



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 10, 2026 – 05:28 PM UTC

PDB ID : 6SPA / pdb_00006spa
Title : A4V MUTANT OF HUMAN SUPEROXIDE DISMUTASE 1 IN C2 SPACE GROUP
Authors : Shahid, M.; Chantadul, V.; Amporndanai, K.; Wright, G.; Antonyuk, S.; Hasnain, S.
Deposited on : 2019-08-31
Resolution : 1.65 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

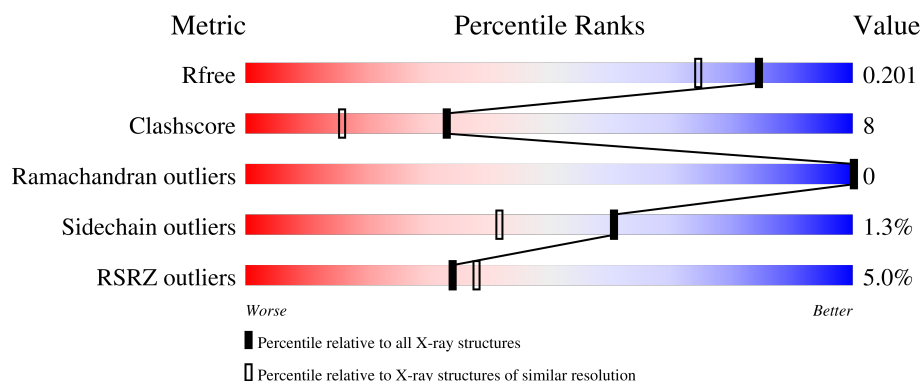
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.65 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.



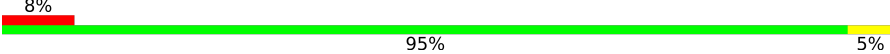
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	2563 (1.66-1.66)
Clashscore	190562	2662 (1.66-1.66)
Ramachandran outliers	187476	2621 (1.66-1.66)
Sidechain outliers	187428	2621 (1.66-1.66)
RSRZ outliers	180081	2564 (1.66-1.66)

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	153	5% 92% 7%
1	C	153	4% 91% 9%
1	E	153	2% 86% 13%
1	G	153	6% 90% 9%
1	J	153	6% 93% 5%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
1	L	153	

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
3	GOL	A	202[A]	-	-	X	-
3	GOL	C	202	-	-	X	-
3	GOL	E	203[A]	-	-	X	X
3	GOL	E	203[B]	-	-	-	X
3	GOL	E	204[A]	-	-	X	-
3	GOL	G	203	-	-	X	-
3	GOL	J	202	-	-	X	-
4	DMS	C	204[A]	-	-	X	-

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 8368 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 Superoxide dismutase [Cu-Zn].

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	153	Total	C	N	O	S	3	7	0
			1145	703	205	232	5			
1	C	153	Total	C	N	O	S	0	5	0
			1144	702	208	229	5			
1	E	153	Total	C	N	O	S	0	6	0
			1141	700	205	231	5			
1	G	153	Total	C	N	O	S	0	7	0
			1153	704	209	235	5			
1	J	153	Total	C	N	O	S	0	9	0
			1163	714	211	233	5			
1	L	153	Total	C	N	O	S	0	7	0
			1147	704	207	231	5			

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	4	VAL	ALA	engineered mutation	UNP P00441
C	4	VAL	ALA	engineered mutation	UNP P00441
E	4	VAL	ALA	engineered mutation	UNP P00441
G	4	VAL	ALA	engineered mutation	UNP P00441
J	4	VAL	ALA	engineered mutation	UNP P00441
L	4	VAL	ALA	engineered mutation	UNP P00441

- Molecule 2 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	1	Total	Zn	0	0
			1	1		
2	C	1	Total	Zn	0	0
			1	1		
2	E	1	Total	Zn	0	0
			1	1		

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	G	1	Total	Zn	0	0
			1	1		
2	J	1	Total	Zn	0	0
			1	1		
2	L	1	Total	Zn	0	0
			1	1		

- Molecule 3 is GLYCEROL (CCD ID: GOL) (formula: $C_3H_8O_3$).



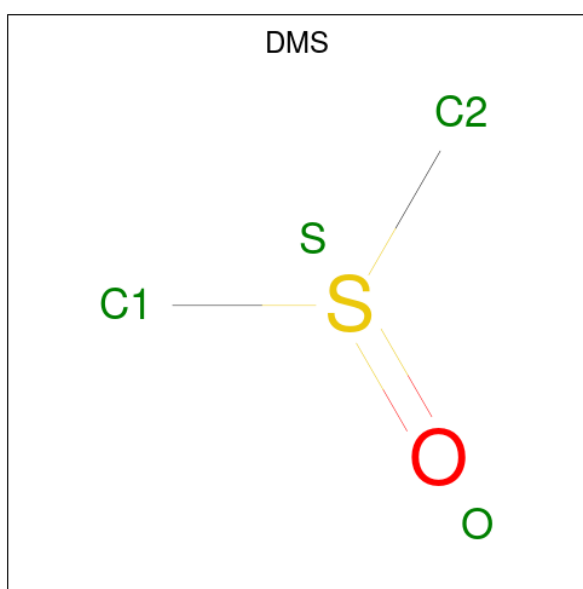
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	1
			6	3	3		
3	A	1	Total	C	O	0	0
			6	3	3		
3	C	1	Total	C	O	0	0
			6	3	3		
3	C	1	Total	C	O	0	0
			6	3	3		
3	E	1	Total	C	O	0	0
			6	3	3		
3	E	1	Total	C	O	0	1
			12	6	6		
3	E	1	Total	C	O	0	1
			6	3	3		
3	G	1	Total	C	O	0	1
			6	3	3		

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	G	1	Total	C	O	0	0
			6	3	3		
3	G	1	Total	C	O	0	1
			6	3	3		
3	J	1	Total	C	O	0	0
			6	3	3		
3	L	1	Total	C	O	0	0
			6	3	3		

- Molecule 4 is DIMETHYL SULFOXIDE (CCD ID: DMS) (formula: C_2H_6OS).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	1	Total	C	O	S	0	1
			4	2	1	1		
4	C	1	Total	C	O	S	0	1
			4	2	1	1		
4	L	1	Total	C	O	S	0	0
			4	2	1	1		

- Molecule 5 is SULFATE ION (CCD ID: SO4) (formula: O_4S).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	G	1	Total	O	S	0	1
			5	4	1		

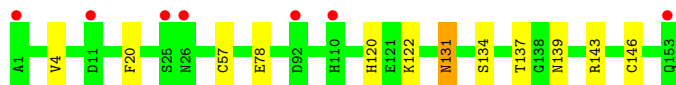
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	210	Total	O	0	14
			216	216		
6	C	229	Total	O	0	12
			238	238		
6	E	231	Total	O	0	9
			237	237		
6	G	221	Total	O	0	20
			231	231		
6	J	230	Total	O	0	15
			237	237		
6	L	211	Total	O	0	8
			215	215		

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.

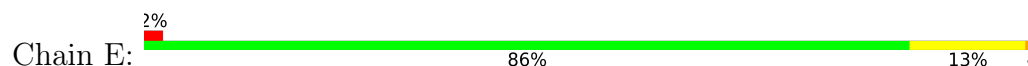
- Molecule 1: Superoxide dismutase [Cu-Zn]



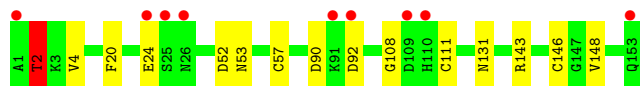
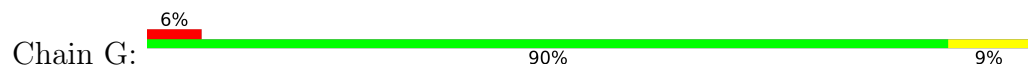
- Molecule 1: Superoxide dismutase [Cu-Zn]



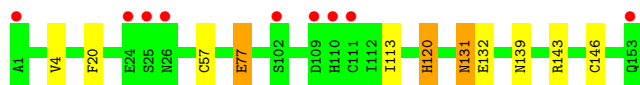
- Molecule 1: Superoxide dismutase [Cu-Zn]



- Molecule 1: Superoxide dismutase [Cu-Zn]



- Molecule 1: Superoxide dismutase [Cu-Zn]



- Molecule 1: Superoxide dismutase [Cu-Zn]



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	112.60Å 195.96Å 75.68Å 90.00° 97.10° 90.00°	Depositor
Resolution (Å)	97.98 – 1.65 97.98 – 1.65	Depositor EDS
% Data completeness (in resolution range)	99.5 (97.98-1.65) 99.5 (97.98-1.65)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.52 (at 1.65Å)	Xtriage
Refinement program	REFMAC 5.8.0238	Depositor
R, R_{free}	0.169 , 0.196 0.178 , 0.201	Depositor DCC
R_{free} test set	9697 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å ²)	21.5	Xtriage
Anisotropy	0.212	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.37 , 54.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.97	EDS
Total number of atoms	8368	wwPDB-VP
Average B, all atoms (Å ²)	27.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.00% 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, DMS, ZN, 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	0.97	0/1178	1.08	2/1586 (0.1%)
1	C	0.97	0/1174	1.05	0/1580
1	E	0.94	0/1174	1.11	3/1581 (0.2%)
1	G	0.96	0/1181	1.14	1/1592 (0.1%)
1	J	0.96	0/1196	1.08	2/1610 (0.1%)
1	L	0.97	0/1177	1.09	0/1584
All	All	0.96	0/7080	1.09	8/9533 (0.1%)

There are no bond length outliers.

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	G	2	THR	CB-CA-C	6.91	121.81	109.38
1	J	120	HIS	CA-C-N	5.43	127.55	120.28
1	J	120	HIS	C-N-CA	5.43	127.55	120.28
1	E	120	HIS	CA-C-N	5.27	127.34	120.28
1	E	120	HIS	C-N-CA	5.27	127.34	120.28
1	A	120	HIS	CA-C-N	5.24	127.72	120.29
1	A	120	HIS	C-N-CA	5.24	127.72	120.29
1	E	20	PHE	CA-CB-CG	5.08	118.88	113.80

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	1145	0	1121	13	0
1	C	1144	0	1125	13	0
1	E	1141	0	1120	25	0
1	G	1153	0	1114	20	0
1	J	1163	0	1144	10	0
1	L	1147	0	1125	7	0
2	A	1	0	0	0	0
2	C	1	0	0	0	0
2	E	1	0	0	0	0
2	G	1	0	0	0	0
2	J	1	0	0	0	0
2	L	1	0	0	0	0
3	A	12	0	16	5	0
3	C	12	0	16	7	0
3	E	24	0	32	10	0
3	G	18	0	24	11	0
3	J	6	0	8	5	0
3	L	6	0	8	3	0
4	A	4	0	6	0	0
4	C	4	0	6	4	0
4	L	4	0	6	3	0
5	G	5	0	0	0	0
6	A	216	0	0	2	0
6	C	238	0	0	9	0
6	E	237	0	0	8	0
6	G	231	0	0	3	0
6	J	237	0	0	4	0
6	L	215	0	0	4	0
All	All	8368	0	6871	104	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 (104) 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:G:53:ASN:HB2	3:G:203:GOL:H31	1.32	1.11
3:E:203[B]:GOL:O2	6:E:301[B]:HOH:O	1.72	1.06
1:G:53:ASN:CB	3:G:203:GOL:H31	1.92	1.00

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:53:ASN:HB2	3:G:203:GOL:C3	1.97	0.94
1:A:57:CYS:HG	1:A:146:CYS:HG	1.04	0.93
1:C:69[A]:ARG:NH1	1:C:78[A]:GLU:OE1	2.04	0.91
1:A:143:ARG:HE	3:A:202[A]:GOL:H12	1.37	0.88
1:E:57:CYS:HG	1:E:146:CYS:HG	0.92	0.88
1:G:57:CYS:HG	1:G:146:CYS:HG	1.11	0.85
1:J:131:ASN:HD21	1:J:139:ASN:HD21	1.25	0.82
1:L:143:ARG:HH21	3:L:203:GOL:H2	1.46	0.80
1:G:143:ARG:HH21	3:G:202[A]:GOL:H2	1.50	0.76
1:G:53:ASN:CG	3:G:203:GOL:H31	2.09	0.76
1:A:131:ASN:HD21	1:A:139:ASN:HD21	1.33	0.74
1:C:143:ARG:HH21	3:C:202:GOL:H2	1.54	0.73
1:E:143:ARG:HH21	3:E:204[A]:GOL:H2	1.54	0.71
1:E:4:VAL:HG22	1:E:20:PHE:HB2	1.73	0.69
6:E:301[B]:HOH:O	1:G:111[B]:CYS:SG	2.50	0.69
1:E:111[A]:CYS:HB2	3:E:203[A]:GOL:H32	1.74	0.69
1:A:4:VAL:HG22	1:A:20:PHE:HB2	1.75	0.68
1:J:4:VAL:HG22	1:J:20:PHE:HB2	1.75	0.68
1:G:4:VAL:HG22	1:G:20:PHE:HB2	1.76	0.67
1:C:4:VAL:HG22	1:C:20:PHE:HB2	1.77	0.66
1:E:9[B]:LYS:CE	6:E:344:HOH:O	2.45	0.65
1:E:107:SER:HA	3:E:203[A]:GOL:H31	1.79	0.65
1:E:76:ASP:OD2	6:E:302[A]:HOH:O	2.14	0.64
1:J:143:ARG:HE	3:J:202:GOL:H11	1.63	0.64
4:L:202:DMS:C1	6:L:313:HOH:O	2.45	0.64
1:E:131:ASN:HD21	1:E:139:ASN:HD21	1.46	0.63
1:L:71:HIS:HE1	1:L:124:ASP:OD1	1.82	0.62
1:A:131:ASN:HD22	1:A:134:SER:H	1.49	0.61
4:C:204[A]:DMS:C2	6:C:459:HOH:O	2.49	0.61
1:G:53:ASN:ND2	6:G:304[B]:HOH:O	2.30	0.60
1:E:107:SER:HA	3:E:203[A]:GOL:C3	2.32	0.60
1:A:143:ARG:HE	3:A:202[A]:GOL:C1	2.13	0.59
4:L:202:DMS:H13	6:L:313:HOH:O	2.02	0.59
1:A:131:ASN:ND2	1:A:134:SER:H	2.01	0.58
1:E:69:ARG:NH2	1:E:77:GLU:OE2	2.38	0.57
3:E:202:GOL:H2	3:E:204[A]:GOL:H31	1.87	0.57
3:J:202:GOL:H12	6:J:318:HOH:O	2.05	0.56
1:A:137:THR:HG21	3:A:202[A]:GOL:H31	1.88	0.55
1:L:4:VAL:HG22	1:L:20:PHE:HB2	1.88	0.55
1:L:143:ARG:NH2	3:L:203:GOL:H2	2.21	0.55
1:C:111[B]:CYS:SG	6:C:432:HOH:O	2.59	0.54

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:143:ARG:HE	3:E:204[A]:GOL:H2	1.73	0.54
1:G:146:CYS:SG	3:G:203:GOL:H2	2.47	0.54
1:E:9[B]:LYS:HE2	6:E:344:HOH:O	2.08	0.53
1:J:4:VAL:CG2	1:J:20:PHE:HB2	2.39	0.53
1:E:75:LYS:NZ	6:E:303:HOH:O	2.43	0.52
1:C:9[A]:LYS:HG2	6:C:424:HOH:O	2.09	0.52
1:A:4:VAL:CG2	1:A:20:PHE:HB2	2.40	0.52
1:J:132[B]:GLU:HG2	6:J:448:HOH:O	2.09	0.52
3:C:203:GOL:H2	6:C:441:HOH:O	2.10	0.51
1:E:131:ASN:HD22	1:E:134:SER:H	1.59	0.51
1:A:78[A]:GLU:HG2	6:A:496[A]:HOH:O	2.11	0.50
1:E:55:ALA:HB3	1:E:59[B]:SER:OG	2.12	0.50
1:E:9[B]:LYS:NZ	6:E:304:HOH:O	2.44	0.50
1:E:4:VAL:CG2	1:E:20:PHE:HB2	2.42	0.50
1:C:4:VAL:CG2	1:C:20:PHE:HB2	2.42	0.49
1:E:111[A]:CYS:CB	3:E:203[A]:GOL:H32	2.41	0.49
1:G:4:VAL:CG2	1:G:20:PHE:HB2	2.43	0.49
1:J:77[A]:GLU:HG3	6:J:414:HOH:O	2.12	0.49
1:C:121[B]:GLU:HA	1:C:144:LEU:HD11	1.95	0.48
1:A:57:CYS:HG	1:A:146:CYS:CB	2.26	0.48
1:E:131:ASN:ND2	1:E:134:SER:H	2.11	0.48
1:G:57:CYS:HG	1:G:146:CYS:CB	2.27	0.47
4:C:204[A]:DMS:H23	6:C:459:HOH:O	2.11	0.47
1:L:4:VAL:CG2	1:L:20:PHE:HB2	2.45	0.47
3:C:202:GOL:H11	6:C:330:HOH:O	2.15	0.46
1:C:143:ARG:NH2	3:C:202:GOL:H2	2.26	0.46
1:E:143:ARG:NH2	3:E:204[A]:GOL:H2	2.26	0.46
4:C:204[A]:DMS:H22	6:C:459:HOH:O	2.12	0.45
1:G:53:ASN:HB2	3:G:203:GOL:H32	1.90	0.45
1:C:69[A]:ARG:NH2	1:C:77:GLU:OE2	2.28	0.45
1:G:2:THR:HG23	6:G:422:HOH:O	2.15	0.45
3:L:203:GOL:H11	6:L:313:HOH:O	2.15	0.45
1:J:57:CYS:SG	1:J:146:CYS:SG	3.03	0.44
1:E:78:GLU:HG2	6:E:517:HOH:O	2.16	0.44
1:G:148:VAL:HG23	3:G:203:GOL:H32	2.00	0.44
1:A:143:ARG:NE	3:A:202[A]:GOL:H12	2.19	0.43
3:C:202:GOL:O3	3:C:203:GOL:H31	2.18	0.43
1:E:52:ASP:O	1:E:59[B]:SER:HB2	2.18	0.43
1:E:8:LEU:C	1:E:9[B]:LYS:HG2	2.42	0.43
1:C:143:ARG:HE	3:C:202:GOL:H2	1.84	0.43
3:G:202[A]:GOL:H11	6:G:337:HOH:O	2.19	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:75:LYS:HA	1:E:75:LYS:HD3	1.85	0.42
1:G:143:ARG:NH2	3:G:202[A]:GOL:H2	2.26	0.42
1:L:111[B]:CYS:O	1:L:111[B]:CYS:SG	2.77	0.42
1:J:120:HIS:HE1	3:J:202:GOL:C1	2.33	0.42
1:G:52:ASP:C	3:G:203:GOL:H11	2.44	0.42
1:J:143:ARG:NE	3:J:202:GOL:H11	2.33	0.42
1:E:4:VAL:HB	1:E:150:GLY:O	2.19	0.42
1:G:90[A]:ASP:OD1	1:G:92[A]:ASP:HB2	2.21	0.41
1:C:111[B]:CYS:SG	6:C:342:HOH:O	2.59	0.41
4:L:202:DMS:H22	6:L:458:HOH:O	2.20	0.41
1:C:96:ASP:O	1:G:131:ASN:HB3	2.20	0.41
1:L:96[B]:ASP:OD1	1:L:96[B]:ASP:C	2.64	0.41
3:C:202:GOL:H32	6:C:330:HOH:O	2.20	0.40
3:E:203[B]:GOL:H11	1:G:108[B]:GLY:H	1.85	0.40
1:A:137:THR:CG2	3:A:202[A]:GOL:H31	2.52	0.40
6:A:408:HOH:O	4:C:204[A]:DMS:H21	2.20	0.40
1:C:70:LYS:HE3	1:C:135:THR:O	2.20	0.40
1:J:4:VAL:HG11	1:J:113:ILE:HG12	2.04	0.40
3:J:202:GOL:H32	6:J:447:HOH:O	2.22	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	157/153 (103%)	156 (99%)	1 (1%)	0	100	100
1	C	156/153 (102%)	154 (99%)	2 (1%)	0	100	100
1	E	157/153 (103%)	155 (99%)	2 (1%)	0	100	100
1	G	158/153 (103%)	155 (98%)	3 (2%)	0	100	100
1	J	159/153 (104%)	158 (99%)	1 (1%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	L	157/153 (103%)	156 (99%)	1 (1%)	0	100	100
All	All	944/918 (103%)	934 (99%)	10 (1%)	0	100	100

There are no Ramachandran outliers to report.

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	125/119 (105%)	123 (98%)	2 (2%)	55	34
1	C	124/119 (104%)	123 (99%)	1 (1%)	73	60
1	E	125/119 (105%)	124 (99%)	1 (1%)	73	60
1	G	125/119 (105%)	123 (98%)	2 (2%)	55	34
1	J	127/119 (107%)	125 (98%)	2 (2%)	55	34
1	L	125/119 (105%)	124 (99%)	1 (1%)	73	60
All	All	751/714 (105%)	742 (99%)	9 (1%)	61	45

All (9) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	122	LYS
1	A	131	ASN
1	C	26	ASN
1	E	131	ASN
1	G	2	THR
1	G	24	GLU
1	J	77[A]	GLU
1	J	131	ASN
1	L	26[A]	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (12) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	26	ASN
1	A	53	ASN
1	A	131	ASN
1	C	26	ASN
1	C	53	ASN
1	E	26	ASN
1	E	131	ASN
1	G	26	ASN
1	J	131	ASN
1	J	153	GLN
1	L	53	ASN
1	L	71	HIS

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 23 ligands modelled in this entry, 6 are monoatomic - leaving 17 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	G	203	-	5,5,5	0.27	0	5,5,5	0.57	0
3	GOL	C	203	-	5,5,5	0.13	0	5,5,5	0.45	0
3	GOL	E	204[A]	-	5,5,5	0.10	0	5,5,5	0.41	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	GOL	G	202[A]	-	5,5,5	0.15	0	5,5,5	0.55	0
3	GOL	J	202	-	5,5,5	0.10	0	5,5,5	0.69	0
3	GOL	G	204[A]	-	5,5,5	0.08	0	5,5,5	0.35	0
3	GOL	C	202	-	5,5,5	0.10	0	5,5,5	0.50	0
3	GOL	E	203[A]	-	5,5,5	0.09	0	5,5,5	0.33	0
3	GOL	E	202	-	5,5,5	0.17	0	5,5,5	0.49	0
3	GOL	L	203	-	5,5,5	0.06	0	5,5,5	0.36	0
4	DMS	A	204[B]	-	3,3,3	0.32	0	3,3,3	0.12	0
4	DMS	L	202	-	3,3,3	0.20	0	3,3,3	0.14	0
4	DMS	C	204[A]	-	3,3,3	0.20	0	3,3,3	0.16	0
3	GOL	A	203	-	5,5,5	0.13	0	5,5,5	0.34	0
5	SO4	G	205[A]	-	4,4,4	0.38	0	6,6,6	0.10	0
3	GOL	E	203[B]	-	5,5,5	0.13	0	5,5,5	0.27	0
3	GOL	A	202[A]	-	5,5,5	0.08	0	5,5,5	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
3	GOL	G	203	-	-	2/4/4/4	-
3	GOL	C	203	-	-	2/4/4/4	-
3	GOL	E	204[A]	-	-	4/4/4/4	-
3	GOL	G	202[A]	-	-	4/4/4/4	-
3	GOL	J	202	-	-	4/4/4/4	-
3	GOL	G	204[A]	-	-	2/4/4/4	-
3	GOL	C	202	-	-	4/4/4/4	-
3	GOL	E	203[A]	-	-	4/4/4/4	-
3	GOL	E	202	-	-	2/4/4/4	-
3	GOL	L	203	-	-	2/4/4/4	-
3	GOL	A	203	-	-	3/4/4/4	-
3	GOL	E	203[B]	-	-	4/4/4/4	-
3	GOL	A	202[A]	-	-	2/4/4/4	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (39) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	C	202	GOL	O1-C1-C2-C3
3	C	202	GOL	C1-C2-C3-O3
3	E	203[A]	GOL	O1-C1-C2-C3
3	E	203[A]	GOL	C1-C2-C3-O3
3	E	203[B]	GOL	C1-C2-C3-O3
3	E	204[A]	GOL	O1-C1-C2-C3
3	E	204[A]	GOL	C1-C2-C3-O3
3	G	202[A]	GOL	C1-C2-C3-O3
3	G	203	GOL	O1-C1-C2-C3
3	J	202	GOL	C1-C2-C3-O3
3	E	203[A]	GOL	O1-C1-C2-O2
3	G	204[A]	GOL	O2-C2-C3-O3
3	A	202[A]	GOL	O1-C1-C2-C3
3	A	203	GOL	O1-C1-C2-C3
3	A	203	GOL	C1-C2-C3-O3
3	C	203	GOL	O1-C1-C2-C3
3	E	203[B]	GOL	O1-C1-C2-C3
3	G	202[A]	GOL	O1-C1-C2-C3
3	G	204[A]	GOL	C1-C2-C3-O3
3	J	202	GOL	O1-C1-C2-C3
3	L	203	GOL	O1-C1-C2-C3
3	A	202[A]	GOL	O1-C1-C2-O2
3	A	203	GOL	O1-C1-C2-O2
3	C	202	GOL	O1-C1-C2-O2
3	C	202	GOL	O2-C2-C3-O3
3	E	203[A]	GOL	O2-C2-C3-O3
3	E	204[A]	GOL	O1-C1-C2-O2
3	E	204[A]	GOL	O2-C2-C3-O3
3	G	202[A]	GOL	O1-C1-C2-O2
3	G	202[A]	GOL	O2-C2-C3-O3
3	G	203	GOL	O1-C1-C2-O2
3	J	202	GOL	O1-C1-C2-O2
3	J	202	GOL	O2-C2-C3-O3
3	C	203	GOL	O1-C1-C2-O2
3	E	203[B]	GOL	O1-C1-C2-O2
3	E	203[B]	GOL	O2-C2-C3-O3
3	L	203	GOL	O1-C1-C2-O2
3	E	202	GOL	C1-C2-C3-O3
3	E	202	GOL	O2-C2-C3-O3

There are no ring outliers.

13 monomers are involved in 48 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	G	203	GOL	8	0
3	C	203	GOL	2	0
3	E	204[A]	GOL	4	0
3	G	202[A]	GOL	3	0
3	J	202	GOL	5	0
3	C	202	GOL	6	0
3	E	203[A]	GOL	4	0
3	E	202	GOL	1	0
3	L	203	GOL	3	0
4	L	202	DMS	3	0
4	C	204[A]	DMS	4	0
3	E	203[B]	GOL	2	0
3	A	202[A]	GOL	5	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	153/153 (100%)	0.07	7 (4%)	37	41	10, 20, 36, 49	10 (6%)
1	C	153/153 (100%)	0.07	6 (3%)	43	48	12, 20, 39, 57	8 (5%)
1	E	153/153 (100%)	-0.01	3 (1%)	65	70	11, 20, 36, 46	9 (5%)
1	G	153/153 (100%)	0.17	9 (5%)	28	32	11, 20, 34, 56	10 (6%)
1	J	153/153 (100%)	0.21	9 (5%)	28	32	12, 21, 39, 53	9 (5%)
1	L	153/153 (100%)	0.24	12 (7%)	19	22	13, 22, 43, 54	7 (4%)
All	All	918/918 (100%)	0.12	46 (5%)	34	38	10, 21, 40, 57	53 (5%)

All (46) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	26	ASN	8.2
1	L	1	ALA	5.9
1	J	1	ALA	5.8
1	G	26	ASN	5.3
1	G	1	ALA	5.2
1	C	1	ALA	4.9
1	C	109	ASP	4.8
1	J	26[A]	ASN	4.7
1	A	1	ALA	4.7
1	J	109	ASP	4.3
1	A	153	GLN	3.6
1	C	11	ASP	3.5
1	G	110[A]	HIS	3.4
1	L	26[A]	ASN	3.3
1	G	91	LYS	3.2
1	G	24	GLU	3.2
1	G	25	SER	3.1
1	L	92	ASP	3.1
1	L	25	SER	3.0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	E	1	ALA	2.9
1	A	26	ASN	2.9
1	A	110	HIS	2.8
1	E	26	ASN	2.8
1	L	109	ASP	2.6
1	L	68	SER	2.5
1	G	92[A]	ASP	2.5
1	J	110	HIS	2.5
1	L	23	LYS	2.5
1	L	110	HIS	2.4
1	J	153	GLN	2.3
1	J	25[A]	SER	2.3
1	L	67	LEU	2.3
1	A	25	SER	2.3
1	E	11	ASP	2.3
1	J	102	SER	2.3
1	A	11	ASP	2.3
1	C	153	GLN	2.3
1	G	153	GLN	2.2
1	L	24	GLU	2.2
1	G	109[A]	ASP	2.2
1	A	92	ASP	2.1
1	J	24	GLU	2.1
1	L	133	GLU	2.1
1	C	110	HIS	2.1
1	L	108	GLY	2.0
1	J	111[A]	CYS	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(Å ²)	Q<0.9
3	GOL	E	203[A]	6/6	0.79	0.43	10,12,13,14	6
3	GOL	E	203[B]	6/6	0.79	0.43	13,15,15,16	6
3	GOL	G	204[A]	6/6	0.80	0.31	21,25,30,33	6
4	DMS	C	204[A]	4/4	0.81	0.36	42,43,45,45	4
4	DMS	L	202	4/4	0.84	0.27	73,76,79,80	0
3	GOL	G	202[A]	6/6	0.85	0.23	25,37,39,40	6
3	GOL	E	202	6/6	0.85	0.20	32,42,46,48	0
5	SO4	G	205[A]	5/5	0.85	0.20	35,35,37,39	5
3	GOL	A	203	6/6	0.86	0.16	44,47,49,50	0
3	GOL	L	203	6/6	0.86	0.19	33,51,53,56	0
3	GOL	E	204[A]	6/6	0.86	0.22	25,40,43,50	6
3	GOL	C	202	6/6	0.86	0.21	29,48,54,61	0
3	GOL	G	203	6/6	0.86	0.25	18,22,24,28	6
4	DMS	A	204[B]	4/4	0.87	0.20	38,45,50,53	0
3	GOL	A	202[A]	6/6	0.87	0.19	21,25,25,29	6
3	GOL	C	203	6/6	0.88	0.20	26,35,36,38	6
3	GOL	J	202	6/6	0.89	0.17	29,47,51,58	0
2	ZN	J	201	1/1	0.99	0.02	19,19,19,19	0
2	ZN	G	201	1/1	1.00	0.01	16,16,16,16	0
2	ZN	A	201	1/1	1.00	0.01	17,17,17,17	0
2	ZN	L	201	1/1	1.00	0.02	19,19,19,19	0
2	ZN	C	201	1/1	1.00	0.01	17,17,17,17	0
2	ZN	E	201	1/1	1.00	0.01	17,17,17,17	0

6.5 Other polymers ⓘ

There are no such residues in this entry.