	A	603	6/6	0.99	0.04	29,31,31,33	0
3	PO4	D	607	5/5	0.99	0.03	46,46,50,54	0
3	PO4	D	609	5/5	0.99	0.04	20,23,27,32	0
2	GOL	A	604	6/6	0.99	0.04	26,41,44,45	0
4	CL	B	601	1/1	0.99	0.05	66,66,66,66	0
4	CL	B	602	1/1	0.99	0.05	50,50,50,50	0
4	CL	D	601	1/1	0.99	0.06	49,49,49,49	0
3	PO4	C	605	5/5	1.00	0.03	28,31,36,38	0
2	GOL	B	603	6/6	1.00	0.03	33,41,44,48	0
3	PO4	D	608	5/5	1.00	0.03	30,31,34,36	0
3	PO4	B	607	5/5	1.00	0.04	31,32,39,42	0

6.5 Other polymers ⓘ

There are no such residues in this entry.