



Full wwPDB X-ray Structure Validation Report ⓘ

Jun 24, 2024 – 09:31 AM EDT

PDB ID : 6QBF
Title : Crystal structure of the pathological D187N variant of calcium-free human gelsolin.
Authors : Scalone, E.; Boni, F.; Milani, M.; Eloise, M.; de Rosa, M.
Deposited on : 2018-12-21
Resolution : 3.50 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 : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.37.1
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) : 2.37.1

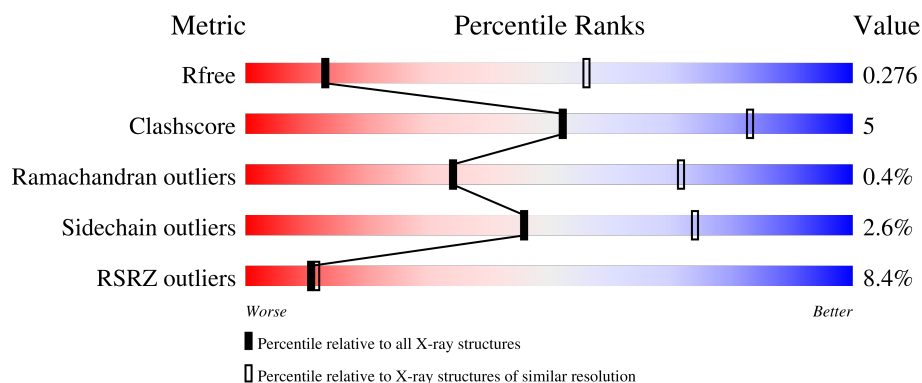
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.50 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}	130704	1659 (3.60-3.40)
Clashscore	141614	1036 (3.58-3.42)
Ramachandran outliers	138981	1005 (3.58-3.42)
Sidechain outliers	138945	1006 (3.58-3.42)
RSRZ outliers	127900	1559 (3.60-3.40)

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	778	
1	B	778	

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 11208 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 Gelsolin.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	714	Total	C	N	O	S	0	1	0
			5562	3516	976	1054	16			
1	B	715	Total	C	N	O	S	0	1	0
			5571	3514	979	1062	16			

There are 48 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-22	MET	-	initiating methionine	UNP P06396
A	-21	GLY	-	expression tag	UNP P06396
A	-20	SER	-	expression tag	UNP P06396
A	-19	SER	-	expression tag	UNP P06396
A	-18	HIS	-	expression tag	UNP P06396
A	-17	HIS	-	expression tag	UNP P06396
A	-16	HIS	-	expression tag	UNP P06396
A	-15	HIS	-	expression tag	UNP P06396
A	-14	HIS	-	expression tag	UNP P06396
A	-13	HIS	-	expression tag	UNP P06396
A	-12	SER	-	expression tag	UNP P06396
A	-11	SER	-	expression tag	UNP P06396
A	-10	GLY	-	expression tag	UNP P06396
A	-9	LEU	-	expression tag	UNP P06396
A	-8	VAL	-	expression tag	UNP P06396
A	-7	PRO	-	expression tag	UNP P06396
A	-6	ARG	-	expression tag	UNP P06396
A	-5	GLY	-	expression tag	UNP P06396
A	-4	SER	-	expression tag	UNP P06396
A	-3	HIS	-	expression tag	UNP P06396
A	-2	MET	-	expression tag	UNP P06396
A	-1	ALA	-	expression tag	UNP P06396
A	0	SER	-	expression tag	UNP P06396
A	187	ASN	ASP	engineered mutation	UNP P06396
B	-22	MET	-	initiating methionine	UNP P06396

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Chain	Residue	Modelled	Actual	Comment	Reference
B	-21	GLY	-	expression tag	UNP P06396
B	-20	SER	-	expression tag	UNP P06396
B	-19	SER	-	expression tag	UNP P06396
B	-18	HIS	-	expression tag	UNP P06396
B	-17	HIS	-	expression tag	UNP P06396
B	-16	HIS	-	expression tag	UNP P06396
B	-15	HIS	-	expression tag	UNP P06396
B	-14	HIS	-	expression tag	UNP P06396
B	-13	HIS	-	expression tag	UNP P06396
B	-12	SER	-	expression tag	UNP P06396
B	-11	SER	-	expression tag	UNP P06396
B	-10	GLY	-	expression tag	UNP P06396
B	-9	LEU	-	expression tag	UNP P06396
B	-8	VAL	-	expression tag	UNP P06396
B	-7	PRO	-	expression tag	UNP P06396
B	-6	ARG	-	expression tag	UNP P06396
B	-5	GLY	-	expression tag	UNP P06396
B	-4	SER	-	expression tag	UNP P06396
B	-3	HIS	-	expression tag	UNP P06396
B	-2	MET	-	expression tag	UNP P06396
B	-1	ALA	-	expression tag	UNP P06396
B	0	SER	-	expression tag	UNP P06396
B	187	ASN	ASP	engineered mutation	UNP P06396

- 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	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

- Molecule 4 is SODIUM ION (three-letter code: NA) (formula: Na).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	B	1	Total Na 1 1	0	0

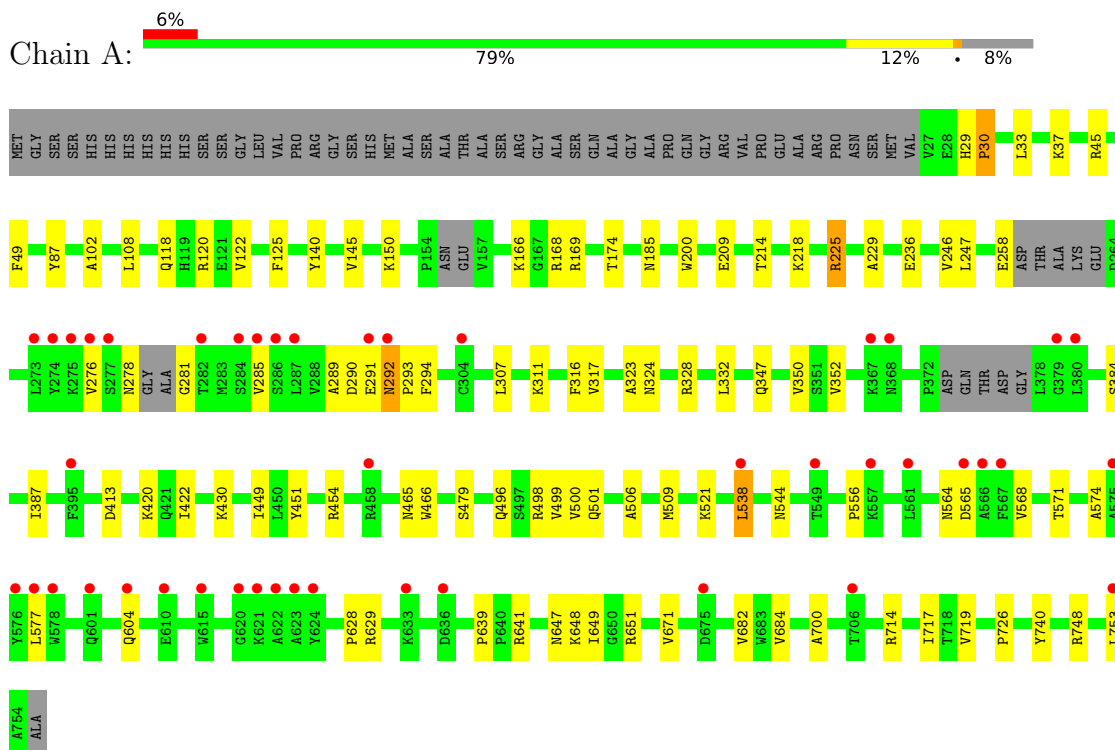
- Molecule 5 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	34	Total O 34 34	0	0
5	B	24	Total O 24 24	0	0

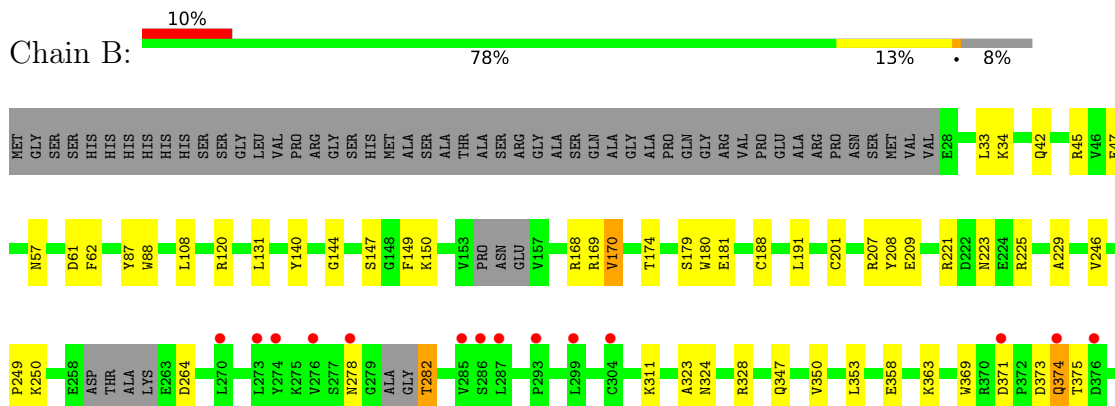
3 Residue-property plots [i](#)

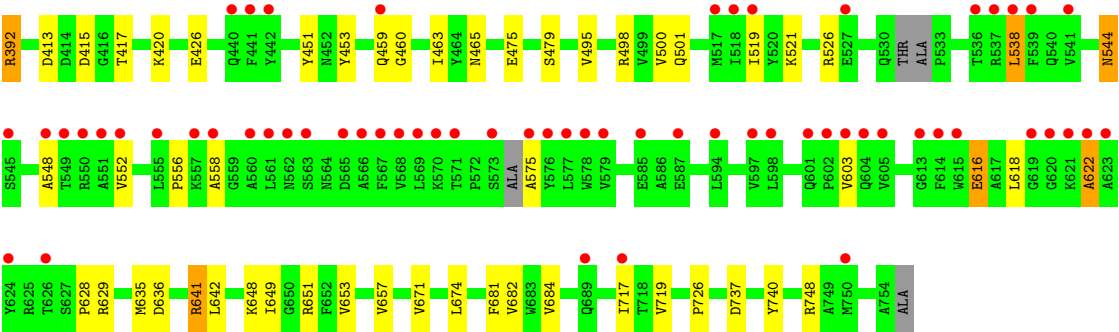
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density.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



- Molecule 1: Gelsolin





4 Data and refinement statistics

Property	Value	Source
Space group	P 4 21 2	Depositor
Cell constants a, b, c, α , β , γ	169.67Å 169.67Å 151.09Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	75.88 – 3.50 75.88 – 3.50	Depositor EDS
% Data completeness (in resolution range)	99.4 (75.88-3.50) 99.4 (75.88-3.50)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.71 (at 3.49Å)	Xtriage
Refinement program	PHENIX (1.10.1_2155: ???)	Depositor
R, R_{free}	0.218 , 0.276 0.218 , 0.276	Depositor DCC
R_{free} test set	1432 reflections (5.06%)	wwPDB-VP
Wilson B-factor (Å ²)	68.8	Xtriage
Anisotropy	0.091	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 80.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.39$, $\langle L^2 \rangle = 0.22$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.88	EDS
Total number of atoms	11208	wwPDB-VP
Average B, all atoms (Å ²)	74.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.92% 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: NA, 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	0.25	0/5690	0.43	0/7705
1	B	0.26	0/5693	0.44	0/7704
All	All	0.25	0/11383	0.43	0/15409

There are no bond length outliers.

There are no bond angle outliers.

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	5431	60	0
1	B	5571	0	5420	60	0
2	A	5	0	0	0	0
2	B	5	0	0	1	0
3	A	6	0	8	0	0
4	B	1	0	0	0	0
5	A	34	0	0	1	0
5	B	24	0	0	1	0
All	All	11208	0	10859	120	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 5.

All (120) 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:648:LYS:HG3	1:A:649:ILE:HG13	1.61	0.80
1:B:648:LYS:HG3	1:B:649:ILE:HG13	1.67	0.75
1:B:392:ARG:NH2	1:B:635:MET:SD	2.64	0.70
1:B:616:GLU:H	1:B:616:GLU:CD	1.98	0.67
1:A:641:ARG:NH2	5:A:901:HOH:O	2.30	0.64
1:B:221:ARG:HG3	1:B:229:ALA:HB3	1.79	0.63
1:B:538:LEU:HD12	1:B:556:PRO:HA	1.80	0.63
1:B:641:ARG:NH2	2:B:801:SO4:O1	2.33	0.61
1:B:740:TYR:O	1:B:748:ARG:NH2	2.34	0.61
1:A:565:ASP:OD2	1:A:629:ARG:NH2	2.33	0.61
1:B:392:ARG:NH1	1:B:636:ASP:OD1	2.34	0.61
1:B:475:GLU:OE2	1:B:526:ARG:NH2	2.34	0.60
1:A:740:TYR:O	1:A:748:ARG:NH2	2.34	0.60
1:A:45:ARG:HH12	1:A:150:LYS:HA	1.69	0.58
1:B:415:ASP:OD2	1:B:417:THR:OG1	2.19	0.58
1:A:218:LYS:HD2	1:A:753:LEU:HD13	1.86	0.57
1:A:496:GLN:HB2	1:A:719:VAL:HB	1.85	0.57
1:A:118:GLN:HB2	1:A:352:VAL:HG22	1.87	0.57
1:A:166:LYS:HZ1	1:A:258:GLU:HA	1.70	0.56
1:B:179:SER:HB3	1:B:181:GLU:HG2	1.86	0.56
1:A:87:TYR:OH	1:A:120[B]:ARG:NH1	2.37	0.56
1:A:185:ASN:ND2	1:A:236:GLU:OE1	2.39	0.55
1:A:500:VAL:HB	1:A:714:ARG:HB3	1.88	0.55
1:B:207:ARG:NH2	5:B:903:HOH:O	2.39	0.55
1:B:45:ARG:NH1	1:B:47:GLU:OE2	2.39	0.55
1:B:45:ARG:NH2	1:B:149:PHE:O	2.39	0.54
1:B:371:ASP:OD1	1:B:371:ASP:N	2.39	0.54
1:B:616:GLU:CD	1:B:616:GLU:N	2.61	0.53
1:A:571:THR:HG23	1:A:574:ALA:H	1.74	0.53
1:B:120[A]:ARG:HB3	1:B:350:VAL:HB	1.90	0.53
1:B:353:LEU:HD13	1:B:358:GLU:HA	1.91	0.53
1:B:674:LEU:HB3	1:B:681:PHE:HB2	1.91	0.53
1:B:120[B]:ARG:HB3	1:B:350:VAL:HB	1.91	0.52
1:B:34:LYS:O	1:B:42:GLN:NE2	2.42	0.52
1:A:289:ALA:HB1	1:A:294:PHE:CD1	2.44	0.52
1:B:616:GLU:N	1:B:616:GLU:OE2	2.43	0.51
1:A:45:ARG:HH21	1:A:145:VAL:HG22	1.75	0.51
1:B:426:GLU:HA	1:B:526:ARG:HH12	1.75	0.51
1:A:538:LEU:HD12	1:A:556:PRO:HA	1.93	0.51
1:B:558:ALA:HB3	1:B:622:ALA:HB3	1.93	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:122:VAL:HG23	1:A:125:PHE:HB2	1.94	0.50
1:A:420:LYS:HB3	1:A:451:TYR:HD1	1.76	0.50
1:A:200:TRP:CZ2	1:A:236:GLU:HG2	2.47	0.50
1:A:292:ASN:CB	1:A:293:PRO:HD3	2.43	0.49
1:A:700:ALA:HB3	1:A:717:ILE:HD13	1.94	0.49
1:A:564:ASN:HD21	1:A:628:PRO:HA	1.78	0.49
1:A:292:ASN:HB3	1:A:293:PRO:CD	2.43	0.49
1:A:671:VAL:HG22	1:A:684:VAL:HG23	1.94	0.49
1:B:374:GLN:O	1:B:374:GLN:NE2	2.45	0.49
1:A:120[A]:ARG:HB3	1:A:350:VAL:HB	1.95	0.49
1:A:577:LEU:HB3	1:A:604:GLN:HA	1.95	0.48
1:A:387:ILE:HD13	1:A:639:PRO:HB3	1.95	0.48
1:B:323:ALA:O	1:B:328:ARG:NH1	2.46	0.48
1:B:140:TYR:HB2	1:B:174:THR:HA	1.95	0.48
1:A:120[B]:ARG:HB3	1:A:350:VAL:HB	1.95	0.48
1:B:180:TRP:NE1	1:B:249:PRO:O	2.47	0.47
1:B:498:ARG:NH1	1:B:500:VAL:HG23	2.30	0.47
1:A:501:GLN:HE22	1:A:521:LYS:HA	1.79	0.47
1:A:682:VAL:HG13	1:A:719:VAL:HA	1.95	0.47
1:B:544:ASN:ND2	1:B:548:ALA:O	2.44	0.47
1:B:558:ALA:N	1:B:618:LEU:HB3	2.30	0.47
1:A:466:TRP:HA	1:A:499:VAL:HG13	1.96	0.47
1:A:506:ALA:HA	1:A:509:MET:HE3	1.97	0.47
1:A:568:VAL:HG22	1:A:577:LEU:HD12	1.96	0.46
1:B:498:ARG:HH21	1:B:717:ILE:HG13	1.80	0.46
1:A:292:ASN:HB3	1:A:293:PRO:HD3	1.98	0.46
1:A:323:ALA:O	1:A:328:ARG:NH1	2.48	0.46
1:A:276:VAL:HG12	1:A:285:VAL:HG12	1.97	0.46
1:A:317:VAL:HB	1:A:352:VAL:HG12	1.97	0.46
1:B:682:VAL:HG13	1:B:719:VAL:HA	1.98	0.46
1:B:168:ARG:HG2	1:B:208:TYR:HD2	1.81	0.46
1:B:498:ARG:HH12	1:B:500:VAL:HG23	1.81	0.45
1:B:737:ASP:HB3	1:B:740:TYR:HB2	1.99	0.45
1:B:168:ARG:HG3	1:B:209:GLU:HG2	1.98	0.45
1:B:463:ILE:N	1:B:495:VAL:O	2.40	0.45
1:A:37:LYS:HD2	1:A:37:LYS:HA	1.72	0.45
1:B:87:TYR:OH	1:B:120[B]:ARG:NH2	2.49	0.45
1:A:214:THR:HG22	1:A:753:LEU:HD12	1.99	0.45
1:A:45:ARG:NH1	1:A:150:LYS:HA	2.32	0.45
1:A:246:VAL:HG23	1:A:247:LEU:HG	1.99	0.44
1:A:294:PHE:HE2	1:A:307:LEU:HD21	1.81	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:420:LYS:HB3	1:B:451:TYR:HD1	1.81	0.44
1:A:422:ILE:HG23	1:A:449:ILE:HG13	2.00	0.44
1:A:292:ASN:CG	1:A:293:PRO:HD3	2.38	0.44
1:B:131:LEU:HD13	1:B:170:VAL:HG11	1.99	0.44
1:B:363:LYS:HD2	1:B:369:TRP:CD1	2.52	0.44
1:A:29:HIS:N	1:A:30:PRO:HD3	2.33	0.44
1:A:384:SER:HB3	1:A:387:ILE:HG12	2.00	0.44
1:B:575:ALA:O	1:B:603:VAL:N	2.42	0.44
1:B:264:ASP:HB3	1:B:653:VAL:HA	2.01	0.43
1:B:519:ILE:HD13	1:B:552:VAL:HG22	1.99	0.43
1:A:278:ASN:HD21	1:A:281:GLY:N	2.17	0.43
1:A:140:TYR:HB2	1:A:174:THR:HA	2.00	0.43
1:B:501:GLN:HE22	1:B:521:LYS:HA	1.83	0.43
1:A:649:ILE:O	1:A:651:ARG:HG3	2.19	0.43
1:B:465:ASN:HD21	1:B:479:SER:HB2	1.84	0.43
1:A:168:ARG:HG3	1:A:209:GLU:HG2	2.00	0.42
1:A:465:ASN:HD21	1:A:479:SER:HB2	1.84	0.42
1:B:629:ARG:HD2	1:B:629:ARG:HA	1.87	0.42
1:B:671:VAL:HG22	1:B:684:VAL:HG23	2.02	0.42
1:B:62:PHE:HB3	1:B:88:TRP:CZ3	2.54	0.42
1:A:413:ASP:OD1	1:A:726:PRO:HB2	2.20	0.42
1:A:307:LEU:HB3	1:A:316:PHE:HB2	2.02	0.41
1:B:413:ASP:OD1	1:B:726:PRO:HB2	2.20	0.41
1:B:519:ILE:HB	1:B:552:VAL:HA	2.02	0.41
1:A:430:LYS:HE3	1:A:430:LYS:HB2	1.93	0.41
1:A:33:LEU:HD12	1:A:33:LEU:H	1.86	0.41
1:A:225:ARG:HG2	1:A:229:ALA:HB2	2.01	0.41
1:B:188:CYS:HA	1:B:201:CYS:HA	2.02	0.41
1:B:191:LEU:HD21	1:B:246:VAL:HG21	2.02	0.41
1:B:57:ASN:O	1:B:223:ASN:HB3	2.21	0.41
1:B:144:GLY:N	1:B:147:SER:OG	2.53	0.41
1:A:498:ARG:HB3	1:A:498:ARG:NH1	2.36	0.41
1:B:33:LEU:H	1:B:33:LEU:HD12	1.85	0.41
1:B:642:LEU:HD23	1:B:657:VAL:HG11	2.03	0.40
1:B:278:ASN:HB2	1:B:282:THR:O	2.22	0.40
1:A:102:ALA:HB1	1:A:332:LEU:HD23	2.02	0.40
1:B:453:TYR:CZ	1:B:460:GLY:HA3	2.56	0.40
1:A:290:ASP:O	1:A:291:GLU:HG3	2.22	0.40
1:A:498:ARG:HB3	1:A:498:ARG:HH11	1.85	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	705/778 (91%)	658 (93%)	45 (6%)	2 (0%)	41	75
1	B	704/778 (90%)	657 (93%)	43 (6%)	4 (1%)	25	64
All	All	1409/1556 (91%)	1315 (93%)	88 (6%)	6 (0%)	34	72

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	292	ASN
1	B	373	ASP
1	B	622	ALA
1	A	30	PRO
1	B	375	THR
1	B	628	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	580/629 (92%)	569 (98%)	11 (2%)	57	80
1	B	581/629 (92%)	562 (97%)	19 (3%)	38	68
All	All	1161/1258 (92%)	1131 (97%)	30 (3%)	46	74

All (30) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	49	PHE
1	A	108	LEU
1	A	169	ARG
1	A	225	ARG
1	A	311	LYS
1	A	324	ASN
1	A	347	GLN
1	A	454	ARG
1	A	538	LEU
1	A	544	ASN
1	A	647	ASN
1	B	61	ASP
1	B	108	LEU
1	B	150	LYS
1	B	169	ARG
1	B	170	VAL
1	B	225	ARG
1	B	250	LYS
1	B	282	THR
1	B	311	LYS
1	B	324	ASN
1	B	347	GLN
1	B	374	GLN
1	B	392	ARG
1	B	459	GLN
1	B	538	LEU
1	B	544	ASN
1	B	616	GLU
1	B	641	ARG
1	B	651	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	185	ASN

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 monosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 4 ligands modelled in this entry, 1 is monoatomic - leaving 3 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	802	-	5,5,5	0.36	0	5,5,5	0.23	0
2	SO4	A	801	-	4,4,4	0.15	0	6,6,6	0.06	0
2	SO4	B	801	-	4,4,4	0.18	0	6,6,6	0.79	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	802	-	-	2/4/4/4	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	802	GOL	O1-C1-C2-C3
3	A	802	GOL	O1-C1-C2-O2

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	801	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	714/778 (91%)	0.56	44 (6%) 20 18	41, 69, 108, 135	0
1	B	715/778 (91%)	0.72	76 (10%) 6 7	43, 74, 120, 160	0
All	All	1429/1556 (91%)	0.64	120 (8%) 11 11	41, 72, 115, 160	0

All (120) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	576	TYR	6.4
1	B	577	LEU	5.7
1	B	594	LEU	5.1
1	B	517	MET	5.0
1	B	569	LEU	4.9
1	B	374	GLN	4.8
1	B	560	ALA	4.8
1	B	578	TRP	4.7
1	B	615	TRP	4.6
1	B	614	PHE	4.2
1	B	566	ALA	4.1
1	B	604	GLN	3.9
1	A	379	GLY	3.8
1	B	549	THR	3.7
1	B	575	ALA	3.7
1	B	587	GLU	3.5
1	B	622	ALA	3.5
1	B	565	ASP	3.4
1	B	562	ASN	3.3
1	B	619	GLY	3.2
1	B	519	ILE	3.2
1	A	276	VAL	3.2
1	B	518	ILE	3.2
1	B	548	ALA	3.2

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Mol	Chain	Res	Type	RSRZ
1	B	278	ASN	3.2
1	A	622	ALA	3.2
1	B	620	GLY	3.2
1	B	557	LYS	3.1
1	B	541	VAL	3.1
1	B	376	ASP	3.0
1	B	579	VAL	3.0
1	B	276	VAL	3.0
1	A	575	ALA	3.0
1	B	621	LYS	3.0
1	B	304	CYS	3.0
1	A	578	TRP	2.9
1	B	287	LEU	2.9
1	B	605	VAL	2.9
1	B	558	ALA	2.9
1	B	371	ASP	2.9
1	B	567	PHE	2.8
1	A	566	ALA	2.8
1	B	537	ARG	2.8
1	B	536	THR	2.8
1	B	585	GLU	2.8
1	A	274	TYR	2.8
1	A	287	LEU	2.8
1	A	576	TYR	2.7
1	A	286	SER	2.7
1	A	623	ALA	2.7
1	A	285	VAL	2.6
1	B	613	GLY	2.6
1	B	623	ALA	2.6
1	A	577	LEU	2.6
1	B	563	SER	2.6
1	A	549	THR	2.6
1	A	615	TRP	2.5
1	B	286	SER	2.5
1	A	277	SER	2.5
1	B	539	PHE	2.5
1	A	273	LEU	2.5
1	A	567	PHE	2.5
1	B	750	MET	2.5
1	B	555	LEU	2.5
1	A	284	SER	2.5
1	B	601	GLN	2.4

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Mol	Chain	Res	Type	RSRZ
1	B	602	PRO	2.4
1	B	550	ARG	2.4
1	A	395	PHE	2.4
1	A	610	GLU	2.4
1	A	604	GLN	2.4
1	B	293	PRO	2.4
1	B	626	THR	2.4
1	B	624	TYR	2.3
1	A	706	THR	2.3
1	B	568	VAL	2.3
1	A	292	ASN	2.3
1	A	565	ASP	2.3
1	A	291	GLU	2.3
1	B	538	LEU	2.3
1	A	304	CYS	2.3
1	B	573	SER	2.3
1	A	561	LEU	2.3
1	B	570	LYS	2.3
1	A	275	LYS	2.2
1	B	717	ILE	2.2
1	B	273	LEU	2.2
1	B	299	LEU	2.2
1	B	689	GLN	2.2
1	B	598	LEU	2.2
1	A	636	ASP	2.2
1	B	571	THR	2.2
1	B	561	LEU	2.2
1	B	551	ALA	2.1
1	A	675	ASP	2.1
1	B	274	TYR	2.1
1	A	368	ASN	2.1
1	B	441	PHE	2.1
1	B	527	GLU	2.1
1	A	753	LEU	2.1
1	A	633	LYS	2.1
1	B	552	VAL	2.1
1	B	597	VAL	2.1
1	A	380	LEU	2.1
1	A	557	LYS	2.1
1	B	270	LEU	2.1
1	A	282	THR	2.1
1	B	285	VAL	2.1

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Mol	Chain	Res	Type	RSRZ
1	A	601	GLN	2.0
1	B	440	GLN	2.0
1	B	603	VAL	2.0
1	B	459	GLN	2.0
1	B	545	SER	2.0
1	A	538	LEU	2.0
1	A	458	ARG	2.0
1	A	620	GLY	2.0
1	A	367	LYS	2.0
1	B	442	TYR	2.0
1	A	621	LYS	2.0
1	A	624	TYR	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 monosaccharides 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	B	801	5/5	0.73	0.39	119,129,134,136	0
3	GOL	A	802	6/6	0.84	0.58	49,78,80,80	0
2	SO4	A	801	5/5	0.88	0.21	106,112,115,119	0
4	NA	B	802	1/1	0.94	0.11	28,28,28,28	0

6.5 Other polymers [i](#)

There are no such residues in this entry.