



Full wwPDB X-ray Structure Validation Report ⓘ

Oct 6, 2026 – 04:09 PM JST

PDB ID : 44WZ / pdb_000044wz
Title : Crystal structure of pyrophosphate-dependent phosphofructokinase from *Promethearchaeum syntrophicum*
Authors : Compton, J.A.; Yosaatmadja, Y.; Bashiri, G.; Patrick, W.M.
Deposited on : 2026-08-16
Resolution : 2.20 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 Phenix2.2
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	2.2
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.015 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.51

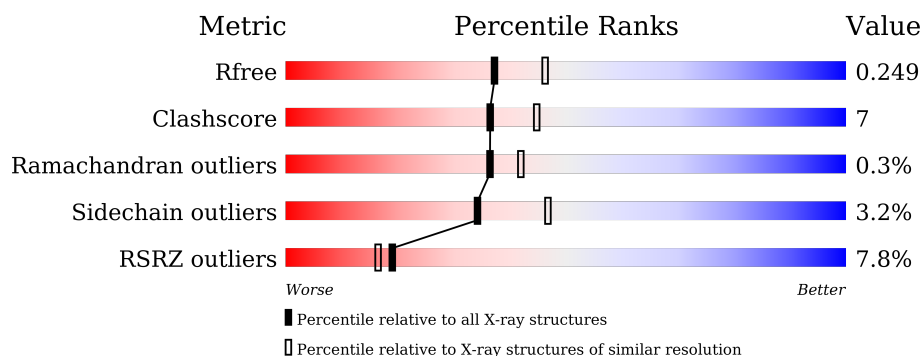
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.20 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	6164 (2.20-2.20)
Clashscore	190562	6851 (2.20-2.20)
Ramachandran outliers	187476	6768 (2.20-2.20)
Sidechain outliers	187428	6769 (2.20-2.20)
RSRZ outliers	180081	6166 (2.20-2.20)

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	424	4% 81% 11% • 6%
1	B	424	11% 83% 11% • 5%
1	C	424	6% 81% 11% • 7%
1	D	424	8% 77% 13% • 7%

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 crite-

ria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	GOL	D	502	-	-	X	-

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 12333 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 6-phosphofructokinase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	399	Total	C	N	O	S	0	4	0
			3080	1956	521	590	13			
1	B	401	Total	C	N	O	S	0	1	0
			3075	1951	520	591	13			
1	C	394	Total	C	N	O	S	0	3	0
			3022	1919	511	578	14			
1	D	393	Total	C	N	O	S	0	3	0
			3029	1920	513	583	13			

There are 80 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-19	MET	-	initiating methionine	UNP A0A5B9D762
A	-18	GLY	-	expression tag	UNP A0A5B9D762
A	-17	SER	-	expression tag	UNP A0A5B9D762
A	-16	SER	-	expression tag	UNP A0A5B9D762
A	-15	HIS	-	expression tag	UNP A0A5B9D762
A	-14	HIS	-	expression tag	UNP A0A5B9D762
A	-13	HIS	-	expression tag	UNP A0A5B9D762
A	-12	HIS	-	expression tag	UNP A0A5B9D762
A	-11	HIS	-	expression tag	UNP A0A5B9D762
A	-10	HIS	-	expression tag	UNP A0A5B9D762
A	-9	SER	-	expression tag	UNP A0A5B9D762
A	-8	SER	-	expression tag	UNP A0A5B9D762
A	-7	GLY	-	expression tag	UNP A0A5B9D762
A	-6	LEU	-	expression tag	UNP A0A5B9D762
A	-5	VAL	-	expression tag	UNP A0A5B9D762
A	-4	PRO	-	expression tag	UNP A0A5B9D762
A	-3	ARG	-	expression tag	UNP A0A5B9D762
A	-2	GLY	-	expression tag	UNP A0A5B9D762
A	-1	SER	-	expression tag	UNP A0A5B9D762
A	0	HIS	-	expression tag	UNP A0A5B9D762
B	-19	MET	-	initiating methionine	UNP A0A5B9D762

Continued on next page...

Continued from previous page...

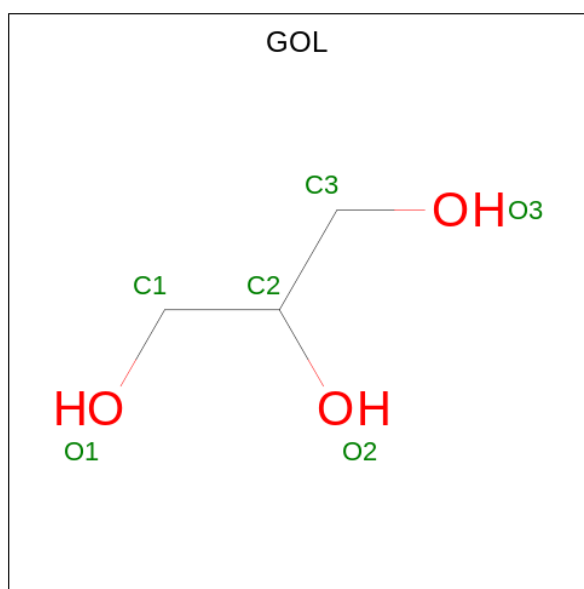
Chain	Residue	Modelled	Actual	Comment	Reference
B	-18	GLY	-	expression tag	UNP A0A5B9D762
B	-17	SER	-	expression tag	UNP A0A5B9D762
B	-16	SER	-	expression tag	UNP A0A5B9D762
B	-15	HIS	-	expression tag	UNP A0A5B9D762
B	-14	HIS	-	expression tag	UNP A0A5B9D762
B	-13	HIS	-	expression tag	UNP A0A5B9D762
B	-12	HIS	-	expression tag	UNP A0A5B9D762
B	-11	HIS	-	expression tag	UNP A0A5B9D762
B	-10	HIS	-	expression tag	UNP A0A5B9D762
B	-9	SER	-	expression tag	UNP A0A5B9D762
B	-8	SER	-	expression tag	UNP A0A5B9D762
B	-7	GLY	-	expression tag	UNP A0A5B9D762
B	-6	LEU	-	expression tag	UNP A0A5B9D762
B	-5	VAL	-	expression tag	UNP A0A5B9D762
B	-4	PRO	-	expression tag	UNP A0A5B9D762
B	-3	ARG	-	expression tag	UNP A0A5B9D762
B	-2	GLY	-	expression tag	UNP A0A5B9D762
B	-1	SER	-	expression tag	UNP A0A5B9D762
B	0	HIS	-	expression tag	UNP A0A5B9D762
C	-19	MET	-	initiating methionine	UNP A0A5B9D762
C	-18	GLY	-	expression tag	UNP A0A5B9D762
C	-17	SER	-	expression tag	UNP A0A5B9D762
C	-16	SER	-	expression tag	UNP A0A5B9D762
C	-15	HIS	-	expression tag	UNP A0A5B9D762
C	-14	HIS	-	expression tag	UNP A0A5B9D762
C	-13	HIS	-	expression tag	UNP A0A5B9D762
C	-12	HIS	-	expression tag	UNP A0A5B9D762
C	-11	HIS	-	expression tag	UNP A0A5B9D762
C	-10	HIS	-	expression tag	UNP A0A5B9D762
C	-9	SER	-	expression tag	UNP A0A5B9D762
C	-8	SER	-	expression tag	UNP A0A5B9D762
C	-7	GLY	-	expression tag	UNP A0A5B9D762
C	-6	LEU	-	expression tag	UNP A0A5B9D762
C	-5	VAL	-	expression tag	UNP A0A5B9D762
C	-4	PRO	-	expression tag	UNP A0A5B9D762
C	-3	ARG	-	expression tag	UNP A0A5B9D762
C	-2	GLY	-	expression tag	UNP A0A5B9D762
C	-1	SER	-	expression tag	UNP A0A5B9D762
C	0	HIS	-	expression tag	UNP A0A5B9D762
D	-19	MET	-	initiating methionine	UNP A0A5B9D762
D	-18	GLY	-	expression tag	UNP A0A5B9D762
D	-17	SER	-	expression tag	UNP A0A5B9D762

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
D	-16	SER	-	expression tag	UNP A0A5B9D762
D	-15	HIS	-	expression tag	UNP A0A5B9D762
D	-14	HIS	-	expression tag	UNP A0A5B9D762
D	-13	HIS	-	expression tag	UNP A0A5B9D762
D	-12	HIS	-	expression tag	UNP A0A5B9D762
D	-11	HIS	-	expression tag	UNP A0A5B9D762
D	-10	HIS	-	expression tag	UNP A0A5B9D762
D	-9	SER	-	expression tag	UNP A0A5B9D762
D	-8	SER	-	expression tag	UNP A0A5B9D762
D	-7	GLY	-	expression tag	UNP A0A5B9D762
D	-6	LEU	-	expression tag	UNP A0A5B9D762
D	-5	VAL	-	expression tag	UNP A0A5B9D762
D	-4	PRO	-	expression tag	UNP A0A5B9D762
D	-3	ARG	-	expression tag	UNP A0A5B9D762
D	-2	GLY	-	expression tag	UNP A0A5B9D762
D	-1	SER	-	expression tag	UNP A0A5B9D762
D	0	HIS	-	expression tag	UNP A0A5B9D762

- Molecule 2 is GLYCEROL (CCD ID: GOL) (formula: $C_3H_8O_3$).



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

Continued on next page...

Continued from previous page...

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

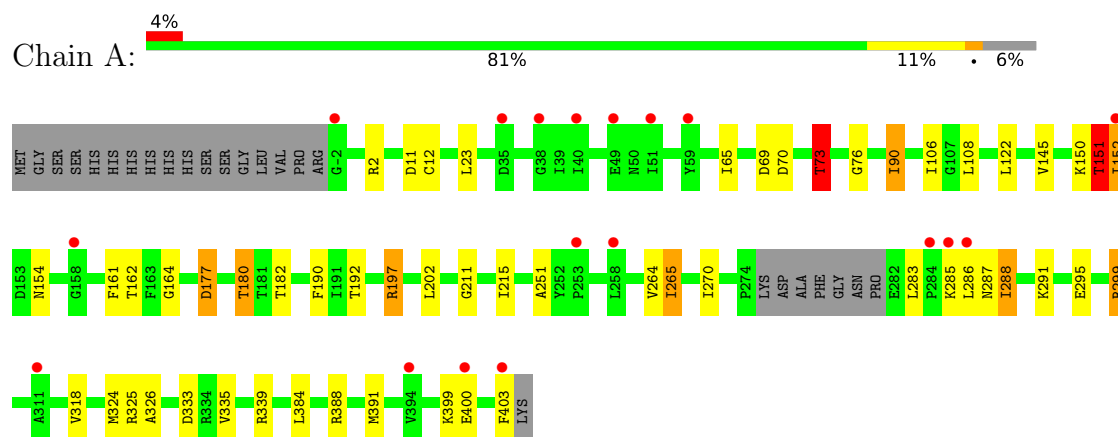
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	24	Total	O	0	0
			24	24		
3	B	28	Total	O	0	0
			28	28		
3	C	21	Total	O	0	0
			21	21		
3	D	24	Total	O	0	0
			24	24		

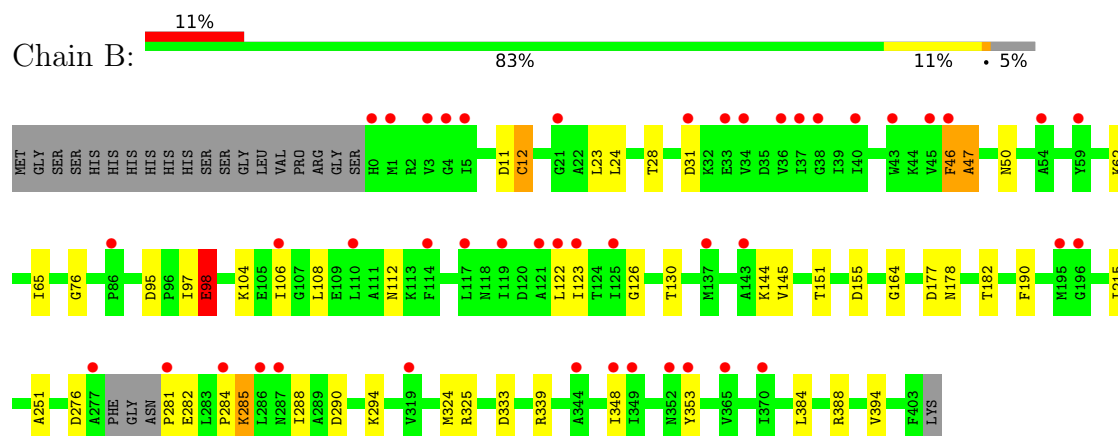
3 Residue-property plots [i](#)

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.

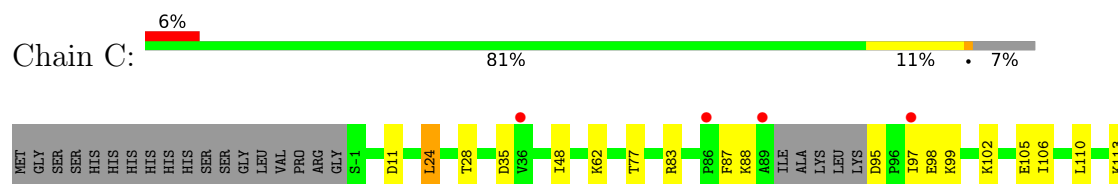
- Molecule 1: 6-phosphofructokinase

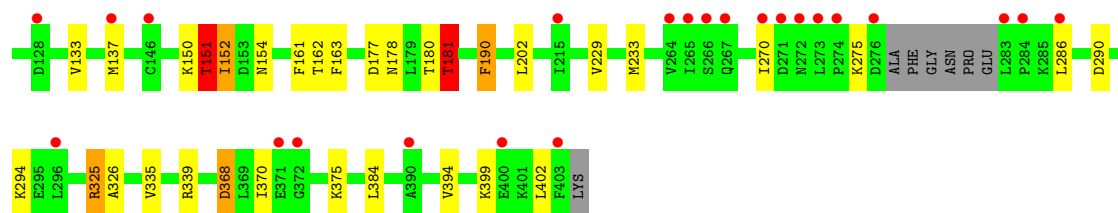


- Molecule 1: 6-phosphofructokinase

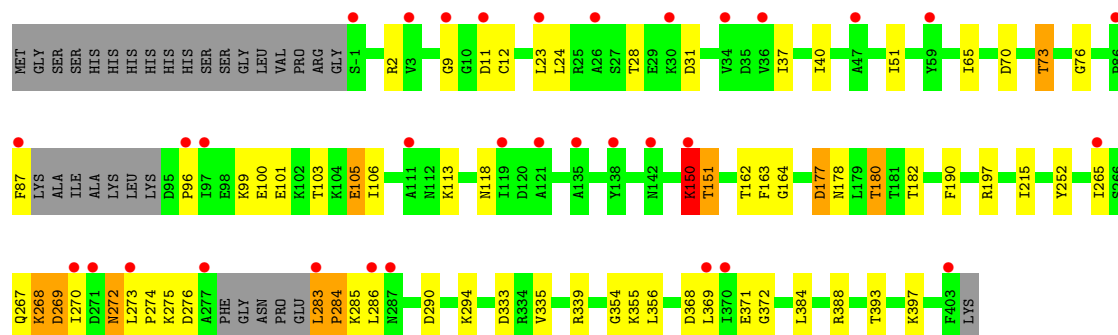
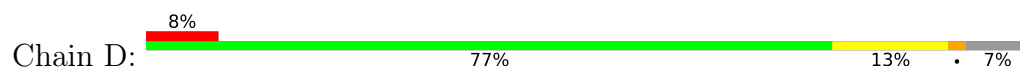


- Molecule 1: 6-phosphofructokinase





● Molecule 1: 6-phosphofructokinase



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	85.97Å 72.36Å 137.34Å 90.00° 90.87° 90.00°	Depositor
Resolution (Å)	45.81 – 2.20 45.81 – 2.20	Depositor EDS
% Data completeness (in resolution range)	100.0 (45.81-2.20) 100.0 (45.81-2.20)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.55 (at 2.20Å)	Xtriage
Refinement program	REFMAC 5.8.0430	Depositor
R, R_{free}	0.220 , 0.249 0.222 , 0.249	Depositor DCC
R_{free} test set	4332 reflections (5.04%)	wwPDB-VP
Wilson B-factor (Å ²)	51.3	Xtriage
Anisotropy	0.075	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 32.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.013 for h,-k,-l	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	12333	wwPDB-VP
Average B, all atoms (Å ²)	66.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.78% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: GOL

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	0.58	0/3145	0.96	5/4253 (0.1%)
1	B	0.58	0/3135	1.00	7/4238 (0.2%)
1	C	0.59	0/3086	0.96	4/4174 (0.1%)
1	D	0.59	0/3092	1.00	7/4178 (0.2%)
All	All	0.58	0/12458	0.98	23/16843 (0.1%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	2
1	B	1	2
1	C	0	2
1	D	0	1
All	All	1	7

There are no bond length outliers.

All (23) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	151	THR	N-CA-C	11.60	125.32	110.24
1	B	98	GLU	CB-CA-C	9.60	129.10	110.67
1	D	276	ASP	CA-CB-CG	9.18	121.78	112.60
1	D	269	ASP	CA-CB-CG	6.79	119.39	112.60
1	B	31	ASP	CA-CB-CG	6.72	119.32	112.60
1	B	155	ASP	N-CA-CB	-6.42	100.99	110.49
1	C	151	THR	CA-CB-OG1	-6.34	100.08	109.60
1	C	181	THR	N-CA-CB	-6.25	100.94	110.01

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	46	PHE	N-CA-C	-6.24	101.04	110.28
1	D	177	ASP	CA-CB-CG	6.17	118.77	112.60
1	A	151	THR	CA-CB-OG1	-5.83	100.86	109.60
1	A	177	ASP	CA-CB-CG	5.80	118.40	112.60
1	A	69	ASP	CA-CB-CG	5.66	118.26	112.60
1	B	95	ASP	CA-CB-CG	5.57	118.17	112.60
1	A	324	MET	CB-CA-C	-5.56	100.00	110.01
1	C	177	ASP	CA-CB-CG	5.55	118.15	112.60
1	D	151	THR	N-CA-CB	-5.48	101.15	109.92
1	B	324	MET	CB-CA-C	-5.37	100.35	110.01
1	B	177	ASP	CA-CB-CG	5.26	117.86	112.60
1	D	150	LYS	N-CA-C	5.19	117.94	111.24
1	A	73	THR	N-CA-CB	-5.08	102.52	110.44
1	D	31	ASP	CA-CB-CG	5.03	117.63	112.60
1	C	190	PHE	CA-CB-CG	-5.02	108.78	113.80

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
1	B	98	GLU	CA

All (7) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	197	ARG	Sidechain
1	A	299[A]	ARG	Sidechain
1	B	325	ARG	Sidechain
1	B	47	ALA	Peptide
1	C	325	ARG	Sidechain
1	C	83	ARG	Sidechain
1	D	150	LYS	Peptide

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	3080	0	3075	54	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	B	3075	0	3056	35	0
1	C	3022	0	2990	34	0
1	D	3029	0	3016	63	0
2	A	6	0	8	0	0
2	B	6	0	8	0	0
2	C	6	0	8	0	0
2	D	12	0	16	9	0
3	A	24	0	0	1	0
3	B	28	0	0	0	0
3	C	21	0	0	0	0
3	D	24	0	0	0	0
All	All	12333	0	12177	176	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 7.

All (176) 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:354:GLY:C	1:D:369:LEU:HD13	1.65	1.22
1:D:354:GLY:C	1:D:369:LEU:CD1	2.18	1.15
1:A:90:ILE:HD11	1:A:106:ILE:HD12	1.32	1.07
1:A:90:ILE:CD1	1:A:106:ILE:HD12	1.83	1.07
1:A:197:ARG:NH1	1:A:286:LEU:CD2	2.19	1.06
1:A:197:ARG:HH12	1:A:286:LEU:CD2	1.69	1.05
1:A:251:ALA:O	1:A:288:ILE:HD12	1.57	1.04
1:A:251:ALA:O	1:A:288:ILE:CD1	2.14	0.95
1:D:354:GLY:O	1:D:369:LEU:HD13	1.66	0.94
1:A:197:ARG:HH12	1:A:286:LEU:HD22	1.35	0.90
1:D:355:LYS:N	1:D:369:LEU:CD1	2.41	0.83
1:A:197:ARG:NH1	1:A:286:LEU:HD23	1.92	0.82
1:C:110:LEU:HB2	1:C:137:MET:SD	2.21	0.80
1:B:123:ILE:CG1	1:B:348:ILE:HD11	2.12	0.80
1:D:265:ILE:HD12	1:D:286:LEU:HD23	1.63	0.78
1:D:150:LYS:O	1:D:163:PHE:O	2.00	0.78
1:C:48:ILE:O	1:C:113:LYS:NZ	2.17	0.77
1:C:151:THR:HG22	1:C:162:THR:HG21	1.67	0.76
1:A:151:THR:HG22	1:A:162:THR:HG21	1.70	0.74
1:D:355:LYS:N	1:D:369:LEU:HD11	2.03	0.73
1:B:123:ILE:CG1	1:B:348:ILE:CD1	2.67	0.73
1:C:95:ASP:OD1	1:C:97:ILE:HG12	1.88	0.73

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:123:ILE:HG13	1:B:348:ILE:HD11	1.71	0.72
1:B:123:ILE:HG13	1:B:348:ILE:CD1	2.20	0.71
1:A:90:ILE:CD1	1:A:106:ILE:CD1	2.66	0.71
1:A:197:ARG:HH12	1:A:286:LEU:HD23	1.52	0.71
1:D:270:ILE:C	1:D:274:PRO:HG2	2.14	0.71
1:A:90:ILE:HD13	1:A:106:ILE:HD12	1.72	0.70
1:D:12:CYS:SG	1:D:164:GLY:HA3	2.31	0.70
1:D:354:GLY:O	1:D:369:LEU:CD1	2.30	0.69
1:B:46:PHE:O	1:B:47:ALA:HB3	1.94	0.68
1:B:123:ILE:HD11	1:B:348:ILE:HD12	1.77	0.67
1:D:37:ILE:CD1	2:D:502:GOL:H2	2.25	0.67
1:D:265:ILE:HD12	1:D:286:LEU:CD2	2.24	0.66
1:D:101:GLU:O	1:D:105:GLU:HG2	1.95	0.66
1:D:37:ILE:HD12	2:D:502:GOL:H2	1.76	0.66
1:B:123:ILE:HG12	1:B:348:ILE:HD11	1.77	0.65
1:A:251:ALA:O	1:A:288:ILE:HD13	1.98	0.64
1:B:182:THR:HA	1:C:11[A]:ASP:OD2	1.99	0.63
1:A:12:CYS:SG	1:A:164:GLY:HA3	2.39	0.63
1:D:354:GLY:CA	1:D:369:LEU:HD13	2.30	0.62
1:B:12:CYS:SG	1:B:164:GLY:HA3	2.39	0.62
1:C:87:PHE:HB2	1:C:133:VAL:HG22	1.81	0.62
1:C:99:LYS:HA	1:C:99:LYS:HE2	1.82	0.62
1:D:270:ILE:O	1:D:274:PRO:HG2	1.99	0.62
1:D:354:GLY:C	1:D:369:LEU:HD11	2.22	0.60
1:C:110:LEU:HD12	1:C:137:MET:CE	2.31	0.60
1:A:211:GLY:HA2	1:A:391:MET:HE1	1.83	0.60
1:B:251:ALA:O	1:B:288:ILE:HG13	2.03	0.59
1:D:9:GLY:HA3	2:D:501:GOL:H11	1.83	0.59
1:D:70:ASP:O	1:D:73:THR:HB	2.02	0.59
1:B:104:LYS:O	1:B:108:LEU:HD13	2.02	0.59
1:A:90:ILE:HD13	1:A:106:ILE:CD1	2.31	0.59
1:D:2:ARG:HD2	2:D:502:GOL:O1	2.03	0.59
1:D:2:ARG:HG3	2:D:502:GOL:O1	2.03	0.59
1:C:95:ASP:HB3	1:C:98:GLU:HG2	1.85	0.58
1:A:265:ILE:N	1:A:265:ILE:HD12	2.19	0.58
1:C:152[B]:ILE:HG23	1:C:202:LEU:HD11	1.85	0.58
1:A:122:LEU:HB3	1:A:145[A]:VAL:HG12	1.84	0.58
1:A:65:ILE:HD13	1:B:394:VAL:HG11	1.87	0.57
1:B:122:LEU:HB3	1:B:145:VAL:HG12	1.85	0.57
1:D:275:LYS:HD2	1:D:285:LYS:O	2.04	0.57
1:D:2:ARG:CG	2:D:502:GOL:O1	2.53	0.56

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:197:ARG:NH1	1:A:286:LEU:HD22	2.02	0.56
1:D:269:ASP:O	1:D:274:PRO:CG	2.53	0.56
1:C:105:GLU:HG3	1:C:106:ILE:HD12	1.88	0.56
1:A:264:VAL:C	1:A:265:ILE:HD12	2.30	0.56
1:C:102:LYS:O	1:C:105:GLU:HG2	2.05	0.55
1:D:368:ASP:O	1:D:371:GLU:HG2	2.07	0.55
1:A:197:ARG:HH11	1:A:286:LEU:CD2	2.17	0.55
1:A:192:THR:HG23	1:A:318:VAL:HG23	1.90	0.54
1:D:273:LEU:N	1:D:274:PRO:CD	2.70	0.54
1:A:70:ASP:O	1:A:73:THR:HB	2.07	0.54
1:A:152:ILE:HG23	1:A:202:LEU:HD11	1.89	0.54
1:A:251:ALA:O	1:A:288:ILE:HG21	2.07	0.54
1:D:2:ARG:CD	2:D:502:GOL:O1	2.56	0.54
1:A:285:LYS:N	1:A:285:LYS:HD2	2.22	0.54
1:B:97:ILE:HG22	1:B:98:GLU:OE2	2.08	0.53
1:C:87:PHE:HB2	1:C:133:VAL:CG2	2.38	0.53
1:D:118:ASN:ND2	2:D:502:GOL:H12	2.22	0.53
1:A:264:VAL:HG12	1:A:264:VAL:O	2.09	0.53
1:A:251:ALA:C	1:A:288:ILE:HD12	2.33	0.52
1:A:285:LYS:N	1:A:285:LYS:CD	2.71	0.52
1:A:295:GLU:OE2	1:A:299[B]:ARG:NH2	2.42	0.52
1:B:282:GLU:O	1:B:284:PRO:HD3	2.10	0.52
1:D:96:PRO:O	1:D:99:LYS:HG2	2.10	0.52
1:A:270:ILE:HG22	1:A:283:LEU:HD13	1.90	0.51
1:B:144:LYS:CD	1:B:353:TYR:CZ	2.93	0.51
1:D:100:GLU:O	1:D:103:THR:HG22	2.11	0.51
1:D:269:ASP:O	1:D:274:PRO:HG3	2.11	0.51
1:C:178:ASN:O	1:C:181:THR:HB	2.11	0.51
1:D:100:GLU:HA	1:D:103:THR:HG22	1.93	0.50
1:D:11:ASP:OD1	1:D:76:GLY:HA2	2.12	0.49
1:A:154:ASN:HD21	1:A:161:PHE:HA	1.77	0.49
1:A:339:ARG:HD2	1:B:384:LEU:HD21	1.94	0.49
1:C:368:ASP:OD2	1:C:370:ILE:HG22	2.12	0.49
1:C:154:ASN:HD21	1:C:161:PHE:HA	1.77	0.49
1:A:11:ASP:OD2	1:D:182:THR:HA	2.13	0.48
1:B:46:PHE:O	1:B:47:ALA:CB	2.57	0.48
1:D:286:LEU:O	1:D:286:LEU:HG	2.13	0.48
1:A:325:ARG:O	1:A:325:ARG:HG2	2.12	0.48
1:B:123:ILE:CD1	1:B:348:ILE:HD12	2.43	0.48
1:D:150:LYS:HA	1:D:163:PHE:CE1	2.48	0.48
1:D:268:LYS:HA	1:D:272:ASN:HB2	1.94	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:265:ILE:N	1:A:265:ILE:CD1	2.76	0.48
1:C:110:LEU:HD12	1:C:137:MET:HE1	1.93	0.48
1:D:197:ARG:CZ	1:D:285:LYS:HB3	2.44	0.48
1:D:356:LEU:HD22	1:D:372:GLY:HA3	1.95	0.48
1:B:11:ASP:OD1	1:B:76:GLY:HA2	2.13	0.48
1:B:144:LYS:HD2	1:B:353:TYR:CZ	2.49	0.48
1:A:11:ASP:OD1	1:A:76:GLY:HA2	2.13	0.47
1:B:276:ASP:N	1:B:281:PRO:O	2.40	0.47
1:D:252:TYR:CD1	1:D:284:PRO:HB3	2.50	0.46
1:A:11:ASP:O	1:A:325:ARG:HD3	2.15	0.46
1:C:110:LEU:CB	1:C:137:MET:SD	2.99	0.46
1:B:97:ILE:HD12	1:B:97:ILE:N	2.31	0.46
1:D:355:LYS:CA	1:D:369:LEU:HD12	2.46	0.46
1:B:123:ILE:CG1	1:B:348:ILE:HD12	2.44	0.46
1:B:215:ILE:HB	1:B:388:ARG:HD2	1.99	0.45
1:D:269:ASP:O	1:D:274:PRO:HD3	2.17	0.45
1:A:182:THR:HA	1:D:11:ASP:OD2	2.17	0.45
1:C:384:LEU:HD21	1:D:339:ARG:HD2	1.99	0.45
1:B:290:ASP:OD2	1:B:294:LYS:HE2	2.17	0.45
1:B:23:LEU:HB3	1:B:65:ILE:HD12	1.98	0.45
1:D:215:ILE:HB	1:D:388:ARG:HD2	1.99	0.45
1:B:24:LEU:O	1:B:28:THR:HG23	2.17	0.44
1:C:110:LEU:HD12	1:C:137:MET:HE3	1.98	0.44
1:C:150:LYS:HB2	1:C:163:PHE:CZ	2.53	0.44
1:A:265:ILE:HD11	1:A:291:LYS:HB3	1.99	0.44
1:C:150:LYS:O	1:C:151:THR:HB	2.17	0.44
1:A:286:LEU:O	1:A:287:ASN:OD1	2.35	0.44
1:D:393:THR:HG22	1:D:397:LYS:HD3	2.00	0.44
1:D:290:ASP:OD2	1:D:294:LYS:HE2	2.18	0.44
1:D:87:PHE:CE1	1:D:106:ILE:CG2	3.01	0.44
1:A:215:ILE:HB	1:A:388:ARG:HD2	2.00	0.43
1:B:144:LYS:HD3	1:B:353:TYR:CZ	2.54	0.43
1:C:151:THR:HG23	1:C:154:ASN:H	1.84	0.43
1:C:270:ILE:H	1:C:270:ILE:HD12	1.84	0.43
1:A:326:ALA:HB1	1:D:178:ASN:O	2.19	0.43
1:D:23:LEU:HB3	1:D:65:ILE:HD12	2.01	0.42
1:C:339:ARG:HD2	1:D:384:LEU:HD21	2.00	0.42
1:A:270:ILE:O	1:A:283:LEU:HD22	2.18	0.42
1:A:335:VAL:O	1:A:339:ARG:HG3	2.19	0.42
1:B:284:PRO:O	1:B:285:LYS:CB	2.67	0.42
1:D:283:LEU:N	1:D:284:PRO:CD	2.81	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:23:LEU:HB3	1:A:65:ILE:HD12	2.02	0.42
1:C:24:LEU:O	1:C:28:THR:HG23	2.19	0.42
1:C:335:VAL:O	1:C:339:ARG:HG3	2.19	0.42
1:A:151:THR:HG23	1:A:154:ASN:H	1.85	0.42
1:C:229:VAL:HG12	1:C:233:MET:HE2	2.00	0.42
1:D:24:LEU:O	1:D:28:THR:HG23	2.19	0.42
1:D:355:LYS:CA	1:D:369:LEU:CD1	2.97	0.42
1:A:286:LEU:O	1:A:287:ASN:CG	2.62	0.42
1:D:197:ARG:CZ	1:D:285:LYS:CB	2.97	0.42
1:B:178:ASN:O	1:C:326:ALA:HB1	2.20	0.42
1:D:164:GLY:H	1:D:333:ASP:CG	2.28	0.42
1:D:283:LEU:N	1:D:284:PRO:HD3	2.35	0.42
1:C:102:LYS:HA	1:C:105:GLU:HG2	2.00	0.42
1:B:164:GLY:H	1:B:333:ASP:CG	2.27	0.41
1:A:2:ARG:NH2	3:A:602:HOH:O	2.52	0.41
1:C:290:ASP:OD2	1:C:294:LYS:HE3	2.20	0.41
1:A:177:ASP:O	1:A:180:THR:HB	2.21	0.41
1:D:118:ASN:CG	2:D:502:GOL:H12	2.46	0.41
1:A:164:GLY:H	1:A:333:ASP:CG	2.29	0.41
1:A:384:LEU:HD21	1:B:339:ARG:HD2	2.03	0.41
1:B:288:ILE:H	1:B:288:ILE:HG12	1.75	0.41
1:C:325:ARG:HG2	1:C:325:ARG:O	2.21	0.41
1:D:177:ASP:O	1:D:180:THR:HB	2.21	0.41
1:C:35:ASP:CG	1:C:62:LYS:HE2	2.46	0.41
1:A:150:LYS:O	1:A:151:THR:HB	2.21	0.40
1:B:126:GLY:HA3	1:B:130:THR:HG21	2.02	0.40
1:D:335:VAL:O	1:D:339:ARG:HG3	2.21	0.40
1:D:51:ILE:HD11	1:D:113:LYS:HD3	2.03	0.40
1:D:151:THR:O	1:D:162:THR:OG1	2.39	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	399/424 (94%)	392 (98%)	6 (2%)	1 (0%)	36	42
1	B	398/424 (94%)	388 (98%)	8 (2%)	2 (0%)	24	27
1	C	391/424 (92%)	378 (97%)	12 (3%)	1 (0%)	36	42
1	D	390/424 (92%)	377 (97%)	12 (3%)	1 (0%)	36	42
All	All	1578/1696 (93%)	1535 (97%)	38 (2%)	5 (0%)	36	42

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	285	LYS
1	B	151	THR
1	C	151	THR
1	A	151	THR
1	D	284	PRO

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	330/355 (93%)	319 (97%)	11 (3%)	33	45
1	B	327/355 (92%)	320 (98%)	7 (2%)	47	63
1	C	320/355 (90%)	305 (95%)	15 (5%)	23	31
1	D	325/355 (92%)	316 (97%)	9 (3%)	38	52
All	All	1302/1420 (92%)	1260 (97%)	42 (3%)	34	47

All (42) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	73	THR
1	A	90	ILE
1	A	108	LEU
1	A	152	ILE
1	A	180	THR
1	A	190	PHE

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	265	ILE
1	A	288	ILE
1	A	399	LYS
1	A	400	GLU
1	A	403	PHE
1	B	12	CYS
1	B	50	ASN
1	B	62	LYS
1	B	98	GLU
1	B	106	ILE
1	B	112	ASN
1	B	190	PHE
1	C	24	LEU
1	C	77	THR
1	C	88	LYS
1	C	152[A]	ILE
1	C	152[B]	ILE
1	C	180	THR
1	C	181	THR
1	C	190	PHE
1	C	275	LYS
1	C	286	LEU
1	C	368	ASP
1	C	375	LYS
1	C	394	VAL
1	C	399	LYS
1	C	402	LEU
1	D	40	ILE
1	D	73	THR
1	D	105	GLU
1	D	180	THR
1	D	190	PHE
1	D	267	GLN
1	D	268	LYS
1	D	272	ASN
1	D	283	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (15) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	0	HIS
1	A	154	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	297	ASN
1	A	307	ASN
1	B	118	ASN
1	B	297	ASN
1	C	58	HIS
1	C	118	ASN
1	C	154	ASN
1	C	287	ASN
1	C	307	ASN
1	D	112	ASN
1	D	297	ASN
1	D	307	ASN
1	D	343	HIS

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](#)

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	GOL	D	502	-	5,5,5	0.14	0	5,5,5	0.39	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	GOL	D	501	-	5,5,5	0.10	0	5,5,5	0.29	0
2	GOL	B	501	-	5,5,5	0.10	0	5,5,5	0.31	0
2	GOL	A	501	-	5,5,5	0.19	0	5,5,5	0.41	0
2	GOL	C	501	-	5,5,5	0.24	0	5,5,5	0.76	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	D	502	-	-	2/4/4/4	-
2	GOL	D	501	-	-	0/4/4/4	-
2	GOL	B	501	-	-	0/4/4/4	-
2	GOL	A	501	-	-	2/4/4/4	-
2	GOL	C	501	-	-	4/4/4/4	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (8) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	501	GOL	C1-C2-C3-O3
2	C	501	GOL	C1-C2-C3-O3
2	C	501	GOL	O1-C1-C2-C3
2	A	501	GOL	O2-C2-C3-O3
2	C	501	GOL	O2-C2-C3-O3
2	D	502	GOL	O1-C1-C2-O2
2	C	501	GOL	O1-C1-C2-O2
2	D	502	GOL	O1-C1-C2-C3

There are no ring outliers.

2 monomers are involved in 9 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	D	502	GOL	8	0
2	D	501	GOL	1	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 [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	399/424 (94%)	0.56	18 (4%)	38	35	22, 60, 113, 154	4 (1%)
1	B	401/424 (94%)	0.79	45 (11%)	10	8	26, 64, 116, 147	1 (0%)
1	C	394/424 (92%)	0.60	27 (6%)	23	20	24, 57, 108, 150	3 (0%)
1	D	393/424 (92%)	0.70	33 (8%)	17	14	29, 62, 122, 154	3 (0%)
All	All	1587/1696 (93%)	0.66	123 (7%)	19	16	22, 60, 118, 154	11 (0%)

All (123) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	283	LEU	5.9
1	B	277	ALA	5.6
1	B	3	VAL	4.8
1	D	283	LEU	4.7
1	C	270	ILE	4.5
1	A	403	PHE	4.3
1	C	273	LEU	4.2
1	D	277	ALA	4.1
1	B	286	LEU	4.1
1	B	45	VAL	4.0
1	B	143	ALA	4.0
1	B	121	ALA	3.9
1	B	123	ILE	3.9
1	B	281	PRO	3.8
1	C	137	MET	3.7
1	B	348	ILE	3.7
1	B	284	PRO	3.6
1	D	26	ALA	3.5
1	D	270	ILE	3.5
1	B	59	TYR	3.5
1	C	265	ILE	3.4

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	C	89	ALA	3.4
1	B	46	PHE	3.3
1	D	273	LEU	3.3
1	B	54	ALA	3.2
1	D	286	LEU	3.2
1	B	43	TRP	3.2
1	C	284	PRO	3.1
1	B	349	ILE	3.1
1	A	311	ALA	3.0
1	B	36	VAL	3.0
1	B	5	ILE	2.9
1	A	40	ILE	2.9
1	C	97	ILE	2.9
1	B	196	GLY	2.9
1	A	286	LEU	2.9
1	B	195	MET	2.9
1	B	117	LEU	2.8
1	D	369	LEU	2.8
1	B	33	GLU	2.8
1	B	344	ALA	2.8
1	B	1	MET	2.8
1	A	152	ILE	2.8
1	B	119	ILE	2.8
1	C	274	PRO	2.8
1	D	97	ILE	2.7
1	D	271[A]	ASP	2.7
1	D	87	PHE	2.7
1	C	276	ASP	2.7
1	A	49	GLU	2.7
1	D	119	ILE	2.7
1	D	265	ILE	2.7
1	D	138	TYR	2.6
1	C	372	GLY	2.6
1	B	122	LEU	2.6
1	C	267	GLN	2.6
1	B	352	ASN	2.6
1	C	371	GLU	2.6
1	D	47	ALA	2.6
1	B	31	ASP	2.6
1	B	4	GLY	2.6
1	A	-2	GLY	2.6
1	A	284	PRO	2.6

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	59	TYR	2.6
1	C	286	LEU	2.5
1	D	370	ILE	2.5
1	B	21	GLY	2.5
1	B	37	ILE	2.5
1	B	370	ILE	2.5
1	D	59	TYR	2.5
1	D	135	ALA	2.5
1	D	96	PRO	2.5
1	A	394	VAL	2.4
1	B	125	ILE	2.4
1	D	3	VAL	2.4
1	D	34	VAL	2.4
1	B	110	LEU	2.4
1	A	35	ASP	2.4
1	C	215	ILE	2.4
1	C	272	ASN	2.4
1	A	38	GLY	2.4
1	B	38	GLY	2.4
1	C	271	ASP	2.3
1	B	0	HIS	2.3
1	B	114	PHE	2.3
1	C	403	PHE	2.3
1	C	390	ALA	2.3
1	C	400	GLU	2.3
1	D	30	LYS	2.3
1	D	150	LYS	2.3
1	B	365	VAL	2.3
1	C	266	SER	2.2
1	C	264	VAL	2.2
1	B	287	ASN	2.2
1	C	128	ASP	2.2
1	B	40	ILE	2.2
1	B	34	VAL	2.2
1	D	36	VAL	2.2
1	C	86	PRO	2.2
1	A	285	LYS	2.2
1	B	86	PRO	2.2
1	D	86	PRO	2.2
1	A	158	GLY	2.2
1	A	258	LEU	2.1
1	D	142	ASN	2.1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	253	PRO	2.1
1	D	121	ALA	2.1
1	B	106	ILE	2.1
1	D	287	ASN	2.1
1	A	400	GLU	2.1
1	C	296	LEU	2.1
1	D	403	PHE	2.1
1	D	9	GLY	2.1
1	A	51	ILE	2.1
1	B	319	VAL	2.1
1	C	36	VAL	2.1
1	D	-1	SER	2.0
1	C	146	CYS	2.0
1	D	111	ALA	2.0
1	D	11	ASP	2.0
1	D	23	LEU	2.0
1	B	353	TYR	2.0
1	B	137	MET	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($\text{\AA}^2$)	Q<0.9
2	GOL	A	501	6/6	0.74	0.19	74,79,83,85	0
2	GOL	D	501	6/6	0.80	0.13	81,90,95,97	0
2	GOL	C	501	6/6	0.86	0.14	73,78,82,86	0
2	GOL	B	501	6/6	0.86	0.12	72,76,79,81	0
2	GOL	D	502	6/6	0.88	0.10	55,62,74,75	0

6.5 Other polymers [i](#)

There are no such residues in this entry.