



Full wwPDB X-ray Structure Validation Report ⓘ

Apr 19, 2026 – 01:32 AM UTC

PDB ID : 5TR2 / pdb_00005tr2
Title : Crystal structure of the D263G missense variant of human PGM1
Authors : Beamer, L.J.; Stiers, K.M.
Deposited on : 2016-10-25
Resolution : 2.50 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

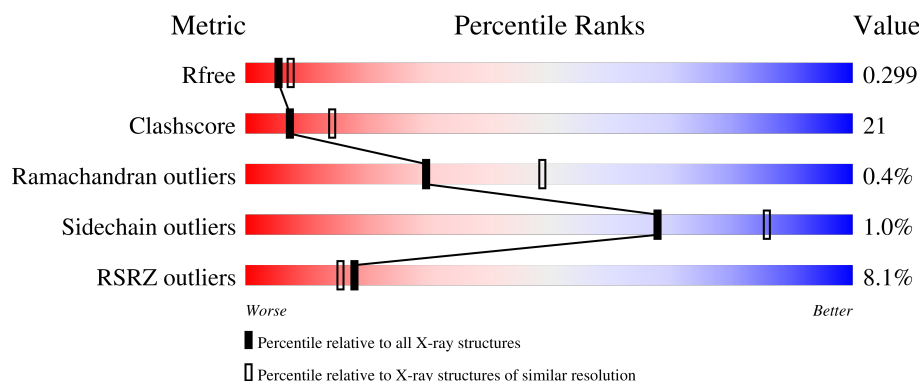
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.50 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	5829 (2.50-2.50)
Clashscore	190562	6492 (2.50-2.50)
Ramachandran outliers	187476	6378 (2.50-2.50)
Sidechain outliers	187428	6380 (2.50-2.50)
RSRZ outliers	180081	5833 (2.50-2.50)

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	585	2% 66% 30% • •
1	B	585	14% 68% 25% • 6%

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	SO4	A	602	-	-	X	-
2	SO4	B	601	-	-	X	-

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 8233 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 Phosphoglucomutase-1.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	561	Total	C	N	O	P	S	0	8	0
			4188	2659	713	798	1	17			
1	B	552	Total	C	N	O	P	S	0	7	0
			3813	2393	670	735	1	14			

There are 48 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-22	MET	-	expression tag	UNP P36871
A	-21	HIS	-	expression tag	UNP P36871
A	-20	HIS	-	expression tag	UNP P36871
A	-19	HIS	-	expression tag	UNP P36871
A	-18	HIS	-	expression tag	UNP P36871
A	-17	HIS	-	expression tag	UNP P36871
A	-16	HIS	-	expression tag	UNP P36871
A	-15	SER	-	expression tag	UNP P36871
A	-14	SER	-	expression tag	UNP P36871
A	-13	GLY	-	expression tag	UNP P36871
A	-12	VAL	-	expression tag	UNP P36871
A	-11	ASP	-	expression tag	UNP P36871
A	-10	LEU	-	expression tag	UNP P36871
A	-9	GLY	-	expression tag	UNP P36871
A	-8	THR	-	expression tag	UNP P36871
A	-7	GLU	-	expression tag	UNP P36871
A	-6	ASN	-	expression tag	UNP P36871
A	-5	LEU	-	expression tag	UNP P36871
A	-4	TYR	-	expression tag	UNP P36871
A	-3	PHE	-	expression tag	UNP P36871
A	-2	GLN	-	expression tag	UNP P36871
A	-1	SER	-	expression tag	UNP P36871
A	0	ASN	-	expression tag	UNP P36871
A	263	GLY	ASP	conflict	UNP P36871
B	-22	MET	-	expression tag	UNP P36871

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
B	-21	HIS	-	expression tag	UNP P36871
B	-20	HIS	-	expression tag	UNP P36871
B	-19	HIS	-	expression tag	UNP P36871
B	-18	HIS	-	expression tag	UNP P36871
B	-17	HIS	-	expression tag	UNP P36871
B	-16	HIS	-	expression tag	UNP P36871
B	-15	SER	-	expression tag	UNP P36871
B	-14	SER	-	expression tag	UNP P36871
B	-13	GLY	-	expression tag	UNP P36871
B	-12	VAL	-	expression tag	UNP P36871
B	-11	ASP	-	expression tag	UNP P36871
B	-10	LEU	-	expression tag	UNP P36871
B	-9	GLY	-	expression tag	UNP P36871
B	-8	THR	-	expression tag	UNP P36871
B	-7	GLU	-	expression tag	UNP P36871
B	-6	ASN	-	expression tag	UNP P36871
B	-5	LEU	-	expression tag	UNP P36871
B	-4	TYR	-	expression tag	UNP P36871
B	-3	PHE	-	expression tag	UNP P36871
B	-2	GLN	-	expression tag	UNP P36871
B	-1	SER	-	expression tag	UNP P36871
B	0	ASN	-	expression tag	UNP P36871
B	263	GLY	ASP	conflict	UNP P36871

- Molecule 2 is SULFATE ION (CCD ID: SO4) (formula: O₄S).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total O S 5 4 1	0	0
2	A	1	Total O S 5 4 1	0	0
2	A	1	Total O S 5 4 1	0	0
2	B	1	Total O S 5 4 1	0	0

- Molecule 3 is CALCIUM ION (CCD ID: CA) (formula: Ca).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total Ca 1 1	0	0
3	B	1	Total Ca 1 1	0	0

- Molecule 4 is GLYCEROL (CCD ID: GOL) (formula: C₃H₈O₃).



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

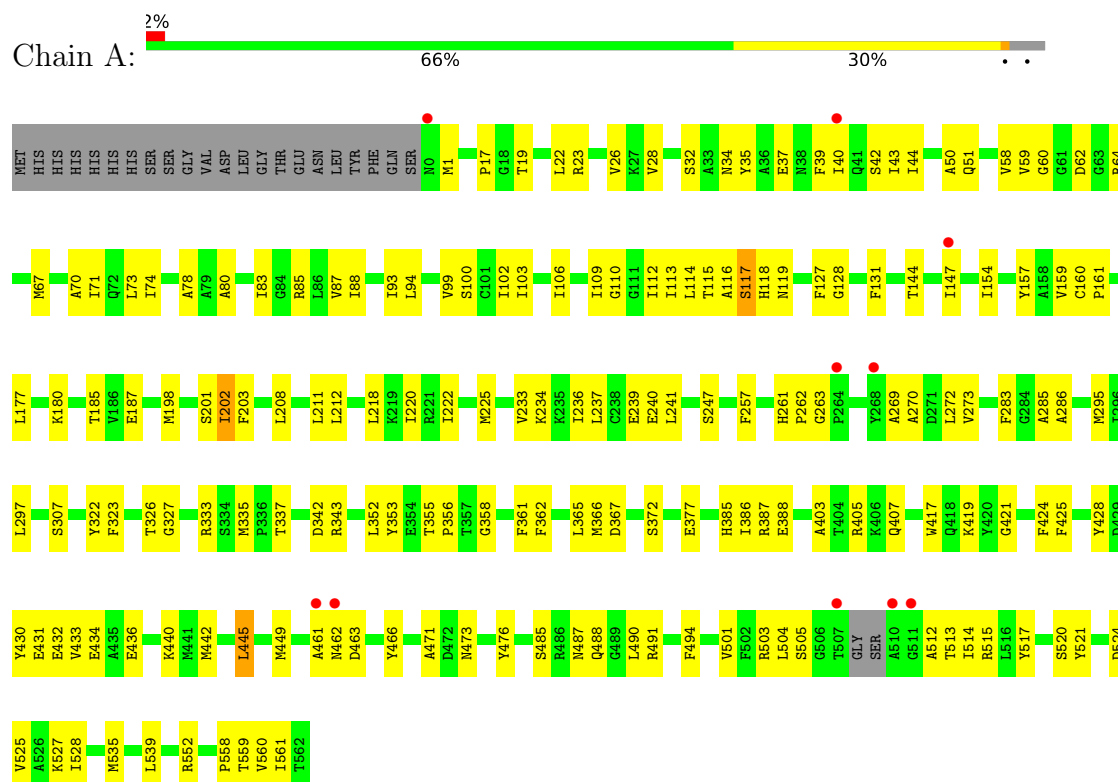
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	125	Total 125	O 125	0	0
5	B	79	Total 79	O 79	0	0

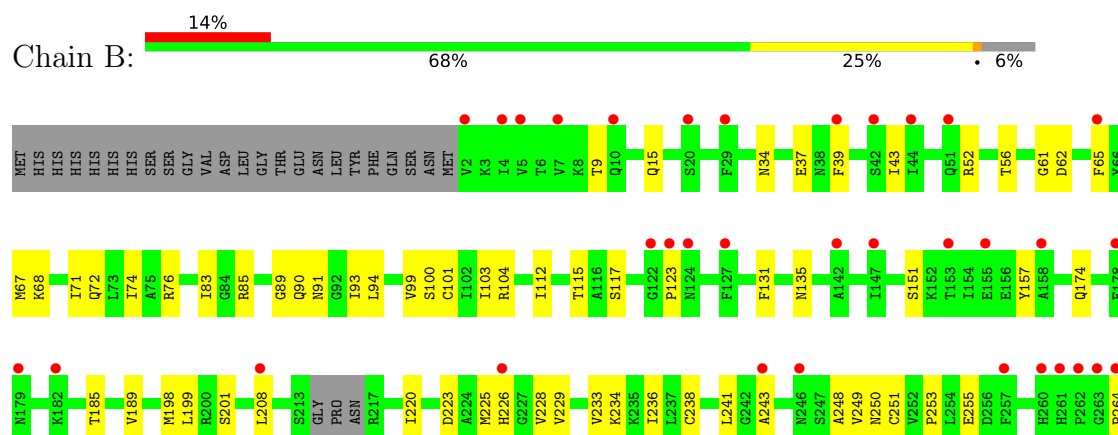
3 Residue-property plots

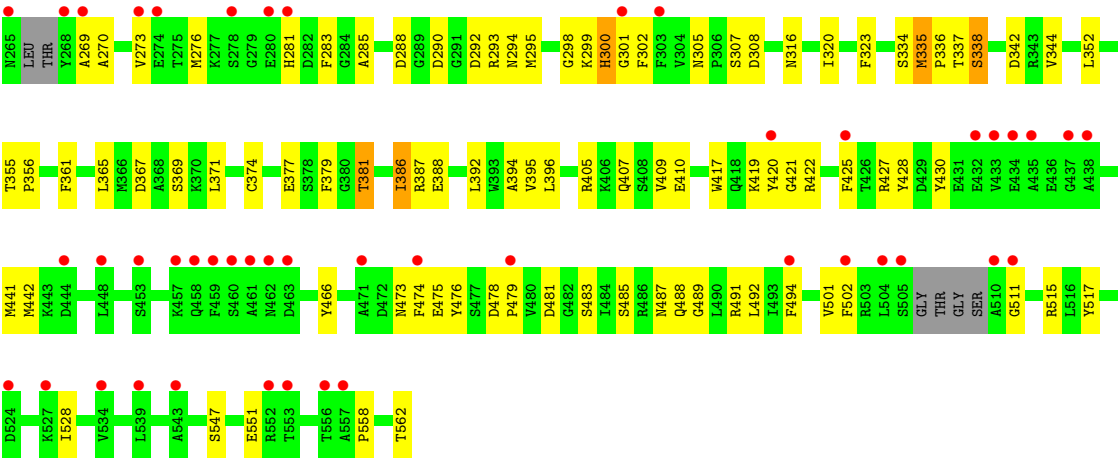
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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: Phosphoglucomutase-1



• Molecule 1: Phosphoglucomutase-1





4 Data and refinement statistics

Property	Value	Source
Space group	P 41 21 2	Depositor
Cell constants a, b, c, α , β , γ	172.12Å 172.12Å 99.00Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	51.84 – 2.50 51.84 – 2.50	Depositor EDS
% Data completeness (in resolution range)	85.0 (51.84-2.50) 85.3 (51.84-2.50)	Depositor EDS
R_{merge}	0.19	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.62 (at 2.51Å)	Xtriage
Refinement program	PHENIX (1.10.1 _2155: 000)	Depositor
R, R_{free}	0.220 , 0.292 0.225 , 0.299	Depositor DCC
R_{free} test set	2217 reflections (3.56%)	wwPDB-VP
Wilson B-factor (Å ²)	44.3	Xtriage
Anisotropy	0.348	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 90.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	8233	wwPDB-VP
Average B, all atoms (Å ²)	56.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.48% 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: SEP, SO4, CA, 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	0.45	0/4277	0.67	2/5805 (0.0%)
1	B	0.36	0/3885	0.59	0/5305
All	All	0.41	0/8162	0.63	2/11110 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	240	GLU	CA-C-N	-5.29	114.19	122.65
1	A	240	GLU	C-N-CA	-5.29	114.19	122.65

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	4188	0	3999	176	0
1	B	3813	0	3190	137	0
2	A	15	0	0	4	0
2	B	5	0	0	3	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
4	A	6	0	8	2	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	A	125	0	0	4	0
5	B	79	0	0	6	0
All	All	8233	0	7197	313	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 21.

All (313) 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:367:ASP:OD1	1:A:387:ARG:NH2	1.95	0.99
1:A:58:VAL:HG22	1:A:103:ILE:HD11	1.49	0.91
1:B:442:MET:HE1	1:B:502:PHE:HB3	1.52	0.91
1:A:43:ILE:HA	1:A:147:ILE:HD13	1.58	0.82
1:A:62:ASP:OD2	1:A:64:ARG:NH1	2.14	0.81
1:A:386[A]:ILE:HG22	1:A:388:GLU:H	1.47	0.80
1:B:220:ILE:HG22	1:B:283:PHE:HB3	1.64	0.80
1:B:342:ASP:OD1	1:B:352:LEU:HD11	1.83	0.79
1:A:323:PHE:HA	1:A:326:THR:HG22	1.64	0.78
1:A:431:GLU:HA	1:A:513:THR:HG22	1.65	0.78
1:A:202:ILE:HB	1:A:322:TYR:HB2	1.68	0.76
1:A:326:THR:HG23	1:A:327:GLY:O	1.85	0.76
1:B:226:HIS:CE1	1:B:250[A]:ASN:HD21	2.04	0.75
1:B:335:MET:HE1	1:B:501:VAL:HG21	1.66	0.75
1:A:58:VAL:HG12	1:A:87:VAL:CG1	2.17	0.74
1:A:58:VAL:HG12	1:A:87:VAL:HG13	1.69	0.74
1:A:43:ILE:CA	1:A:147:ILE:HD13	2.18	0.74
1:A:211:LEU:HD13	1:A:403:ALA:HB2	1.72	0.72
1:A:78:ALA:HA	1:A:83:ILE:HD12	1.72	0.71
1:A:43:ILE:CA	1:A:147:ILE:CD1	2.68	0.71
1:B:473:ASN:OD1	1:B:487:ASN:HA	1.91	0.70
1:A:64:ARG:NH1	1:A:116:ALA:H	1.88	0.70
1:B:9:THR:HA	1:B:34:ASN:HD22	1.57	0.70
1:A:43:ILE:HA	1:A:147:ILE:CD1	2.22	0.69
1:A:34:ASN:ND2	1:A:37:GLU:OE2	2.27	0.68
1:A:71:ILE:HA	1:A:74:ILE:HD12	1.76	0.68
1:B:264:PRO:HD3	1:B:288:ASP:HB3	1.76	0.67
1:A:405:ARG:NH2	1:A:407:GLN:OE1	2.24	0.67
1:A:434:GLU:OE1	1:A:436:GLU:N	2.27	0.67
1:B:377:GLU:HG3	1:B:425:PHE:HZ	1.59	0.67
1:A:159:VAL:HG13	1:A:161:PRO:HD3	1.77	0.66

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:505[B]:SER:OG	1:A:513:THR:OG1	2.11	0.66
1:A:358:GLY:HA2	4:A:605:GOL:H31	1.76	0.66
1:A:37:GLU:OE1	1:A:73:LEU:HD11	1.94	0.66
1:A:26:VAL:HG12	1:A:127:PHE:HB2	1.79	0.65
1:A:70:ALA:HB3	1:A:114:LEU:HD21	1.78	0.65
1:A:17:PRO:HG2	1:A:147:ILE:HG21	1.78	0.64
1:B:37:GLU:N	1:B:37:GLU:OE1	2.30	0.64
1:A:342:ASP:HA	1:A:352:LEU:HD13	1.80	0.64
1:A:211:LEU:HG	1:A:218:LEU:HD22	1.80	0.64
1:B:491:ARG:HA	1:B:501:VAL:HG22	1.80	0.64
1:A:432:GLU:H	1:A:513:THR:HG22	1.62	0.64
1:A:527:LYS:HB3	1:A:535:MET:HE2	1.80	0.64
1:B:515:ARG:NH1	2:B:601:SO4:O4	2.30	0.63
1:B:283:PHE:CZ	1:B:395:VAL:HG23	2.34	0.63
1:B:377:GLU:HG3	1:B:425:PHE:CZ	2.33	0.63
1:A:559:THR:HG22	1:A:560:VAL:HG23	1.80	0.63
1:B:292:ASP:OD2	1:B:293:ARG:HG3	1.99	0.63
1:B:466:TYR:HB3	1:B:494:PHE:CD1	2.33	0.63
1:A:377:GLU:HG3	1:A:425:PHE:CZ	2.34	0.63
1:A:295:MET:HE3	1:A:297:LEU:HD21	1.81	0.62
1:B:441:MET:HE3	1:B:442:MET:HE3	1.81	0.62
1:B:61:GLY:N	1:B:67[B]:MET:HE1	2.15	0.62
1:A:58:VAL:HG11	1:A:102:ILE:HG22	1.82	0.62
1:B:298:GLY:CA	1:B:409:VAL:HG11	2.30	0.62
1:B:90:GLN:HG2	1:B:91:ASN:OD1	2.00	0.61
1:A:236:ILE:O	1:A:241:LEU:HD23	2.00	0.61
1:A:270:ALA:HA	1:A:273:VAL:HB	1.83	0.61
1:A:257:PHE:CG	1:A:262:PRO:HG3	2.34	0.61
1:B:515:ARG:NH1	2:B:601:SO4:S	2.62	0.61
1:A:237:LEU:HA	1:A:241:LEU:HD21	1.83	0.61
1:B:298:GLY:N	1:B:302:PHE:O	2.33	0.60
1:A:17:PRO:HG2	1:A:147:ILE:CG2	2.31	0.60
1:A:503:ARG:NH2	2:A:602:SO4:O3	2.35	0.60
1:A:67:MET:HE1	1:A:93:ILE:HD13	1.84	0.60
1:A:177:LEU:HB2	1:A:180:LYS:HB2	1.84	0.60
1:A:362:PHE:O	1:A:366:MET:HG3	2.00	0.60
1:B:335:MET:HG3	1:B:336:PRO:HD3	1.84	0.59
1:A:440:LYS:HD2	1:A:552:ARG:HD2	1.84	0.59
1:A:211:LEU:HD13	1:A:403:ALA:CB	2.33	0.59
1:A:43:ILE:HD11	1:A:131:PHE:CD2	2.38	0.59
1:A:356:PRO:HG2	1:A:361:PHE:CZ	2.37	0.59

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:527:LYS:HB3	1:A:535:MET:CE	2.33	0.59
1:B:71:ILE:HA	1:B:74:ILE:HD12	1.84	0.58
1:B:421:GLY:HA2	1:B:528:ILE:HD11	1.85	0.58
1:B:405[B]:ARG:NH1	1:B:407:GLN:OE1	2.34	0.57
1:B:112:ILE:HG22	1:B:131:PHE:HD2	1.68	0.57
1:A:385:HIS:CD2	1:A:386[A]:ILE:HG12	2.39	0.57
1:A:428:TYR:CD2	1:A:558:PRO:HG3	2.39	0.57
1:B:62:ASP:OD1	1:B:115:THR:OG1	2.21	0.57
1:A:333:ARG:HD2	1:A:337:THR:HB	1.87	0.57
1:B:101:CYS:HA	1:B:386:ILE:HD11	1.85	0.57
1:B:473:ASN:HD22	1:B:489:GLY:C	2.12	0.57
1:A:43:ILE:N	1:A:147:ILE:CD1	2.68	0.57
1:A:109:ILE:HD12	1:A:110:GLY:N	2.20	0.57
1:A:505[A]:SER:HB3	1:A:513:THR:OG1	2.05	0.56
1:B:236:ILE:O	1:B:241:LEU:HD12	2.05	0.56
1:B:386:ILE:HG22	1:B:388:GLU:H	1.70	0.56
1:B:427:ARG:HB3	1:B:562:THR:OG1	2.05	0.56
1:A:501:VAL:HG23	1:A:517:TYR:CD1	2.40	0.56
1:B:68:LYS:O	1:B:72:GLN:HG2	2.05	0.56
1:B:344:VAL:HA	1:B:420:TYR:CZ	2.41	0.56
1:A:234:LYS:O	1:A:239:GLU:HG3	2.06	0.56
1:B:9:THR:HA	1:B:34:ASN:ND2	2.19	0.56
1:A:44:ILE:HG12	1:A:83:ILE:HD11	1.88	0.56
1:A:62:ASP:OD1	1:A:64:ARG:HG3	2.06	0.56
1:B:335:MET:SD	1:B:474:PHE:HD1	2.29	0.55
1:B:337:THR:HA	1:B:377:GLU:HB2	1.87	0.55
1:B:104[A]:ARG:HD3	1:B:135:ASN:O	2.06	0.55
1:A:356:PRO:HG2	1:A:361:PHE:CE1	2.42	0.55
1:B:199:LEU:HD23	1:B:396:LEU:HD22	1.89	0.55
1:A:40:ILE:HD12	1:A:73:LEU:CD2	2.37	0.54
1:B:229:VAL:O	1:B:233:VAL:HG23	2.07	0.54
1:B:37:GLU:HB3	1:B:157:TYR:CE2	2.42	0.54
1:A:40:ILE:HD12	1:A:73:LEU:HD22	1.89	0.54
1:B:294:ASN:O	1:B:379:PHE:HB3	2.08	0.54
1:A:501:VAL:CG2	1:A:517:TYR:HB2	2.38	0.54
1:A:269:ALA:HB3	1:A:295:MET:HE1	1.90	0.54
1:B:515:ARG:NH1	2:B:601:SO4:O1	2.37	0.54
1:B:298:GLY:HA3	1:B:409:VAL:HG11	1.89	0.53
1:A:212:LEU:HD12	1:A:241:LEU:CD1	2.39	0.53
1:A:471:ALA:HA	1:A:491:ARG:O	2.08	0.53
1:B:99:VAL:O	1:B:103:ILE:HG13	2.08	0.53

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:505[A]:SER:HB3	1:A:513:THR:HG1	1.74	0.53
1:B:189:VAL:HG11	5:B:768:HOH:O	2.08	0.53
1:A:261:HIS:ND1	2:A:603:SO4:O2	2.25	0.53
1:A:43:ILE:HB	1:A:147:ILE:CD1	2.39	0.52
1:A:43:ILE:CB	1:A:147:ILE:HD13	2.40	0.52
1:B:419:LYS:HE3	1:B:420:TYR:CG	2.44	0.52
1:B:234:LYS:O	1:B:238:CYS:HB2	2.09	0.52
1:A:40:ILE:HD13	1:A:74:ILE:HG13	1.92	0.52
1:A:220:ILE:HD12	1:A:247:SER:HB3	1.91	0.52
1:A:527:LYS:HD3	1:A:535:MET:HE1	1.91	0.52
1:B:39:PHE:O	1:B:43:ILE:HG12	2.09	0.52
1:B:298:GLY:HA2	1:B:409:VAL:HG11	1.92	0.52
1:A:22:LEU:O	1:A:128:GLY:HA2	2.10	0.52
1:A:43:ILE:HD11	1:A:131:PHE:CG	2.45	0.52
1:A:485:SER:HB3	1:A:488:GLN:NE2	2.25	0.52
1:A:212:LEU:HD23	1:A:218:LEU:HD21	1.93	0.51
1:A:237:LEU:HA	1:A:241:LEU:CD2	2.40	0.51
1:A:445:LEU:HD13	1:A:449:MET:SD	2.50	0.51
1:A:43:ILE:HB	1:A:147:ILE:HD13	1.91	0.51
1:B:112:ILE:HG22	1:B:131:PHE:CD2	2.46	0.51
1:A:67:MET:HG3	1:A:114:LEU:HD22	1.93	0.51
1:A:50:ALA:HB3	1:A:51:GLN:NE2	2.25	0.51
1:A:212:LEU:HD23	1:A:218:LEU:CD2	2.40	0.51
1:B:65:PHE:CE2	1:B:123:PRO:HA	2.45	0.51
1:A:430:TYR:HB2	1:A:514:ILE:HB	1.92	0.51
1:B:476:TYR:CE2	1:B:478:ASP:HA	2.45	0.51
1:A:211:LEU:CD2	1:A:218:LEU:CD2	2.90	0.50
1:A:501:VAL:HG22	1:A:517:TYR:HB2	1.92	0.50
1:A:43:ILE:HD13	1:A:112:ILE:HD11	1.93	0.50
1:B:290:ASP:OD1	1:B:290:ASP:N	2.32	0.50
1:B:474:PHE:HD2	1:B:475:GLU:N	2.09	0.50
1:B:52:ARG:HB3	1:B:83:ILE:HD13	1.92	0.50
1:B:299:LYS:C	1:B:301:GLY:H	2.19	0.50
1:A:60:GLY:HA3	1:A:94:LEU:HB2	1.93	0.50
1:B:174:GLN:HG2	1:B:185:THR:HG22	1.92	0.50
1:B:381:THR:OG1	1:B:394:ALA:HB2	2.12	0.50
1:B:335:MET:N	1:B:355:THR:O	2.45	0.50
1:A:34:ASN:ND2	1:A:157:TYR:OH	2.45	0.50
1:A:220:ILE:HG22	1:A:283:PHE:HB3	1.92	0.50
1:B:344:VAL:HA	1:B:420:TYR:CE1	2.46	0.50
1:A:42:SER:C	1:A:147:ILE:HD12	2.37	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:144:THR:HA	1:A:147:ILE:HG22	1.94	0.49
1:B:76:ARG:NH2	5:B:701:HOH:O	2.19	0.49
1:B:466:TYR:CD2	1:B:494:PHE:HD1	2.30	0.49
1:A:37:GLU:HG3	1:A:73:LEU:HD21	1.95	0.49
1:A:62:ASP:OD2	1:A:115:THR:OG1	2.21	0.49
1:A:307:SER:HB3	1:A:337:THR:HG23	1.93	0.49
1:A:356:PRO:HD3	1:A:476:TYR:CG	2.48	0.49
1:A:520:SER:HB2	1:A:539:LEU:HD12	1.95	0.49
1:A:64:ARG:NH2	1:A:119:ASN:O	2.30	0.49
1:B:223:ASP:OD2	1:B:225:MET:N	2.43	0.49
1:A:211:LEU:CD1	1:A:403:ALA:HA	2.42	0.49
1:B:356:PRO:HG2	1:B:361:PHE:CZ	2.48	0.49
1:B:283:PHE:CE1	1:B:395:VAL:HG23	2.48	0.48
1:B:473:ASN:ND2	1:B:489:GLY:H	2.11	0.48
1:A:43:ILE:N	1:A:147:ILE:HD11	2.28	0.48
1:A:19:THR:HG21	4:A:605:GOL:H32	1.95	0.48
1:B:89:GLY:HA3	1:B:94:LEU:HG	1.96	0.48
1:A:501:VAL:HG23	1:A:517:TYR:HD1	1.77	0.48
1:A:211:LEU:CG	1:A:218:LEU:HD22	2.43	0.48
1:A:417:TRP:O	1:A:421:GLY:N	2.46	0.48
1:B:334:SER:HG	1:B:337:THR:HG1	1.61	0.48
1:A:485:SER:HB3	1:A:488:GLN:HE21	1.79	0.48
1:B:409:VAL:HG13	1:B:410:GLU:N	2.29	0.48
1:A:118:HIS:O	1:A:262:PRO:HD2	2.13	0.48
1:B:56:THR:OG1	1:B:85:ARG:HB3	2.14	0.48
1:A:222:ILE:HG13	1:A:237:LEU:HD13	1.95	0.48
1:A:58:VAL:HG23	1:A:99:VAL:HG13	1.96	0.47
1:B:427:ARG:HD2	1:B:517:TYR:CE2	2.49	0.47
1:B:417:TRP:CE2	1:B:422:ARG:HD2	2.49	0.47
1:B:72:GLN:O	1:B:76:ARG:HG3	2.14	0.47
1:B:473:ASN:HD21	1:B:489:GLY:H	1.62	0.47
1:B:316:ASN:HD21	1:B:405[B]:ARG:HE	1.63	0.47
1:B:74:ILE:HG12	1:B:112:ILE:HD11	1.97	0.47
1:A:272:LEU:HD22	1:A:286:ALA:HB2	1.97	0.47
1:A:58:VAL:HG22	1:A:103:ILE:CD1	2.34	0.46
1:B:56:THR:HA	1:B:85:ARG:O	2.15	0.46
1:B:223:ASP:HA	1:B:249:VAL:O	2.15	0.46
1:A:525:VAL:HA	1:A:528:ILE:CG2	2.45	0.46
1:A:225:MET:HE1	1:A:263:GLY:O	2.15	0.46
1:A:377:GLU:HG3	1:A:425:PHE:HZ	1.80	0.46
1:A:515:ARG:NE	2:A:602:SO4:O3	2.46	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:305:ASN:HB3	1:B:308:ASP:HB2	1.98	0.46
1:A:28:VAL:O	1:A:32:SER:HB3	2.15	0.46
1:A:42:SER:C	1:A:147:ILE:CD1	2.89	0.46
1:B:67[A]:MET:HE1	1:B:93:ILE:HD13	1.98	0.46
1:B:305:ASN:OD1	1:B:307:SER:N	2.49	0.46
1:B:485:SER:HB3	1:B:488:GLN:HE21	1.81	0.46
1:A:211:LEU:HD13	1:A:403:ALA:CA	2.46	0.46
1:B:283:PHE:HZ	1:B:395:VAL:HG23	1.81	0.46
1:A:211:LEU:CD2	1:A:218:LEU:HD22	2.46	0.46
1:A:208:LEU:HB3	1:A:241:LEU:CD1	2.45	0.45
1:B:481:ASP:OD1	1:B:483:SER:N	2.48	0.45
1:B:377:GLU:OE1	1:B:427:ARG:HD3	2.16	0.45
1:B:425:PHE:HE2	5:B:748:HOH:O	1.98	0.45
1:A:387:ARG:NE	5:A:701:HOH:O	2.14	0.45
1:A:323:PHE:HE2	1:A:372:SER:HB3	1.80	0.45
1:B:371:LEU:HD21	1:B:374:CYS:HB3	1.97	0.45
1:B:253:PRO:HB3	5:B:706:HOH:O	2.15	0.45
1:A:473:ASN:CG	1:A:487:ASN:HA	2.41	0.45
1:B:367:ASP:OD2	1:B:387:ARG:NE	2.38	0.45
1:A:17:PRO:HG3	1:A:39:PHE:CZ	2.51	0.45
1:A:202:ILE:HD11	1:A:203:PHE:CZ	2.51	0.45
1:A:59:VAL:HG22	1:A:88:ILE:HG12	1.98	0.45
1:A:505[B]:SER:HB2	2:A:602:SO4:O1	2.17	0.45
1:B:392:LEU:HA	1:B:395:VAL:HG12	1.98	0.45
1:B:441:MET:HG3	1:B:547:SER:O	2.16	0.45
1:A:419:LYS:NZ	5:A:723:HOH:O	2.49	0.45
1:B:356:PRO:HG2	1:B:361:PHE:CE2	2.52	0.45
1:B:369:SER:HA	5:B:720:HOH:O	2.17	0.45
1:A:461:ALA:O	1:A:463:ASP:N	2.50	0.44
1:B:208:LEU:HB2	1:B:241:LEU:HD22	1.99	0.44
1:B:386:ILE:HA	1:B:386:ILE:HD13	1.57	0.44
1:A:100:SER:OG	1:A:386[A]:ILE:HG23	2.17	0.44
1:B:67[B]:MET:HE3	1:B:71:ILE:HD11	1.98	0.44
1:A:94:LEU:HD13	1:A:99:VAL:HG22	1.99	0.44
1:A:103:ILE:HD13	1:A:103:ILE:HA	1.74	0.44
1:A:117:SEP:OG	1:A:118:HIS:N	2.50	0.44
1:A:198:MET:O	1:A:201[A]:SER:OG	2.33	0.44
1:B:248:ALA:HB1	1:B:251:CYS:SG	2.57	0.44
1:B:281:HIS:CE1	1:B:300:HIS:N	2.85	0.44
1:B:316:ASN:ND2	1:B:405[A]:ARG:HD3	2.32	0.44
1:B:417:TRP:HB3	1:B:528:ILE:HG21	1.99	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:365:LEU:C	5:B:704:HOH:O	2.60	0.44
1:A:466:TYR:HB3	1:A:494:PHE:CD2	2.53	0.44
1:B:67[B]:MET:CE	1:B:71:ILE:HD11	2.48	0.44
1:A:1:MET:HE2	1:A:1:MET:HB2	1.82	0.44
1:A:64:ARG:CZ	1:A:116:ALA:HB3	2.48	0.44
1:B:198:MET:O	1:B:201[A]:SER:OG	2.35	0.44
1:B:427:ARG:HE	1:B:515:ARG:HD3	1.82	0.44
1:B:428:TYR:CD1	1:B:558:PRO:HG3	2.52	0.44
1:A:87:VAL:HA	1:A:187:GLU:O	2.17	0.44
1:A:64:ARG:NH2	1:A:117:SEP:O	2.43	0.43
1:A:433:VAL:HG22	1:A:512:ALA:O	2.17	0.43
1:B:307:SER:CB	1:B:338:SER:HB3	2.47	0.43
1:B:492[A]:LEU:HB3	1:B:494:PHE:HE2	1.82	0.43
1:A:118:HIS:HB3	5:A:796:HOH:O	2.17	0.43
1:B:270:ALA:HA	1:B:273:VAL:HG22	2.00	0.43
1:B:276:MET:O	1:B:281:HIS:CE1	2.71	0.43
1:A:461:ALA:C	1:A:463:ASP:H	2.26	0.43
1:A:23:ARG:HH22	1:A:117:SEP:HB2	1.82	0.43
1:A:58:VAL:CG2	1:A:103:ILE:HD11	2.33	0.43
1:A:295:MET:HE2	1:A:295:MET:HB3	1.89	0.43
1:A:424:PHE:CE2	1:A:535:MET:HG3	2.53	0.43
1:A:17:PRO:HG3	1:A:39:PHE:HZ	1.83	0.43
1:A:212:LEU:HD23	1:A:212:LEU:HA	1.78	0.43
1:A:323:PHE:CE2	1:A:372:SER:HB3	2.54	0.43
1:A:102:ILE:O	1:A:106:ILE:HG12	2.19	0.43
1:B:466:TYR:HB3	1:B:494:PHE:HD1	1.82	0.43
1:B:478:ASP:HB3	1:B:481:ASP:OD1	2.19	0.43
1:A:212:LEU:CD2	1:A:218:LEU:HD21	2.48	0.43
1:A:343:ARG:NH2	1:A:521:TYR:CZ	2.87	0.43
1:B:72:GLN:HB2	1:B:76:ARG:HH12	1.83	0.43
1:B:65:PHE:N	1:B:255:GLU:O	2.46	0.43
1:B:220:ILE:HD11	1:B:243:ALA:CB	2.48	0.43
1:A:211:LEU:CD2	1:A:218:LEU:HD21	2.49	0.43
1:A:343:ARG:CZ	1:A:521:TYR:CZ	3.01	0.43
1:B:285:ALA:HA	1:B:295:MET:O	2.19	0.43
1:A:39:PHE:O	1:A:43:ILE:HG22	2.19	0.42
1:B:15:GLN:OE1	1:B:151:SER:HB2	2.19	0.42
1:A:237:LEU:HD23	1:A:241:LEU:HD21	2.02	0.42
1:B:72:GLN:HG2	1:B:72:GLN:H	1.66	0.42
1:B:335:MET:HG3	1:B:336:PRO:CD	2.50	0.42
1:A:233:VAL:O	1:A:237:LEU:HB2	2.19	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:478:ASP:HA	1:B:479:PRO:HD3	1.85	0.42
1:A:442:MET:HG3	1:A:504:LEU:HD13	2.01	0.42
1:B:551:GLU:OE1	1:B:551:GLU:N	2.47	0.42
1:A:335:MET:N	1:A:355:THR:O	2.47	0.42
1:A:461:ALA:C	1:A:463:ASP:N	2.78	0.42
1:A:40:ILE:HD13	1:A:74:ILE:CG1	2.50	0.42
1:B:62:ASP:HA	1:B:228:VAL:HB	2.02	0.42
1:B:112:ILE:HD13	1:B:112:ILE:HG21	1.74	0.42
1:B:208:LEU:HD23	1:B:208:LEU:HA	1.87	0.42
1:B:220:ILE:HD11	1:B:243:ALA:HB1	2.01	0.42
1:B:198:MET:HE2	1:B:198:MET:HB3	1.81	0.41
1:B:386:ILE:HG22	1:B:388:GLU:O	2.20	0.41
1:A:99:VAL:HG11	1:A:113:ILE:HG12	2.02	0.41
1:A:285:ALA:HA	1:A:295:MET:O	2.20	0.41
1:B:392:LEU:HD12	1:B:395:VAL:HG13	2.03	0.41
1:B:430:TYR:CE1	1:B:558:PRO:HA	2.55	0.41
1:A:58:VAL:HG11	1:A:102:ILE:CG2	2.49	0.41
1:A:35:TYR:HB3	5:A:708:HOH:O	2.20	0.41
1:B:269:ALA:O	1:B:273:VAL:HG13	2.20	0.41
1:A:80:ALA:HB2	1:A:160:CYS:SG	2.60	0.41
1:B:335:MET:HE3	1:B:335:MET:O	2.21	0.41
1:B:208:LEU:HB2	1:B:241:LEU:CD2	2.51	0.41
1:B:270:ALA:O	1:B:273:VAL:HG22	2.20	0.41
1:A:85:ARG:HA	1:A:185:THR:O	2.20	0.41
1:A:353:TYR:CD1	1:A:365:LEU:HD13	2.56	0.41
1:A:490:LEU:O	1:A:501:VAL:HA	2.21	0.41
1:A:180:LYS:HD3	1:A:180:LYS:HA	1.87	0.41
1:A:198:MET:HB3	1:A:198:MET:HE2	1.84	0.40
1:B:100:SER:OG	1:B:386:ILE:HG23	2.22	0.40
1:A:58:VAL:CG2	1:A:99:VAL:HG13	2.51	0.40
1:A:257:PHE:CD2	1:A:262:PRO:HG3	2.56	0.40
1:A:59:VAL:HG11	1:A:74:ILE:HG21	2.03	0.40
1:A:473:ASN:ND2	1:A:487:ASN:HA	2.36	0.40
1:A:524:ASP:HB3	1:A:527:LYS:HG3	2.03	0.40
1:B:295:MET:HG3	1:B:379:PHE:HE2	1.87	0.40
1:B:320:ILE:HB	1:B:323:PHE:HD2	1.86	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	564/585 (96%)	545 (97%)	17 (3%)	2 (0%)	30	49
1	B	550/585 (94%)	506 (92%)	42 (8%)	2 (0%)	30	49
All	All	1114/1170 (95%)	1051 (94%)	59 (5%)	4 (0%)	30	49

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	154	ILE
1	B	300	HIS
1	A	462	ASN
1	B	511	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	417/481 (87%)	413 (99%)	4 (1%)	68	86
1	B	304/481 (63%)	300 (99%)	4 (1%)	61	82
All	All	721/962 (75%)	713 (99%)	8 (1%)	68	84

All (8) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	202	ILE
1	A	445	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	561[A]	ILE
1	A	561[B]	ILE
1	B	335	MET
1	B	338	SER
1	B	381	THR
1	B	386	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (8) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	34	ASN
1	A	51	GLN
1	A	246	ASN
1	B	72	GLN
1	B	316	ASN
1	B	439	ASN
1	B	473	ASN
1	B	488	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

2 non-standard protein/DNA/RNA residues are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
1	SEP	B	117	3,1	8,9,10	1.56	1 (12%)	7,12,14	2.45	1 (14%)
1	SEP	A	117	3,1	8,9,10	1.53	2 (25%)	7,12,14	1.61	1 (14%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral

centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	SEP	B	117	3,1	-	2/6/8/10	-
1	SEP	A	117	3,1	-	5/6/8/10	-

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	117	SEP	P-O1P	3.21	1.60	1.50
1	A	117	SEP	P-O1P	2.91	1.59	1.50
1	A	117	SEP	P-O2P	2.18	1.62	1.54

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	117	SEP	OG-CB-CA	5.68	113.67	108.14
1	A	117	SEP	OG-CB-CA	3.46	111.51	108.14

There are no chirality outliers.

All (7) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	A	117	SEP	C-CA-CB-OG
1	A	117	SEP	CB-OG-P-O2P
1	A	117	SEP	CB-OG-P-O3P
1	B	117	SEP	N-CA-CB-OG
1	A	117	SEP	CB-OG-P-O1P
1	B	117	SEP	CB-OG-P-O1P
1	A	117	SEP	N-CA-CB-OG

There are no ring outliers.

1 monomer is involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	A	117	SEP	3	0

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry

Of 7 ligands modelled in this entry, 2 are monoatomic - leaving 5 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	SO4	A	602	-	4,4,4	0.18	0	6,6,6	0.32	0
2	SO4	A	601	-	4,4,4	0.28	0	6,6,6	0.16	0
4	GOL	A	605	-	5,5,5	0.27	0	5,5,5	0.52	0
2	SO4	A	603	-	4,4,4	0.28	0	6,6,6	0.21	0
2	SO4	B	601	-	4,4,4	0.25	0	6,6,6	0.11	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
4	GOL	A	605	-	-	0/4/4/4	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

4 monomers are involved in 9 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	602	SO4	3	0
4	A	605	GOL	2	0
2	A	603	SO4	1	0
2	B	601	SO4	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	560/585 (95%)	0.12	10 (1%) 67 64	14, 42, 76, 118	8 (1%)
1	B	551/585 (94%)	0.98	80 (14%) 6 5	22, 67, 121, 175	7 (1%)
All	All	1111/1170 (94%)	0.54	90 (8%) 18 15	14, 52, 108, 175	15 (1%)

All (90) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	260	HIS	5.8
1	B	179	ASN	5.1
1	B	461	ALA	4.9
1	B	557	ALA	4.8
1	B	44	ILE	4.7
1	B	5	VAL	4.4
1	B	268	TYR	4.2
1	B	471	ALA	4.0
1	B	127	PHE	4.0
1	B	434	GLU	3.9
1	B	263	GLY	3.7
1	B	124	ASN	3.6
1	B	158	ALA	3.6
1	A	462	ASN	3.6
1	B	246	ASN	3.6
1	B	261	HIS	3.6
1	B	264	PRO	3.6
1	B	269	ALA	3.5
1	B	448	LEU	3.5
1	B	433	VAL	3.5
1	B	20	SER	3.4
1	B	420	TYR	3.4
1	B	265	ASN	3.3
1	A	264	PRO	3.3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	B	556	THR	3.3
1	B	527	LYS	3.3
1	B	51	GLN	3.2
1	B	432	GLU	3.2
1	B	147	ILE	3.2
1	B	65	PHE	3.1
1	B	278	SER	3.0
1	B	7	VAL	3.0
1	B	10	GLN	3.0
1	B	438	ALA	3.0
1	B	502	PHE	3.0
1	B	39	PHE	2.9
1	B	504	LEU	2.9
1	B	474	PHE	2.9
1	B	505	SER	2.8
1	B	511	GLY	2.8
1	A	40	ILE	2.8
1	B	462	ASN	2.8
1	B	510	ALA	2.8
1	B	123	PRO	2.7
1	B	280	GLU	2.7
1	B	425	PHE	2.7
1	A	507	THR	2.7
1	B	281	HIS	2.7
1	B	524	ASP	2.6
1	B	178	GLU	2.6
1	B	494	PHE	2.6
1	B	435	ALA	2.6
1	B	29	PHE	2.5
1	B	2	VAL	2.5
1	B	226	HIS	2.5
1	A	461	ALA	2.5
1	B	543	ALA	2.5
1	B	444	ASP	2.5
1	B	257	PHE	2.5
1	A	511	GLY	2.5
1	A	510	ALA	2.5
1	B	301	GLY	2.4
1	B	155	GLU	2.4
1	B	553	THR	2.4
1	B	534	VAL	2.4
1	B	182	LYS	2.3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	B	142	ALA	2.3
1	B	262	PRO	2.3
1	B	552	ARG	2.3
1	A	0	ASN	2.2
1	B	208	LEU	2.2
1	B	459	PHE	2.2
1	B	460	SER	2.2
1	B	463	ASP	2.2
1	B	457	LYS	2.1
1	B	458	GLN	2.1
1	B	153	THR	2.1
1	B	4	ILE	2.1
1	A	268	TYR	2.1
1	B	42	SER	2.1
1	B	479	PRO	2.1
1	B	243	ALA	2.1
1	B	303	PHE	2.1
1	B	122	GLY	2.1
1	B	437	GLY	2.1
1	B	274	GLU	2.1
1	A	147	ILE	2.0
1	B	453	SER	2.0
1	B	273	VAL	2.0
1	B	539	LEU	2.0

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

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. 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
1	SEP	B	117	10/11	0.95	0.08	33,65,70,74	0
1	SEP	A	117	10/11	0.96	0.07	36,42,48,59	0

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	SO4	A	603	5/5	0.74	0.12	49,60,65,66	5
2	SO4	B	601	5/5	0.86	0.10	103,103,111,112	0
2	SO4	A	602	5/5	0.91	0.10	52,53,62,64	0
4	GOL	A	605	6/6	0.92	0.11	59,61,63,65	0
2	SO4	A	601	5/5	0.94	0.07	51,59,65,65	5
3	CA	B	602	1/1	0.99	0.03	39,39,39,39	0
3	CA	A	604	1/1	1.00	0.02	25,25,25,25	0

6.5 Other polymers [i](#)

There are no such residues in this entry.