



Full wwPDB X-ray Structure Validation Report ⓘ

May 27, 2020 – 12:45 am BST

PDB ID : 5VIN
Title : Crystal Structure of the R515Q missense variant of human PGM1
Authors : Stiers, K.M.; Beamer, L.J.
Deposited on : 2017-04-17
Resolution : 2.60 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 following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.11
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0158
CCP4 : 7.0.044 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.11

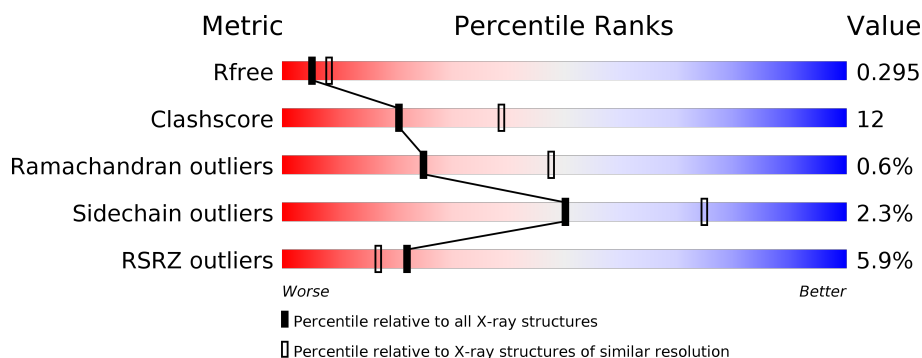
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.60 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}	130704	3163 (2.60-2.60)
Clashscore	141614	3518 (2.60-2.60)
Ramachandran outliers	138981	3455 (2.60-2.60)
Sidechain outliers	138945	3455 (2.60-2.60)
RSRZ outliers	127900	3104 (2.60-2.60)

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 on 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	<div> <div>3%</div> <div> <div></div> <div>75%</div> <div>20%</div> <div>• •</div> </div> </div>
1	B	585	<div> <div>9%</div> <div> <div></div> <div>72%</div> <div>22%</div> <div>• •</div> </div> </div>

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 8281 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	564	Total	C	N	O	S	0	5	0
			4200	2670	714	799	17			
1	B	560	Total	C	N	O	S	0	3	0
			3887	2445	679	747	16			

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	515	GLN	ARG	engineered mutation	UNP P36871
B	-22	MET	-	expression tag	UNP P36871

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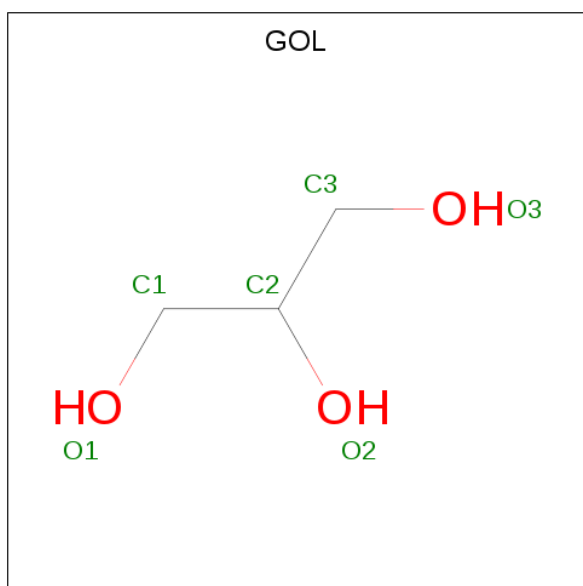
Chain	Residue	Modelled	Actual	Comment	Reference
B	-21	HIS	-	expression tag	UNP P36871
B	-20	HIS	-	expression tag	UNP P36871
B	-19	HIS	-	expression tag	UNP P36871
B	-18	HIS	-	expression tag	UNP P36871
B	-17	HIS	-	expression tag	UNP P36871
B	-16	HIS	-	expression tag	UNP P36871
B	-15	SER	-	expression tag	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	515	GLN	ARG	engineered mutation	UNP P36871

- Molecule 2 is SULFATE ION (three-letter code: 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	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	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
2	B	1	Total O S 5 4 1	0	0
2	B	1	Total O S 5 4 1	0	0
2	B	1	Total O S 5 4 1	0	0

- Molecule 3 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).



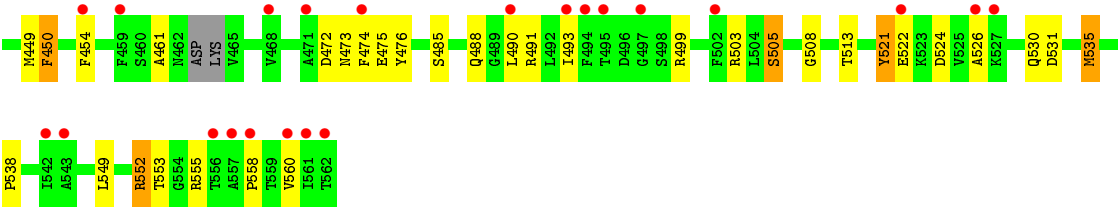
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total C O 6 3 3	0	0
3	A	1	Total C O 6 3 3	0	0
3	A	1	Total C O 6 3 3	0	0
3	A	1	Total C O 6 3 3	0	0
3	B	1	Total C O 6 3 3	0	0
3	B	1	Total C O 6 3 3	0	0

- Molecule 4 is COBALT (II) ION (three-letter code: CO) (formula: Co).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	B	1	Total Co 1 1	0	0
4	A	1	Total Co 1 1	0	0

- Molecule 5 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	63	Total O 63 63	0	0
5	B	28	Total O 28 28	0	0



4 Data and refinement statistics

Property	Value	Source
Space group	P 41 21 2	Depositor
Cell constants a, b, c, α , β , γ	173.96 Å 173.96 Å 99.48 Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	61.50 – 2.60 61.50 – 2.60	Depositor EDS
% Data completeness (in resolution range)	98.9 (61.50-2.60) 99.0 (61.50-2.60)	Depositor EDS
R_{merge}	0.18	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.81 (at 2.61 Å)	Xtriage
Refinement program	PHENIX 1.11.1 _2575	Depositor
R, R_{free}	0.239 , 0.295 0.239 , 0.295	Depositor DCC
R_{free} test set	2385 reflections (5.08%)	wwPDB-VP
Wilson B-factor (Å ²)	50.5	Xtriage
Anisotropy	0.721	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 75.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.46$, $\langle L^2 \rangle = 0.28$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	8281	wwPDB-VP
Average B, all atoms (Å ²)	71.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.37% 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

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: GOL, CO, SO4

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	0.50	1/4299 (0.0%)	0.76	5/5841 (0.1%)
1	B	0.51	2/3972 (0.1%)	0.79	4/5413 (0.1%)
All	All	0.51	3/8271 (0.0%)	0.77	9/11254 (0.1%)

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	35	TYR	CD2-CE2	-5.43	1.31	1.39
1	A	238	CYS	CB-SG	-5.35	1.73	1.81
1	B	101	CYS	CB-SG	-5.20	1.73	1.81

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	503	ARG	NE-CZ-NH1	-7.13	116.73	120.30
1	A	503	ARG	NE-CZ-NH2	6.60	123.60	120.30
1	A	218	LEU	CB-CG-CD1	-6.37	100.17	111.00
1	A	539	LEU	CB-CG-CD1	-5.75	101.23	111.00
1	B	349	LYS	CA-CB-CG	-5.59	101.10	113.40
1	B	218	LEU	CA-CB-CG	5.33	127.56	115.30
1	A	441	MET	CG-SD-CE	5.14	108.43	100.20
1	B	535	MET	CA-CB-CG	-5.07	104.68	113.30
1	B	343	ARG	CB-CG-CD	-5.04	98.51	111.60

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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	4200	0	4034	84	0
1	B	3887	0	3327	108	0
2	A	45	0	0	0	0
2	B	20	0	0	1	0
3	A	24	0	32	2	0
3	B	12	0	16	1	0
4	A	1	0	0	0	0
4	B	1	0	0	0	0
5	A	63	0	0	8	0
5	B	28	0	0	1	0
All	All	8281	0	7409	192	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 12.

All (192) 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:B:472:ASP:OD2	1:B:473:ASN:N	2.03	0.91
1:B:503:ARG:HH21	3:B:606:GOL:H32	1.35	0.90
1:B:270:ALA:O	1:B:273:VAL:HG12	1.71	0.90
1:B:76:ARG:NH1	1:B:163:LEU:O	2.07	0.87
1:B:444:ASP:OD2	1:B:552[A]:ARG:NH2	2.12	0.82
1:B:32:SER:HB3	1:B:35:TYR:CD2	2.14	0.81
1:B:59:VAL:HG22	1:B:88:ILE:HG12	1.61	0.79
1:B:218:LEU:HD23	1:B:282:ASP:HB2	1.65	0.79
1:B:211:LEU:HD11	1:B:218:LEU:HD12	1.64	0.78
1:B:552[A]:ARG:HH11	1:B:552[A]:ARG:HB3	1.51	0.76
1:A:199:LEU:HD23	1:A:396:LEU:HD12	1.69	0.74
1:B:491:ARG:HE	1:B:493:ILE:HD11	1.52	0.74
1:B:335:MET:N	1:B:355:THR:O	2.22	0.71
1:B:292:ASP:OD1	1:B:389[B]:LYS:NZ	2.23	0.69
1:A:426:THR:OG1	5:A:701:HOH:O	2.09	0.69
1:A:466:TYR:CZ	1:A:539:LEU:HD11	2.27	0.69
1:B:48:GLU:HB3	1:B:51:GLN:OE1	1.92	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:225:MET:HE3	1:B:263:ASP:N	2.08	0.68
1:B:218:LEU:CD2	1:B:282:ASP:HB2	2.23	0.68
1:A:70:ALA:O	1:A:74:ILE:HD12	1.92	0.68
1:B:521:TYR:HD1	1:B:522:GLU:N	1.91	0.67
1:B:68:LYS:H	1:B:68:LYS:HD3	1.58	0.67
1:A:380:GLY:O	5:A:702:HOH:O	2.12	0.66
1:A:166:ASP:OD2	5:A:703:HOH:O	2.15	0.64
1:A:321:PRO:HA	1:A:324:GLN:HG3	1.79	0.64
1:B:32:SER:O	1:B:35:TYR:HB2	1.98	0.63
1:A:15:GLN:OE1	1:A:151:SER:HB2	1.99	0.63
1:B:226:HIS:CD2	1:B:250:ASN:HB3	2.34	0.62
1:A:501:VAL:CG1	1:A:517:TYR:HB2	2.30	0.62
1:B:450:PHE:HD1	1:B:450:PHE:O	1.83	0.62
1:A:501:VAL:HG13	1:A:517:TYR:HB2	1.82	0.62
1:A:461:ALA:HB1	1:A:538:PRO:HB3	1.82	0.61
1:A:68:LYS:NZ	1:A:91:ASN:O	2.34	0.61
1:A:15:GLN:HG2	1:A:35:TYR:CZ	2.36	0.60
1:B:449:MET:HE1	1:B:490:LEU:HD22	1.82	0.60
1:B:218:LEU:HD11	1:B:402:LEU:HD22	1.82	0.59
1:B:85:ARG:HG2	1:B:86:LEU:N	2.17	0.59
1:B:446:GLU:HA	1:B:449:MET:HE2	1.85	0.59
1:B:474:PHE:CD1	1:B:491:ARG:NH1	2.70	0.58
1:A:130:LYS:NZ	5:A:707:HOH:O	2.32	0.58
1:B:433:VAL:HA	1:B:555:ARG:HH21	1.69	0.58
1:B:505:SER:HB3	1:B:513:THR:H	1.68	0.57
1:A:533:GLN:NE2	5:A:701:HOH:O	2.19	0.57
1:B:429:ASP:HB2	1:B:560:VAL:HG23	1.86	0.57
1:A:26:VAL:HG12	1:A:125:GLY:O	2.04	0.57
1:A:474:PHE:HD1	1:A:491:ARG:NH1	2.03	0.57
1:B:68:LYS:N	1:B:68:LYS:HD3	2.20	0.56
1:B:530:GLN:CB	1:B:535:MET:HG3	2.36	0.56
1:A:525:VAL:HA	1:A:528:ILE:HG13	1.88	0.56
1:A:339:GLY:HA2	1:A:342:ASP:OD1	2.06	0.55
1:B:491:ARG:NE	1:B:493:ILE:HD11	2.22	0.55
1:B:55:ALA:HB1	1:B:109:ILE:HD13	1.87	0.55
1:B:333:ARG:HB2	1:B:337:THR:HG23	1.89	0.55
1:B:461:ALA:HB3	1:B:538:PRO:HB3	1.88	0.55
1:B:237:LEU:HD23	1:B:241:LEU:HD12	1.89	0.54
1:A:405:ARG:HH21	1:A:407:GLN:NE2	2.04	0.54
1:B:44:ILE:O	1:B:47:VAL:HG12	2.08	0.54
1:B:53:GLN:O	1:B:84:GLY:HA3	2.07	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:333:ARG:HB2	1:B:337:THR:CG2	2.38	0.54
1:A:507:THR:O	1:A:509:SER:N	2.36	0.53
1:B:23:ARG:HH22	1:B:508:GLY:H	1.57	0.53
1:B:222:ILE:HD12	1:B:237:LEU:CD1	2.39	0.53
1:A:37:GLU:HA	1:A:73:LEU:HD21	1.91	0.53
1:B:245:ALA:N	2:B:604:SO4:O4	2.42	0.53
1:B:428:TYR:CD2	1:B:558:PRO:HG3	2.45	0.52
1:B:433:VAL:CA	1:B:555:ARG:HH21	2.22	0.52
1:B:222:ILE:HD12	1:B:237:LEU:HD13	1.92	0.52
1:B:28:VAL:O	1:B:35:TYR:HE2	1.92	0.52
1:B:371:LEU:HD21	1:B:374:CYS:HB3	1.92	0.52
1:B:343:ARG:CZ	1:B:521:TYR:HE2	2.22	0.52
1:A:14:ASP:OD2	1:A:24:LYS:NZ	2.42	0.52
1:B:338:SER:HB3	1:B:425:PHE:CD1	2.45	0.52
1:B:43:ILE:HD11	1:B:131:PHE:CD1	2.45	0.51
1:B:306:PRO:HG3	1:B:379:PHE:CD2	2.46	0.51
1:B:430:TYR:O	1:B:513:THR:HA	2.10	0.51
1:B:505:SER:CB	1:B:513:THR:H	2.23	0.51
1:B:392:LEU:HD12	1:B:395:VAL:CG2	2.40	0.51
1:B:429:ASP:HB2	1:B:560:VAL:CG2	2.41	0.51
1:A:331:PHE:HB3	1:A:341:LEU:HD21	1.92	0.50
1:B:28:VAL:O	1:B:35:TYR:CE2	2.64	0.50
1:B:335:MET:HB2	1:B:474:PHE:CE2	2.46	0.50
1:B:392:LEU:HD12	1:B:395:VAL:HG23	1.94	0.49
1:B:485:SER:HB2	1:B:488:GLN:OE1	2.12	0.49
1:B:440:LYS:CB	1:B:552[A]:ARG:HH22	2.26	0.48
1:B:334:SER:HB3	1:B:376:GLU:HG2	1.95	0.48
1:A:528:ILE:HD12	1:A:529:ASN:N	2.29	0.48
1:B:39:PHE:O	1:B:43:ILE:HG22	2.14	0.48
1:A:427:ARG:HD3	1:A:429:ASP:OD1	2.14	0.48
1:B:225:MET:HE3	1:B:262:PRO:C	2.35	0.48
1:A:474:PHE:HB2	1:A:491:ARG:HD2	1.96	0.48
1:A:503:ARG:HH11	1:A:503:ARG:HD3	1.47	0.47
1:B:138:PRO:HD2	1:B:359:TRP:CD1	2.49	0.47
1:B:337:THR:HB	1:B:377:GLU:N	2.29	0.47
1:B:337:THR:HB	1:B:377:GLU:H	1.79	0.47
1:B:211:LEU:HD22	1:B:403:ALA:HB2	1.95	0.47
1:B:549:LEU:O	1:B:553:THR:HG22	2.15	0.47
1:B:56:THR:HA	1:B:85:ARG:O	2.15	0.47
1:A:366:MET:HG3	1:A:371:LEU:HD23	1.97	0.47
1:B:88:ILE:O	1:B:188:ILE:HA	2.15	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:405:ARG:HH21	1:A:407:GLN:HE22	1.62	0.47
1:B:209:LYS:O	1:B:213:SER:OG	2.31	0.46
1:B:85:ARG:HA	1:B:185:THR:O	2.15	0.46
1:B:237:LEU:HD21	1:B:396:LEU:HD21	1.97	0.46
1:B:68:LYS:CD	1:B:68:LYS:H	2.24	0.46
1:A:472:ASP:OD1	1:A:491:ARG:HD3	2.15	0.46
1:A:222:ILE:HG13	1:A:237:LEU:HD13	1.97	0.46
1:A:502:PHE:CZ	1:A:516:LEU:HD13	2.51	0.46
1:A:503:ARG:NH1	1:A:517:TYR:OH	2.48	0.46
1:B:531:ASP:O	1:B:535:MET:HG2	2.15	0.46
1:A:221:ARG:O	1:A:284:GLY:HA2	2.16	0.45
1:A:40:ILE:HG22	1:A:77:ILE:HG21	1.99	0.45
1:B:141:GLU:O	1:B:144:THR:HG22	2.16	0.45
1:B:343:ARG:HA	1:B:343:ARG:HD3	1.73	0.45
1:A:223:ASP:O	1:A:286:ALA:HA	2.17	0.45
1:A:115:THR:OG1	1:A:290:ASP:HB3	2.17	0.45
1:B:377:GLU:OE1	1:B:427:ARG:HD2	2.17	0.45
1:A:-1:SER:C	1:A:1:MET:H	2.21	0.45
1:B:55:ALA:HB1	1:B:109:ILE:CD1	2.46	0.45
1:A:402:LEU:HD23	1:A:412:ILE:HD12	1.99	0.45
1:A:23[B]:ARG:HA	1:A:127:PHE:O	2.17	0.44
1:A:499:ARG:NE	5:A:713:HOH:O	2.44	0.44
1:B:218:LEU:HD22	1:B:220:ILE:HG22	1.98	0.44
1:A:464:LYS:HG2	1:A:465:VAL:N	2.32	0.44
1:A:114:LEU:HD22	1:A:114:LEU:N	2.32	0.44
1:A:449:MET:HE2	1:A:449:MET:HB2	1.52	0.44
1:A:466:TYR:CE1	1:A:539:LEU:HD11	2.53	0.44
1:B:234:LYS:NZ	1:B:252:VAL:HG22	2.33	0.44
1:B:14:ASP:OD1	1:B:14:ASP:N	2.49	0.44
1:A:217:ARG:HH21	3:A:610:GOL:C3	2.31	0.44
1:A:466:TYR:HB3	1:A:494:PHE:CD1	2.53	0.44
1:B:416:HIS:CE1	1:B:420:TYR:CD2	3.05	0.44
1:A:270:ALA:HA	1:A:273:VAL:HG12	2.00	0.43
1:A:422:ARG:HD3	1:A:424:PHE:CZ	2.53	0.43
1:B:552[A]:ARG:NH1	1:B:552[A]:ARG:HB3	2.27	0.43
1:A:23[A]:ARG:HA	1:A:127:PHE:O	2.18	0.43
1:A:76:ARG:NH1	5:A:704:HOH:O	2.16	0.43
1:B:450:PHE:O	1:B:450:PHE:CD1	2.66	0.43
1:A:504:LEU:HD11	1:A:512:ALA:HB1	2.00	0.43
1:B:225:MET:HE2	1:B:225:MET:HB2	1.95	0.43
1:A:15:GLN:HG2	1:A:35:TYR:OH	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:129:ILE:HD12	1:B:129:ILE:O	2.19	0.43
1:A:469:GLU:HB2	1:A:495:THR:HG22	2.01	0.43
1:A:270:ALA:O	1:A:273:VAL:HG12	2.17	0.43
1:A:55:ALA:HB1	1:A:109:ILE:HD13	1.99	0.43
1:A:441:MET:HE3	1:A:442:MET:HE3	2.00	0.42
1:A:505:SER:CB	1:A:513:THR:HB	2.49	0.42
1:B:62:ASP:HA	1:B:228:VAL:CG2	2.49	0.42
1:B:334:SER:OG	1:B:337:THR:HG22	2.19	0.42
1:B:34:ASN:O	1:B:38:ASN:ND2	2.52	0.42
1:B:449:MET:HA	1:B:454:PHE:CD1	2.55	0.42
1:A:399:LEU:HD23	1:A:402:LEU:HD12	2.01	0.42
1:A:552:ARG:HA	1:A:552:ARG:NE	2.33	0.42
1:B:352:LEU:HD13	1:B:352:LEU:C	2.40	0.42
1:A:-1:SER:O	1:A:1:MET:N	2.45	0.42
1:A:441:MET:HE1	1:A:514:ILE:HD13	2.00	0.42
1:A:419:LYS:HD3	1:A:420:TYR:CE2	2.55	0.42
1:A:172:LYS:NZ	5:A:716:HOH:O	2.52	0.42
1:A:1:MET:HA	1:A:176:ASP:O	2.20	0.42
1:A:321:PRO:O	1:A:324:GLN:HB2	2.20	0.42
1:A:343:ARG:HA	1:A:343:ARG:NH1	2.35	0.42
1:A:502:PHE:CE2	1:A:516:LEU:HD13	2.54	0.42
1:A:356:PRO:HB2	1:A:361:PHE:CE2	2.55	0.42
1:B:58:VAL:HG22	1:B:87:VAL:HG22	2.01	0.42
1:B:29:PHE:HA	1:B:35:TYR:CE2	2.54	0.42
1:B:398:TRP:O	1:B:402:LEU:HD12	2.20	0.42
1:A:208:LEU:HD13	1:A:396:LEU:HD22	2.02	0.41
1:A:356:PRO:HD3	1:A:476:TYR:CG	2.55	0.41
1:B:64:ARG:HH21	1:B:116:ALA:H	1.66	0.41
1:A:53:GLN:O	1:A:84:GLY:HA3	2.19	0.41
1:B:356:PRO:HD3	1:B:476:TYR:CG	2.55	0.41
1:B:386:ILE:HD11	1:B:390:ASP:HB2	2.02	0.41
1:B:433:VAL:HA	1:B:555:ARG:NH2	2.34	0.41
1:B:44:ILE:HG21	1:B:81:ASN:CB	2.50	0.41
1:A:329:ARG:HG3	1:A:372:SER:OG	2.20	0.41
1:B:58:VAL:HG21	1:B:102:ILE:HG22	2.02	0.41
1:A:332:ALA:O	1:A:374:CYS:HA	2.21	0.41
1:A:492[A]:LEU:HB2	1:A:500:ILE:HB	2.02	0.41
1:A:217:ARG:HH21	3:A:610:GOL:H32	1.85	0.41
1:B:524:ASP:OD1	1:B:526:ALA:HB3	2.21	0.41
1:A:343:ARG:HD2	1:A:343:ARG:HH11	1.76	0.41
1:B:115:THR:OG1	1:B:290:ASP:HB3	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:488:GLN:HA	1:B:488:GLN:NE2	2.36	0.41
1:A:198:MET:HG2	1:A:202:ILE:HD12	2.03	0.40
1:A:449:MET:HG2	1:A:454:PHE:CE2	2.56	0.40
1:A:469:GLU:HB2	1:A:495:THR:CG2	2.51	0.40
1:A:313:ILE:HG21	1:A:313:ILE:HD13	1.88	0.40
1:B:342:ASP:OD1	1:B:352:LEU:HD11	2.21	0.40
1:A:525:VAL:HA	1:A:528:ILE:CG1	2.51	0.40
1:B:475:GLU:HG2	5:B:709:HOH:O	2.20	0.40
1:B:335:MET:O	1:B:499:ARG:NH2	2.53	0.40
1:B:40:ILE:HA	1:B:43:ILE:CG2	2.51	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	567/585 (97%)	551 (97%)	10 (2%)	6 (1%)	14	30
1	B	559/585 (96%)	539 (96%)	19 (3%)	1 (0%)	47	71
All	All	1126/1170 (96%)	1090 (97%)	29 (3%)	7 (1%)	25	47

All (7) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	462	ASN
1	A	507	THR
1	B	505	SER
1	A	0	ASN
1	A	463	ASP
1	A	508	GLY
1	A	487	ASN

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	423/483 (88%)	416 (98%)	7 (2%)	60	81
1	B	321/483 (66%)	308 (96%)	13 (4%)	31	57
All	All	744/966 (77%)	724 (97%)	20 (3%)	50	71

All (20) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	261	HIS
1	A	338	SER
1	A	342	ASP
1	A	346[A]	SER
1	A	346[B]	SER
1	A	453	SER
1	A	524	ASP
1	B	35	TYR
1	B	68	LYS
1	B	201	SER
1	B	210	GLU
1	B	282	ASP
1	B	329	ARG
1	B	389[A]	LYS
1	B	389[B]	LYS
1	B	445	LEU
1	B	450	PHE
1	B	521	TYR
1	B	552[A]	ARG
1	B	552[B]	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	407	GLN
1	B	281	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 carbohydrates in this entry.

5.6 Ligand geometry [i](#)

Of 21 ligands modelled in this entry, 2 are monoatomic - leaving 19 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	$\# Z > 2$
3	GOL	A	611	-	5,5,5	0.45	0	5,5,5	0.24	0
2	SO4	A	607	-	4,4,4	0.15	0	6,6,6	0.06	0
2	SO4	B	602	-	4,4,4	0.14	0	6,6,6	0.17	0
2	SO4	A	609	-	4,4,4	0.16	0	6,6,6	0.14	0
2	SO4	A	605	-	4,4,4	0.16	0	6,6,6	0.13	0
2	SO4	A	608	-	4,4,4	0.16	0	6,6,6	0.25	0
3	GOL	A	610	-	5,5,5	0.37	0	5,5,5	0.69	0
2	SO4	B	601	-	4,4,4	0.17	0	6,6,6	0.10	0
2	SO4	A	601	-	4,4,4	0.12	0	6,6,6	0.10	0
2	SO4	A	606	-	4,4,4	0.15	0	6,6,6	0.28	0
2	SO4	A	602	-	4,4,4	0.13	0	6,6,6	0.23	0
3	GOL	B	606	-	5,5,5	0.40	0	5,5,5	0.67	0
2	SO4	A	603	-	4,4,4	0.16	0	6,6,6	0.28	0
2	SO4	B	603	-	4,4,4	0.15	0	6,6,6	0.06	0
2	SO4	B	604	-	4,4,4	0.14	0	6,6,6	0.15	0
3	GOL	B	605	-	5,5,5	0.38	0	5,5,5	0.26	0
3	GOL	A	613	-	5,5,5	0.36	0	5,5,5	0.62	0
2	SO4	A	604	-	4,4,4	0.14	0	6,6,6	0.29	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	GOL	A	612	-	5,5,5	0.36	0	5,5,5	0.45	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
3	GOL	A	612	-	-	2/4/4/4	-
3	GOL	A	611	-	-	1/4/4/4	-
3	GOL	B	606	-	-	4/4/4/4	-
3	GOL	A	610	-	-	4/4/4/4	-
3	GOL	A	613	-	-	1/4/4/4	-
3	GOL	B	605	-	-	2/4/4/4	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (14) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	610	GOL	O1-C1-C2-C3
3	A	610	GOL	C1-C2-C3-O3
3	B	606	GOL	C1-C2-C3-O3
3	B	605	GOL	O1-C1-C2-C3
3	A	612	GOL	O1-C1-C2-C3
3	B	606	GOL	O1-C1-C2-C3
3	A	613	GOL	O1-C1-C2-C3
3	A	610	GOL	O1-C1-C2-O2
3	B	606	GOL	O2-C2-C3-O3
3	A	610	GOL	O2-C2-C3-O3
3	B	605	GOL	O1-C1-C2-O2
3	A	612	GOL	O1-C1-C2-O2
3	A	611	GOL	O1-C1-C2-C3
3	B	606	GOL	O1-C1-C2-O2

There are no ring outliers.

3 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	610	GOL	2	0
3	B	606	GOL	1	0
2	B	604	SO4	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 ⓘ

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	564/585 (96%)	-0.02	15 (2%) 54 48	28, 56, 98, 144	0
1	B	560/585 (95%)	0.40	51 (9%) 9 6	40, 81, 137, 185	0
All	All	1124/1170 (96%)	0.19	66 (5%) 22 17	28, 66, 123, 185	0

All (66) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	5	VAL	7.0
1	B	158	ALA	6.4
1	B	16	LYS	5.4
1	B	494	PHE	4.8
1	B	15	GLN	4.2
1	B	471	ALA	4.1
1	B	121	GLY	3.9
1	A	158	ALA	3.7
1	A	9	THR	3.6
1	B	468	VAL	3.6
1	B	42	SER	3.5
1	B	560	VAL	3.5
1	B	454	PHE	3.4
1	B	558	PRO	3.4
1	B	495	THR	3.3
1	B	493	ILE	3.3
1	B	154	ILE	3.2
1	B	127	PHE	3.2
1	B	562	THR	3.1
1	B	428	TYR	3.1
1	A	17	PRO	3.1
1	B	556	THR	3.0
1	B	177	LEU	3.0
1	B	424	PHE	2.9

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Mol	Chain	Res	Type	RSRZ
1	A	506	GLY	2.9
1	B	157	TYR	2.9
1	B	497	GLY	2.8
1	A	40	ILE	2.7
1	B	38	ASN	2.7
1	B	527	LYS	2.7
1	B	502	PHE	2.7
1	B	557	ALA	2.6
1	B	6	THR	2.6
1	B	526	ALA	2.6
1	A	509	SER	2.6
1	B	1	MET	2.5
1	B	276	MET	2.5
1	A	5	VAL	2.5
1	B	40	ILE	2.5
1	A	510	ALA	2.4
1	B	150	ILE	2.4
1	A	526	ALA	2.4
1	B	542	ILE	2.4
1	B	159	VAL	2.4
1	A	39	PHE	2.3
1	B	459	PHE	2.3
1	B	522	GLU	2.3
1	B	163	LEU	2.3
1	A	8	LYS	2.2
1	B	260	HIS	2.2
1	B	148	PHE	2.2
1	A	147	ILE	2.2
1	B	47	VAL	2.2
1	B	561	ILE	2.2
1	B	474	PHE	2.2
1	B	490	LEU	2.2
1	B	44	ILE	2.1
1	B	222	ILE	2.1
1	A	511	GLY	2.1
1	B	339	GLY	2.1
1	A	83	ILE	2.1
1	B	165	VAL	2.1
1	A	22	LEU	2.1
1	B	543	ALA	2.0
1	B	438	ALA	2.0
1	B	181	PHE	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 carbohydrates 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(\AA^2)	Q<0.9
2	SO4	A	608	5/5	0.60	0.37	138,141,143,144	0
3	GOL	A	612	6/6	0.69	0.30	65,79,90,97	0
3	GOL	B	605	6/6	0.75	0.26	114,115,123,130	0
2	SO4	B	601	5/5	0.75	0.20	137,137,141,145	0
2	SO4	B	603	5/5	0.78	0.17	151,151,152,153	0
3	GOL	A	611	6/6	0.79	0.20	66,74,84,92	0
2	SO4	A	602	5/5	0.80	0.25	127,130,133,137	0
3	GOL	A	613	6/6	0.81	0.18	84,95,100,106	0
3	GOL	B	606	6/6	0.83	0.13	73,89,94,95	0
2	SO4	A	604	5/5	0.83	0.28	103,105,113,117	0
2	SO4	A	605	5/5	0.83	0.17	145,148,149,153	0
2	SO4	A	609	5/5	0.84	0.27	154,155,156,159	0
2	SO4	B	602	5/5	0.85	0.16	131,133,134,135	0
2	SO4	B	604	5/5	0.85	0.17	144,149,151,151	0
2	SO4	A	607	5/5	0.89	0.16	139,141,142,145	0
3	GOL	A	610	6/6	0.93	0.23	58,60,77,91	0
2	SO4	A	601	5/5	0.94	0.19	99,101,104,104	0
2	SO4	A	606	5/5	0.95	0.17	81,85,90,101	0
4	CO	B	607	1/1	0.95	0.28	79,79,79,79	0
2	SO4	A	603	5/5	0.97	0.14	71,86,92,98	0
4	CO	A	614	1/1	0.99	0.25	55,55,55,55	0

6.5 Other polymers [i](#)

There are no such residues in this entry.