



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 1, 2026 – 01:23 AM UTC

PDB ID : 3ZW8 / pdb_00003zw8
Title : Crystal Structure Of Rat Peroxisomal Multifunctional Enzyme Type 1 (rpMFE1) In Apo Form
Authors : Kasaragod, P.; Schmitz, W.; Hiltunen, J.K.; Wierenga, R.K.
Deposited on : 2011-07-28
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

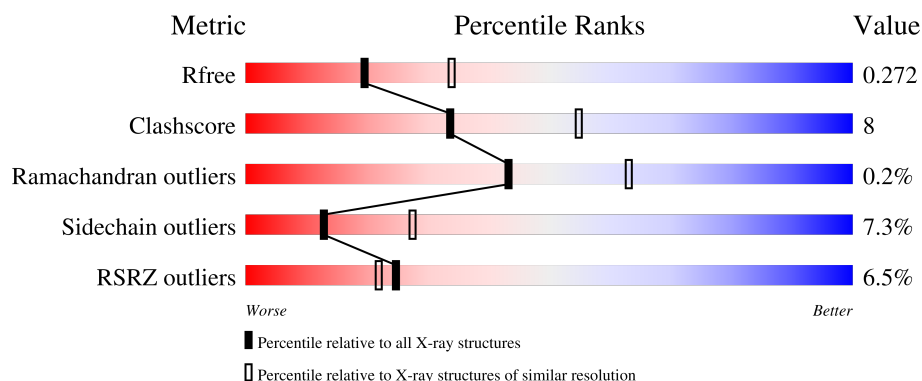
1 Overall quality at a glance

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	742	8% 78% 17% ..
1	B	742	5% 75% 20% ..

2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 11373 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 PEROXISOMAL BIFUNCTIONAL ENZYME.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	725	Total	C	N	O	S	0	0	0
			5562	3553	976	1010	23			
1	B	720	Total	C	N	O	S	0	0	0
			5530	3535	968	1004	23			

There are 40 discrepancies between the modelled and reference sequences:

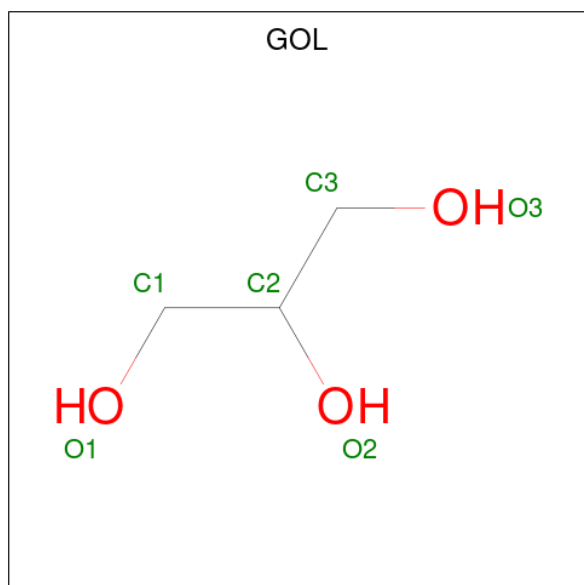
Chain	Residue	Modelled	Actual	Comment	Reference
A	-19	MET	-	expression tag	UNP P07896
A	-18	GLY	-	expression tag	UNP P07896
A	-17	SER	-	expression tag	UNP P07896
A	-16	SER	-	expression tag	UNP P07896
A	-15	HIS	-	expression tag	UNP P07896
A	-14	HIS	-	expression tag	UNP P07896
A	-13	HIS	-	expression tag	UNP P07896
A	-12	HIS	-	expression tag	UNP P07896
A	-11	HIS	-	expression tag	UNP P07896
A	-10	HIS	-	expression tag	UNP P07896
A	-9	SER	-	expression tag	UNP P07896
A	-8	SER	-	expression tag	UNP P07896
A	-7	GLY	-	expression tag	UNP P07896
A	-6	LEU	-	expression tag	UNP P07896
A	-5	VAL	-	expression tag	UNP P07896
A	-4	PRO	-	expression tag	UNP P07896
A	-3	ARG	-	expression tag	UNP P07896
A	-2	GLY	-	expression tag	UNP P07896
A	-1	SER	-	expression tag	UNP P07896
A	0	HIS	-	expression tag	UNP P07896
B	-19	MET	-	expression tag	UNP P07896
B	-18	GLY	-	expression tag	UNP P07896
B	-17	SER	-	expression tag	UNP P07896
B	-16	SER	-	expression tag	UNP P07896
B	-15	HIS	-	expression tag	UNP P07896

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
B	-14	HIS	-	expression tag	UNP P07896
B	-13	HIS	-	expression tag	UNP P07896
B	-12	HIS	-	expression tag	UNP P07896
B	-11	HIS	-	expression tag	UNP P07896
B	-10	HIS	-	expression tag	UNP P07896
B	-9	SER	-	expression tag	UNP P07896
B	-8	SER	-	expression tag	UNP P07896
B	-7	GLY	-	expression tag	UNP P07896
B	-6	LEU	-	expression tag	UNP P07896
B	-5	VAL	-	expression tag	UNP P07896
B	-4	PRO	-	expression tag	UNP P07896
B	-3	ARG	-	expression tag	UNP P07896
B	-2	GLY	-	expression tag	UNP P07896
B	-1	SER	-	expression tag	UNP P07896
B	0	HIS	-	expression tag	UNP P07896

- 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		

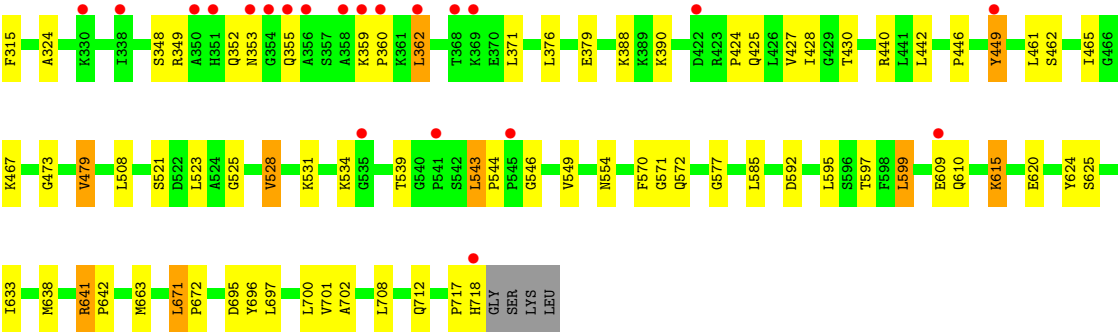
- Molecule 3 is SULFATE ION (CCD ID: SO4) (formula: O_4S).



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

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	148	Total	O	0	0
			148	148		
4	B	97	Total	O	0	0
			97	97		



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	65.22Å 125.68Å 226.43Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	100.00 – 2.50 100.00 – 2.50	Depositor EDS
% Data completeness (in resolution range)	86.2 (100.00-2.50) 86.2 (100.00-2.50)	Depositor EDS
R_{merge}	0.13	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	5.03 (at 2.51Å)	Xtriage
Refinement program	REFMAC 5.5.0109	Depositor
R, R_{free}	0.230 , 0.277 0.227 , 0.272	Depositor DCC
R_{free} test set	2872 reflections (5.09%)	wwPDB-VP
Wilson B-factor (Å ²)	25.9	Xtriage
Anisotropy	0.582	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 32.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.44$, $\langle L^2 \rangle = 0.26$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.89	EDS
Total number of atoms	11373	wwPDB-VP
Average B, all atoms (Å ²)	29.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.90% 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: SO4, 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	1.00	2/5691 (0.0%)	1.10	14/7709 (0.2%)
1	B	0.93	2/5658 (0.0%)	1.10	11/7666 (0.1%)
All	All	0.97	4/11349 (0.0%)	1.10	25/15375 (0.2%)

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	273	ALA	CA-CB	-6.41	1.43	1.53
1	B	266	ALA	N-CA	5.29	1.52	1.46
1	B	479	VAL	CA-CB	5.08	1.60	1.55
1	A	226	VAL	CA-CB	5.01	1.59	1.53

All (25) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	671	LEU	CA-C-N	-8.50	109.93	119.28
1	B	671	LEU	C-N-CA	-8.50	109.93	119.28
1	A	72	GLY	N-CA-C	7.56	119.86	111.85
1	B	24	VAL	CB-CA-C	-7.55	101.33	111.15
1	B	625	SER	N-CA-C	-7.52	103.17	111.36
1	A	671	LEU	CA-C-N	-7.32	111.22	119.28
1	A	671	LEU	C-N-CA	-7.32	111.22	119.28
1	A	227	LEU	N-CA-C	7.27	119.84	111.11
1	A	226	VAL	CB-CA-C	6.79	119.88	111.25
1	B	107	GLY	N-CA-C	-6.42	106.70	114.66
1	A	270	ALA	N-CA-C	-6.41	104.29	111.28
1	B	93	ILE	N-CA-C	6.34	116.95	107.51
1	A	18	ASN	CA-C-N	5.93	123.99	119.66
1	A	18	ASN	C-N-CA	5.93	123.99	119.66
1	A	555	SER	N-CA-C	5.83	118.98	108.48

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	592	ASP	CA-C-N	5.78	125.64	119.28
1	B	592	ASP	C-N-CA	5.78	125.64	119.28
1	A	445	ILE	N-CA-C	5.67	113.76	108.15
1	A	641	ARG	N-CA-C	5.61	113.27	108.22
1	A	592	ASP	CA-C-N	5.54	125.89	119.47
1	A	592	ASP	C-N-CA	5.54	125.89	119.47
1	B	135	THR	N-CA-CB	-5.34	101.53	110.39
1	B	528	VAL	N-CA-C	5.31	115.52	110.42
1	A	-2	GLY	N-CA-C	5.16	118.23	110.18
1	B	226	VAL	N-CA-C	5.11	115.46	107.99

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	5562	0	5667	75	0
1	B	5530	0	5636	99	0
2	A	6	0	8	2	0
3	A	15	0	0	0	0
3	B	15	0	0	2	0
4	A	148	0	0	12	0
4	B	97	0	0	25	0
All	All	11373	0	11311	173	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 8.

All (173) 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:635:GLU:HG2	4:A:2115:HOH:O	1.71	0.90
1:B:136:GLN:HG3	1:B:248:ILE:HD12	1.58	0.83
1:B:554:ASN:HB2	4:B:2077:HOH:O	1.77	0.82

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:589:HIS:HE1	4:A:2108:HOH:O	1.63	0.80
1:A:135:THR:HG21	1:A:235:SER:OG	1.82	0.80
1:A:136:GLN:HG3	1:A:248:ILE:HD12	1.63	0.79
1:B:219:VAL:HG22	1:B:229:PRO:HB2	1.64	0.79
1:B:145:PRO:HD2	4:B:2025:HOH:O	1.84	0.77
1:B:162:ALA:C	4:B:2027:HOH:O	2.27	0.77
1:B:122:PRO:O	1:B:125:THR:HB	1.85	0.77
1:B:663:MET:HA	1:B:663:MET:HE2	1.67	0.76
1:A:603:ARG:HD3	4:A:2112:HOH:O	1.85	0.76
1:A:71:PRO:HD2	1:A:259:ARG:HD2	1.67	0.75
1:B:135:THR:HG21	1:B:235:SER:OG	1.85	0.74
1:A:122:PRO:O	1:A:125:THR:HB	1.87	0.74
1:A:62:ASP:HB3	4:A:2008:HOH:O	1.89	0.73
1:A:382:PHE:HE1	1:A:531:LYS:HZ3	1.38	0.70
1:B:135:THR:HB	1:B:251:GLU:OE2	1.92	0.69
1:A:382:PHE:CE1	1:A:531:LYS:NZ	2.60	0.68
1:B:160:ASP:OD1	1:B:164:ARG:NH2	2.28	0.66
1:B:168:LEU:HG	4:B:2027:HOH:O	1.95	0.65
1:A:382:PHE:HE1	1:A:531:LYS:NZ	1.94	0.65
1:B:554:ASN:CB	4:B:2077:HOH:O	2.40	0.64
1:B:348:SER:O	1:B:352:GLN:HG3	1.96	0.64
1:B:250:GLU:HB2	4:B:2034:HOH:O	1.99	0.63
1:B:440:ARG:O	1:B:467:LYS:HB3	1.98	0.63
1:A:663:MET:HA	1:A:663:MET:HE2	1.83	0.61
1:B:158:SER:HB3	1:B:355:GLN:HG2	1.82	0.61
1:B:717:PRO:HA	4:B:2084:HOH:O	2.00	0.60
1:B:219:VAL:CG2	1:B:229:PRO:HB2	2.32	0.59
1:B:68:ALA:HB2	1:B:260:ALA:HA	1.84	0.59
1:A:135:THR:HB	1:A:251:GLU:OE1	2.04	0.58
1:A:160:ASP:OD1	1:A:164:ARG:NH2	2.37	0.58
1:A:96:VAL:HG13	1:A:98:LEU:HG	1.87	0.57
1:A:675:LEU:HD12	1:A:701:VAL:HG11	1.87	0.57
1:B:168:LEU:N	4:B:2027:HOH:O	2.38	0.56
1:B:615:LYS:HE3	4:B:2067:HOH:O	2.06	0.56
1:A:294:GLN:HB3	4:A:2053:HOH:O	2.05	0.55
1:B:425:GLN:CD	4:B:2057:HOH:O	2.50	0.55
1:B:245:GLU:HG3	4:B:2037:HOH:O	2.06	0.55
1:B:424:PRO:HD2	4:B:2057:HOH:O	2.05	0.55
1:B:708:LEU:C	1:B:708:LEU:HD23	2.32	0.54
1:A:428:ILE:HG13	1:A:446:PRO:HA	1.90	0.54
1:B:33:ARG:NH1	1:B:81:GLU:OE1	2.35	0.54

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:425:GLN:HA	1:B:449:TYR:O	2.08	0.54
1:B:129:LEU:HD12	1:B:129:LEU:C	2.33	0.53
1:B:641:ARG:HB2	1:B:642:PRO:HD2	1.91	0.53
1:A:525:GLY:O	1:A:528:VAL:HG12	2.08	0.53
1:A:497:GLU:OE1	1:A:611:ARG:NH1	2.42	0.53
1:B:162:ALA:CB	4:B:2027:HOH:O	2.57	0.53
1:B:525:GLY:O	1:B:528:VAL:HG12	2.09	0.53
1:B:97:ALA:HB3	1:B:119:VAL:HG12	1.91	0.52
1:B:162:ALA:HB1	4:B:2027:HOH:O	2.09	0.52
1:B:633:ILE:HG23	1:B:638:MET:HB2	1.92	0.52
1:B:125:THR:HG21	4:B:2021:HOH:O	2.10	0.52
1:B:349:ARG:O	1:B:353:ASN:HB2	2.08	0.52
1:A:-1:SER:N	1:A:31:GLU:OE2	2.43	0.52
1:A:219:VAL:HG22	1:A:229:PRO:HB2	1.92	0.52
1:B:137:LEU:O	1:B:138:LEU:C	2.53	0.52
1:A:131:GLY:H	2:A:1721:GOL:H32	1.76	0.51
1:B:110:TYR:CE2	1:B:187:ILE:HD13	2.45	0.51
1:B:700:LEU:O	1:B:701:VAL:C	2.52	0.51
1:B:3:GLU:HA	1:B:3:GLU:OE1	2.10	0.51
1:B:108:CYS:O	1:B:111:ARG:NH1	2.42	0.51
1:B:620:GLU:HG2	1:B:624:TYR:CE2	2.46	0.51
1:B:133:ARG:HD2	1:B:248:ILE:CG1	2.41	0.50
1:A:-2:GLY:HA2	1:A:31:GLU:OE2	2.12	0.50
1:A:183:PHE:O	1:A:186:LYS:HG2	2.12	0.50
1:B:571:GLY:HA2	1:B:577:GLY:HA3	1.93	0.50
1:B:712:GLN:HA	1:B:712:GLN:OE1	2.12	0.49
1:B:137:LEU:O	1:B:140:ARG:HB2	2.13	0.49
1:B:717:PRO:CA	4:B:2084:HOH:O	2.60	0.49
1:B:223:TYR:O	1:B:226:VAL:HG13	2.13	0.48
1:B:283:PRO:HA	1:B:718:HIS:HE1	1.77	0.48
1:A:601:GLN:HG3	4:B:2052:HOH:O	2.13	0.48
1:A:543:LEU:HD11	1:A:547:THR:HG21	1.95	0.48
1:A:571:GLY:HA2	1:A:577:GLY:HA3	1.94	0.48
1:B:379:GLU:OE1	1:B:388:LYS:HD3	2.14	0.48
1:A:433:PHE:CE1	1:A:441:LEU:HD13	2.49	0.48
1:A:362:LEU:HD12	1:A:362:LEU:O	2.14	0.47
1:B:6:ARG:HH12	1:B:10:SER:HA	1.78	0.47
1:A:565:CYS:O	1:B:570:PHE:CE2	2.67	0.47
1:A:348:SER:HB2	4:A:2057:HOH:O	2.13	0.47
1:B:479:VAL:HG22	1:B:633:ILE:HG21	1.96	0.47
1:B:428:ILE:HG13	1:B:446:PRO:HA	1.97	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:151:ILE:HD12	1:B:236:ILE:HD11	1.97	0.47
1:B:136:GLN:NE2	4:B:2024:HOH:O	2.45	0.46
1:A:440:ARG:O	1:A:467:LYS:HB3	2.15	0.46
1:B:37:GLN:HB3	4:B:2003:HOH:O	2.15	0.46
1:A:133:ARG:HD2	1:A:248:ILE:HD11	1.98	0.46
1:B:219:VAL:HG11	1:B:230:GLU:HA	1.97	0.46
1:B:18:ASN:O	1:B:22:ASN:HA	2.15	0.46
1:A:6:ARG:HH12	1:A:10:SER:HA	1.81	0.46
1:A:110:TYR:CE2	1:A:187:ILE:HD13	2.51	0.45
1:B:135:THR:HG22	1:B:136:GLN:OE1	2.17	0.45
1:B:138:LEU:HB3	1:B:139:PRO:HD3	1.97	0.45
1:A:-4:PRO:N	4:A:2003:HOH:O	2.49	0.45
1:A:274:GLU:OE2	1:A:651:HIS:NE2	2.41	0.45
1:A:135:THR:HG22	1:A:136:GLN:OE1	2.15	0.45
1:B:24:VAL:HG11	1:B:75:LEU:HD13	1.98	0.44
1:B:252:GLU:O	1:B:256:MET:HG3	2.17	0.44
1:B:304:LEU:HD11	1:B:324:ALA:HB1	2.00	0.44
1:A:133:ARG:HD2	1:A:248:ILE:CG1	2.47	0.44
1:B:269:TYR:O	1:B:270:ALA:C	2.61	0.44
1:B:157:LEU:HG	1:B:161:GLU:HG2	1.99	0.44
1:B:595:LEU:HG	1:B:599:LEU:HD22	2.00	0.43
1:B:145:PRO:CD	4:B:2025:HOH:O	2.57	0.43
1:A:121:LEU:O	1:A:154:GLY:HA2	2.18	0.43
1:A:599:LEU:O	1:A:603:ARG:HG3	2.18	0.43
1:A:671:LEU:O	1:A:672:PRO:C	2.55	0.43
1:B:97:ALA:O	1:B:119:VAL:HA	2.18	0.43
1:A:123:GLU:HB3	1:A:128:ILE:HG13	2.01	0.43
1:A:689:PRO:HD2	4:A:2105:HOH:O	2.18	0.43
1:B:68:ALA:CB	1:B:260:ALA:HA	2.48	0.43
1:B:696:TYR:O	1:B:697:LEU:C	2.61	0.43
1:B:280:TRP:O	1:B:288:TRP:HD1	2.02	0.43
1:A:274:GLU:CD	1:A:657:ARG:HH21	2.26	0.43
1:B:140:ARG:HD3	1:B:197:ILE:O	2.19	0.43
1:B:315:PHE:HE1	1:B:461:LEU:HD11	1.83	0.43
1:A:304:LEU:HD11	1:A:324:ALA:HB1	2.01	0.42
1:B:430:THR:HB	1:B:442:LEU:HD11	2.01	0.42
1:A:352:GLN:HE21	1:A:352:GLN:C	2.27	0.42
1:A:572:GLN:HE21	1:A:572:GLN:HB3	1.56	0.42
1:B:546:GLY:HA2	4:B:2075:HOH:O	2.20	0.42
1:A:422:ASP:HB2	4:A:2069:HOH:O	2.18	0.42
1:A:473:GLY:HA2	4:A:2076:HOH:O	2.18	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:462:SER:HA	1:B:465:ILE:HG12	2.01	0.42
1:B:671:LEU:O	1:B:672:PRO:C	2.58	0.42
1:A:379:GLU:OE1	1:A:388:LYS:HD3	2.19	0.42
1:B:135:THR:HG21	1:B:235:SER:HG	1.84	0.42
1:B:168:LEU:CG	4:B:2027:HOH:O	2.62	0.42
1:B:543:LEU:HD22	1:B:544:PRO:HD2	2.00	0.42
1:A:578:TRP:O	1:A:595:LEU:HD22	2.19	0.42
1:B:166:GLY:HA2	4:B:2028:HOH:O	2.19	0.42
1:A:441:LEU:HD12	1:A:652:GLY:HA3	2.02	0.42
1:A:131:GLY:H	2:A:1721:GOL:C3	2.31	0.42
1:A:243:PRO:HB2	1:A:245:GLU:OE2	2.20	0.42
1:B:263:GLN:HG3	4:B:2044:HOH:O	2.19	0.42
1:B:362:LEU:O	1:B:362:LEU:HD12	2.20	0.42
1:A:395:LEU:O	1:A:396:SER:C	2.63	0.42
1:B:534:LYS:HG3	1:B:539:THR:HG23	2.02	0.42
1:B:196:ARG:NH1	3:B:3001:SO4:O1	2.53	0.41
1:A:51:CYS:HB3	1:A:92:ALA:HB3	2.02	0.41
1:B:60:GLY:HA3	3:B:1719:SO4:O4	2.20	0.41
1:A:67:SER:HB2	1:A:70:THR:OG1	2.20	0.41
1:A:708:LEU:HA	1:A:711:TRP:CE2	2.55	0.41
1:B:212:PHE:CZ	1:B:237:GLN:HA	2.54	0.41
1:B:473:GLY:HA3	1:B:638:MET:SD	2.60	0.41
1:B:137:LEU:O	1:B:140:ARG:N	2.50	0.41
1:B:140:ARG:NE	1:B:200:LYS:O	2.54	0.41
1:B:359:LYS:HA	1:B:360:PRO:HD3	1.94	0.41
1:A:483:MET:HE3	1:A:630:ALA:HB2	2.02	0.41
1:B:148:LEU:HD13	1:B:215:ALA:HB2	2.02	0.41
1:A:462:SER:HA	1:A:465:ILE:HG12	2.03	0.41
1:B:376:LEU:HD23	1:B:376:LEU:C	2.46	0.41
1:B:465:ILE:HG13	1:B:467:LYS:HG3	2.01	0.41
1:B:702:ALA:O	4:B:2094:HOH:O	2.22	0.41
1:A:129:LEU:C	1:A:129:LEU:HD12	2.45	0.41
1:A:495:LEU:O	1:A:496:GLU:C	2.64	0.41
1:A:635:GLU:CG	4:A:2115:HOH:O	2.49	0.41
1:A:500:LYS:O	1:A:501:PRO:C	2.64	0.41
1:A:299:VAL:HA	1:A:376:LEU:O	2.21	0.40
1:A:441:LEU:HD11	1:A:648:ILE:HG23	2.03	0.40
1:A:641:ARG:HD3	1:A:643:GLU:OE1	2.21	0.40
1:A:219:VAL:HG11	1:A:230:GLU:HA	2.03	0.40
1:A:33:ARG:NH1	1:A:81:GLU:OE1	2.42	0.40
1:A:118:ARG:HD2	4:A:2019:HOH:O	2.20	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:582:ASP:OD1	1:A:586:GLY:HA3	2.22	0.40
1:A:592:ASP:HA	1:A:593:PRO:HD3	1.86	0.40
1:B:52:GLY:HA3	1:B:56:ASN:O	2.22	0.40
1:B:110:TYR:HA	1:B:169:ASP:OD2	2.22	0.40
1:A:359:LYS:HA	1:A:360:PRO:HD3	1.99	0.40
1:B:129:LEU:HD11	1:B:255:PHE:HB2	2.03	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	723/742 (97%)	681 (94%)	40 (6%)	2 (0%)	36	55
1	B	718/742 (97%)	675 (94%)	42 (6%)	1 (0%)	48	68
All	All	1441/1484 (97%)	1356 (94%)	82 (6%)	3 (0%)	43	63

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	-1	SER
1	A	70	THR
1	B	65	GLY

5.3.2 Protein sidechains [i](#)

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	594/609 (98%)	551 (93%)	43 (7%)	13	28
1	B	591/609 (97%)	547 (93%)	44 (7%)	13	27
All	All	1185/1218 (97%)	1098 (93%)	87 (7%)	13	27

All (87) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	3	GLU
1	A	5	LEU
1	A	24	VAL
1	A	63	ILE
1	A	70	THR
1	A	77	SER
1	A	96	VAL
1	A	125	THR
1	A	135	THR
1	A	157	LEU
1	A	165	LEU
1	A	172	VAL
1	A	188	ILE
1	A	210	SER
1	A	219	VAL
1	A	221	LYS
1	A	226	VAL
1	A	234	ARG
1	A	245	GLU
1	A	248	ILE
1	A	258	LEU
1	A	306	THR
1	A	351	HIS
1	A	352	GLN
1	A	353	ASN
1	A	359	LYS
1	A	362	LEU
1	A	371	LEU
1	A	390	LYS
1	A	441	LEU
1	A	449	TYR
1	A	514	LYS
1	A	521	SER
1	A	523	LEU
1	A	572	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	585	LEU
1	A	597	THR
1	A	609	GLU
1	A	610	GLN
1	A	641	ARG
1	A	675	LEU
1	A	676	GLU
1	A	695	ASP
1	B	0	HIS
1	B	3	GLU
1	B	5	LEU
1	B	63	ILE
1	B	70	THR
1	B	73	LEU
1	B	77	SER
1	B	96	VAL
1	B	125	THR
1	B	135	THR
1	B	157	LEU
1	B	165	LEU
1	B	172	VAL
1	B	186	LYS
1	B	188	ILE
1	B	210	SER
1	B	214	GLU
1	B	219	VAL
1	B	226	VAL
1	B	245	GLU
1	B	248	ILE
1	B	258	LEU
1	B	279	LYS
1	B	282	THR
1	B	362	LEU
1	B	371	LEU
1	B	390	LYS
1	B	427	VAL
1	B	449	TYR
1	B	508	LEU
1	B	521	SER
1	B	523	LEU
1	B	531	LYS
1	B	543	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	549	VAL
1	B	572	GLN
1	B	585	LEU
1	B	597	THR
1	B	599	LEU
1	B	609	GLU
1	B	610	GLN
1	B	615	LYS
1	B	641	ARG
1	B	695	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (22) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	0	HIS
1	A	94	GLN
1	A	185	GLN
1	A	278	ASN
1	A	294	GLN
1	A	352	GLN
1	A	353	ASN
1	A	355	GLN
1	A	489	ASN
1	A	572	GLN
1	A	589	HIS
1	A	606	HIS
1	B	94	GLN
1	B	185	GLN
1	B	242	HIS
1	B	294	GLN
1	B	489	ASN
1	B	536	GLN
1	B	572	GLN
1	B	606	HIS
1	B	679	GLN
1	B	718	HIS

5.3.3 RNA ⓘ

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](#)

7 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	$\# Z > 2$
3	SO4	B	1719	-	4,4,4	0.37	0	6,6,6	0.44	0
3	SO4	A	1723	-	4,4,4	0.23	0	6,6,6	0.17	0
3	SO4	B	1720	-	4,4,4	0.23	0	6,6,6	0.25	0
3	SO4	B	3001	-	4,4,4	0.36	0	6,6,6	0.58	0
2	GOL	A	1721	-	5,5,5	0.29	0	5,5,5	1.44	1 (20%)
3	SO4	A	1722	-	4,4,4	0.43	0	6,6,6	0.73	0
3	SO4	A	3001	-	4,4,4	0.27	0	6,6,6	0.48	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	A	1721	-	-	2/4/4/4	-

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	1721	GOL	C3-C2-C1	-2.72	101.81	111.80

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	1721	GOL	C1-C2-C3-O3
2	A	1721	GOL	O2-C2-C3-O3

There are no ring outliers.

3 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	1719	SO4	1	0
3	B	3001	SO4	1	0
2	A	1721	GOL	2	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	725/742 (97%)	0.37	58 (8%)	18 16	2, 26, 60, 104	0
1	B	720/742 (97%)	0.37	36 (5%)	34 30	3, 27, 60, 104	0
All	All	1445/1484 (97%)	0.37	94 (6%)	25 22	2, 27, 60, 104	0

All (94) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	356	ALA	7.1
1	A	69	PHE	5.3
1	A	70	THR	5.1
1	A	348	SER	5.0
1	B	355	GLN	4.8
1	A	68	ALA	4.6
1	B	351	HIS	4.6
1	B	358	ALA	4.4
1	B	356	ALA	4.2
1	B	354	GLY	4.1
1	A	-3	ARG	4.0
1	A	411	ALA	4.0
1	B	718	HIS	3.7
1	B	-1	SER	3.6
1	A	347	ALA	3.5
1	A	367	SER	3.5
1	A	422	ASP	3.4
1	B	369	LYS	3.3
1	A	329	PRO	3.3
1	A	449	TYR	3.3
1	A	365	SER	3.2
1	A	718	HIS	3.1
1	B	330	LYS	3.1
1	B	353	ASN	3.0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	355	GLN	2.9
1	A	331	GLN	2.9
1	B	0	HIS	2.9
1	B	609	GLU	2.8
1	B	350	ALA	2.8
1	A	5	LEU	2.8
1	B	12	ALA	2.8
1	B	8	PRO	2.7
1	B	185	GLN	2.7
1	A	340	THR	2.7
1	B	362	LEU	2.6
1	A	351	HIS	2.6
1	B	535	GLY	2.6
1	A	245	GLU	2.6
1	A	353	ASN	2.6
1	A	67	SER	2.6
1	A	-2	GLY	2.6
1	A	242	HIS	2.6
1	A	-4	PRO	2.5
1	A	71	PRO	2.5
1	B	449	TYR	2.5
1	A	177	VAL	2.5
1	A	349	ARG	2.5
1	B	188	ILE	2.5
1	A	345	LYS	2.5
1	A	536	GLN	2.5
1	A	278	ASN	2.5
1	A	357	SER	2.5
1	B	360	PRO	2.4
1	A	0	HIS	2.4
1	A	1	MET	2.4
1	A	337	LYS	2.4
1	B	43	HIS	2.4
1	A	324	ALA	2.4
1	B	545	PRO	2.4
1	A	369	LYS	2.4
1	B	186	LYS	2.4
1	A	354	GLY	2.4
1	B	63	ILE	2.4
1	A	64	HIS	2.4
1	A	334	ALA	2.4
1	A	364	PHE	2.4

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	609	GLU	2.4
1	B	11	LEU	2.3
1	A	438	VAL	2.3
1	B	4	TYR	2.3
1	A	332	LEU	2.3
1	A	350	ALA	2.3
1	A	65	GLY	2.3
1	A	339	ILE	2.2
1	B	5	LEU	2.2
1	A	382	PHE	2.2
1	B	541	PRO	2.2
1	A	327	SER	2.2
1	B	64	HIS	2.1
1	A	3	GLU	2.1
1	A	336	LYS	2.1
1	B	359	LYS	2.1
1	A	185	GLN	2.1
1	A	437	HIS	2.1
1	B	178	GLU	2.1
1	B	368	THR	2.1
1	B	338	ILE	2.1
1	A	-1	SER	2.1
1	A	358	ALA	2.0
1	B	65	GLY	2.0
1	B	422	ASP	2.0
1	A	425	GLN	2.0
1	A	398	LEU	2.0
1	A	416	ASP	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
3	SO4	B	1720	5/5	0.72	0.17	90,90,90,91	0
3	SO4	A	1723	5/5	0.75	0.18	97,98,99,99	0
3	SO4	B	3001	5/5	0.84	0.14	61,62,63,63	0
3	SO4	B	1719	5/5	0.88	0.16	72,72,73,73	0
3	SO4	A	1722	5/5	0.90	0.13	46,47,49,50	0
2	GOL	A	1721	6/6	0.96	0.08	12,15,16,17	0
3	SO4	A	3001	5/5	0.98	0.09	19,20,23,24	0

6.5 Other polymers [i](#)

There are no such residues in this entry.