



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 06:21 AM UTC

PDB ID : 5VSA / pdb_00005vsa
Title : Crystal structure of SsoPox AsA1 mutant (C258L-I261F-W263A)
Authors : Hiblot, J.; Gotthard, G.; Jacquet, P.; Daude, D.; Bergonzi, C.; Chabriere, E.; Elias, M.
Deposited on : 2017-05-11
Resolution : 2.00 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

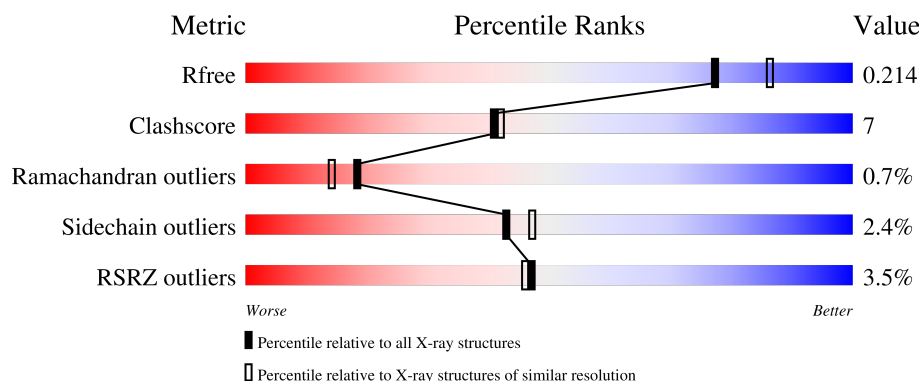
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

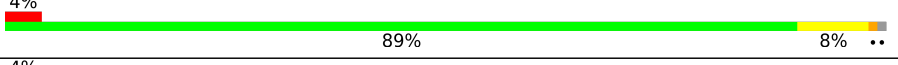
The reported resolution of this entry is 2.00 Å.

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	10052 (2.00-2.00)
Clashscore	190562	11152 (2.00-2.00)
Ramachandran outliers	187476	11031 (2.00-2.00)
Sidechain outliers	187428	11029 (2.00-2.00)
RSRZ outliers	180081	10067 (2.00-2.00)

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	314	
1	B	314	
1	C	314	
1	D	314	

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
4	GOL	A	403	-	X	-	-

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 10768 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 Aryldialkylphosphatase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	305	Total	C	N	O	S	0	2	0
			2453	1574	419	454	6			
1	B	314	Total	C	N	O	S	0	1	0
			2514	1615	425	468	6			
1	C	310	Total	C	N	O	S	0	2	0
			2503	1606	427	464	6			
1	D	314	Total	C	N	O	S	0	0	0
			2509	1610	425	468	6			

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	258	LEU	CYS	engineered mutation	UNP Q97VT7
A	261	PHE	ILE	engineered mutation	UNP Q97VT7
A	263	ALA	TRP	engineered mutation	UNP Q97VT7
B	258	LEU	CYS	engineered mutation	UNP Q97VT7
B	261	PHE	ILE	engineered mutation	UNP Q97VT7
B	263	ALA	TRP	engineered mutation	UNP Q97VT7
C	258	LEU	CYS	engineered mutation	UNP Q97VT7
C	261	PHE	ILE	engineered mutation	UNP Q97VT7
C	263	ALA	TRP	engineered mutation	UNP Q97VT7
D	258	LEU	CYS	engineered mutation	UNP Q97VT7
D	261	PHE	ILE	engineered mutation	UNP Q97VT7
D	263	ALA	TRP	engineered mutation	UNP Q97VT7

- Molecule 2 is FE (II) ION (CCD ID: FE2) (formula: Fe).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	1	Total	Fe	0	0
			1	1		
2	B	1	Total	Fe	0	0
			1	1		

Continued on next page...

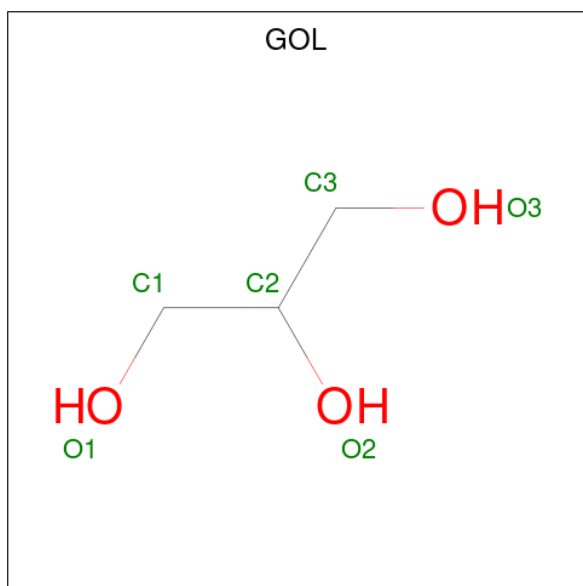
Continued from previous page...

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	C	1	Total	Fe	0	0
			1	1		
2	D	1	Total	Fe	0	0
			1	1		

- Molecule 3 is COBALT (II) ION (CCD ID: CO) (formula: Co).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	1	Total	Co	0	0
			1	1		
3	B	1	Total	Co	0	0
			1	1		
3	C	1	Total	Co	0	0
			1	1		
3	D	1	Total	Co	0	0
			1	1		

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



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

Continued on next page...

Continued from previous page...

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

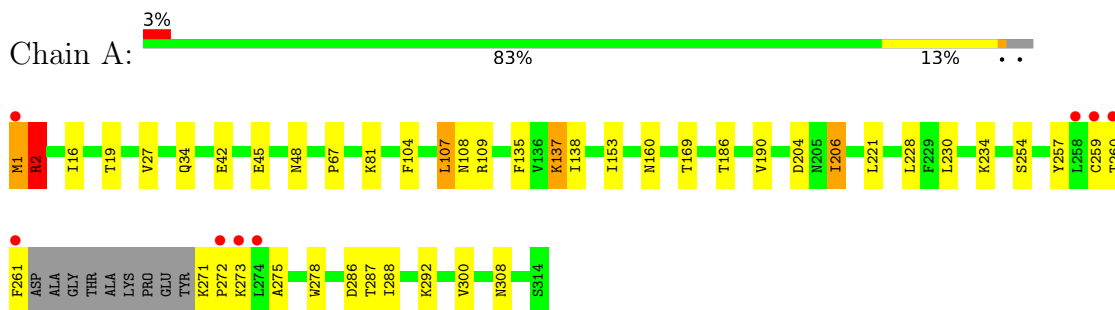
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	189	Total	O	0	0
			189	189		
5	B	203	Total	O	0	0
			203	203		
5	C	191	Total	O	0	0
			191	191		
5	D	150	Total	O	0	0
			150	150		

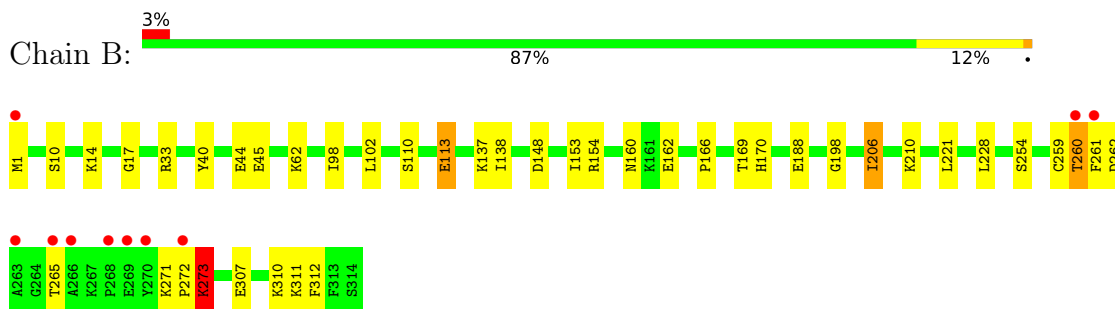
3 Residue-property plots [i](#)

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.

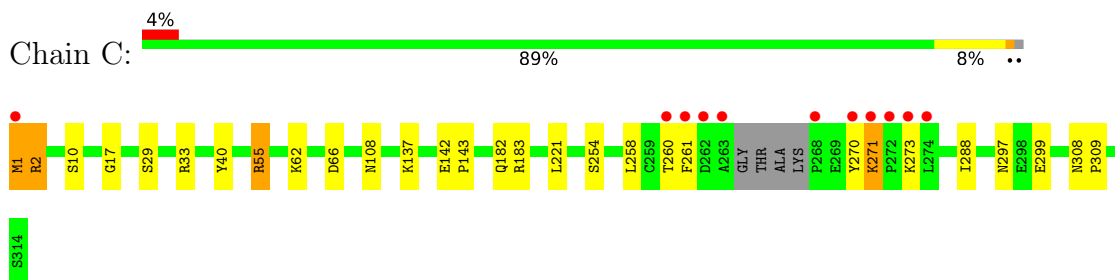
- Molecule 1: Aryldialkylphosphatase



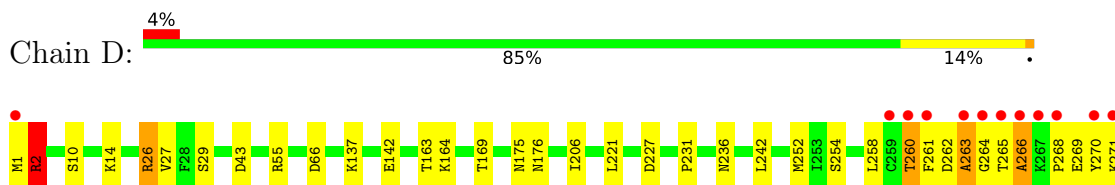
- Molecule 1: Aryldialkylphosphatase

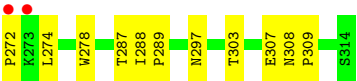


- Molecule 1: Aryldialkylphosphatase



- Molecule 1: Aryldialkylphosphatase





4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	86.60Å 103.10Å 151.80Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	48.81 – 2.00 48.81 – 2.00	Depositor EDS
% Data completeness (in resolution range)	98.6 (48.81-2.00) 98.6 (48.81-2.00)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.95 (at 2.00Å)	Xtriage
Refinement program	REFMAC 5.8.0158	Depositor
R, R_{free}	0.158 , 0.204 0.170 , 0.214	Depositor DCC
R_{free} test set	4556 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	23.2	Xtriage
Anisotropy	0.106	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.37 , 39.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	10768	wwPDB-VP
Average B, all atoms (Å ²)	30.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.73% 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: FE2, CO, GOL, KCX

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	1.20	5/2489 (0.2%)	1.00	1/3357 (0.0%)
1	B	1.18	1/2554 (0.0%)	1.07	3/3449 (0.1%)
1	C	1.16	2/2542 (0.1%)	1.00	0/3428
1	D	1.17	5/2546 (0.2%)	1.03	4/3437 (0.1%)
All	All	1.18	13/10131 (0.1%)	1.03	8/13671 (0.1%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1
1	B	0	1
1	C	0	1
1	D	0	1
All	All	0	4

All (13) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	260	THR	CA-C	7.88	1.61	1.52
1	C	288	ILE	CA-CB	5.73	1.57	1.54
1	A	288	ILE	CA-C	5.50	1.57	1.52
1	D	308	ASN	CA-C	5.44	1.59	1.52
1	A	308	ASN	N-CA	-5.42	1.41	1.46
1	A	300	VAL	C-O	-5.38	1.17	1.24
1	C	182	GLN	C-O	-5.37	1.18	1.24
1	A	109	ARG	C-O	-5.32	1.17	1.24
1	D	2	ARG	C-O	-5.29	1.17	1.24
1	D	262	ASP	CA-C	5.25	1.59	1.52

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	135	PHE	C-O	5.23	1.29	1.23
1	B	160	ASN	N-CA	-5.18	1.40	1.46
1	D	297	ASN	N-CA	5.14	1.52	1.45

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	262	ASP	N-CA-C	10.96	122.97	111.14
1	B	261	PHE	N-CA-C	6.35	118.72	109.07
1	D	142	GLU	CA-C-N	-5.84	113.80	119.87
1	D	142	GLU	C-N-CA	-5.84	113.80	119.87
1	D	260	THR	CB-CA-C	5.66	119.42	109.80
1	A	287	THR	N-CA-C	5.51	116.97	110.97
1	B	162	GLU	N-CA-C	5.22	117.06	111.36
1	D	263	ALA	N-CA-C	5.11	116.89	110.24

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	221	LEU	Peptide
1	B	221	LEU	Peptide
1	C	221	LEU	Peptide
1	D	221	LEU	Peptide

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	2453	0	2496	42	0
1	B	2514	0	2551	28	0
1	C	2503	0	2537	28	0
1	D	2509	0	2540	41	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
2	C	1	0	0	0	0
2	D	1	0	0	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	A	1	0	0	0	0
3	B	1	0	0	0	0
3	C	1	0	0	0	0
3	D	1	0	0	0	0
4	A	18	0	24	0	0
4	B	12	0	16	0	0
4	C	12	0	16	0	0
4	D	6	0	8	0	0
5	A	189	0	0	7	0
5	B	203	0	0	6	0
5	C	191	0	0	3	0
5	D	150	0	0	7	0
All	All	10768	0	10188	132	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 7.

All (132) 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:2[B]:ARG:HH21	1:A:2[B]:ARG:CG	1.51	1.18
1:A:2[A]:ARG:HH21	1:A:2[A]:ARG:HG2	1.07	1.10
1:A:2[B]:ARG:NH2	1:A:2[B]:ARG:HG3	1.55	1.09
1:D:258:LEU:HD13	1:D:261:PHE:CD2	1.89	1.08
1:A:2[A]:ARG:HH21	1:A:2[A]:ARG:CG	1.66	1.07
1:C:62:LYS:HE2	5:C:618:HOH:O	1.52	1.07
1:A:45:GLU:O	1:A:260:THR:HG21	1.57	1.04
1:C:55[A]:ARG:HG3	1:C:55[A]:ARG:HH21	1.21	1.00
1:A:2[B]:ARG:HH21	1:A:2[B]:ARG:HG3	0.85	0.99
1:A:48:ASN:HB2	1:A:260:THR:HG22	1.43	0.97
1:C:55[A]:ARG:HH21	1:C:55[A]:ARG:CG	1.81	0.94
1:A:1:MET:SD	1:A:1:MET:N	2.37	0.93
1:A:2[A]:ARG:HG2	1:A:2[A]:ARG:NH2	1.80	0.85
1:C:55[B]:ARG:HG2	1:C:55[B]:ARG:HH11	1.40	0.85
1:A:108:ASN:ND2	1:D:265:THR:HG22	1.96	0.80
1:B:1:MET:N	1:B:1:MET:SD	2.56	0.78
1:A:2[B]:ARG:CG	1:A:2[B]:ARG:NH2	2.25	0.78
1:D:2:ARG:HH11	1:D:2:ARG:HB3	1.50	0.76
1:B:311:LYS:HD3	5:B:648:HOH:O	1.86	0.75
1:C:55[B]:ARG:HH11	1:C:55[B]:ARG:CG	1.99	0.75
1:D:258:LEU:HD13	1:D:261:PHE:HD2	1.46	0.72

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:55[A]:ARG:CG	1:C:55[A]:ARG:NH2	2.47	0.70
1:C:1:MET:N	1:C:10:SER:OG	2.24	0.69
1:A:16[B]:ILE:HG22	5:A:551:HOH:O	1.94	0.67
1:D:14:LYS:HE2	5:D:595:HOH:O	1.94	0.67
1:A:27:VAL:H	1:A:261:PHE:CB	2.07	0.67
1:A:107:LEU:HB3	1:D:265:THR:HG23	1.75	0.66
1:B:1:MET:N	1:B:10:SER:OG	2.27	0.66
1:C:297:ASN:HD22	1:C:299:GLU:H	1.42	0.66
1:D:29:SER:HB3	5:D:527:HOH:O	1.96	0.65
1:A:34:GLN:NE2	5:A:501:HOH:O	2.27	0.65
1:B:98:ILE:HD13	1:B:102[B]:LEU:HD22	1.81	0.63
1:D:43:ASP:HB3	5:D:571:HOH:O	1.98	0.63
1:C:55[A]:ARG:NH2	1:C:55[A]:ARG:CB	2.62	0.63
1:A:108:ASN:HD22	1:D:265:THR:HA	1.64	0.62
1:C:55[A]:ARG:NH2	1:C:55[A]:ARG:HB2	2.15	0.61
1:D:1:MET:SD	1:D:1:MET:N	2.66	0.61
1:D:236:ASN:ND2	1:D:287:THR:HG23	2.16	0.61
1:A:2[A]:ARG:CG	1:A:2[A]:ARG:NH2	2.37	0.61
1:C:55[B]:ARG:NH1	1:C:55[B]:ARG:HB3	2.17	0.60
1:C:258:LEU:HD13	1:C:261:PHE:CD1	2.35	0.60
1:B:259:CYS:O	1:B:260:THR:HG23	2.02	0.58
1:B:265:THR:HG23	1:C:108:ASN:ND2	2.18	0.58
1:D:258:LEU:HD12	1:D:278:TRP:HH2	1.69	0.57
1:B:206:ILE:HG23	1:B:210:LYS:HE3	1.88	0.55
1:B:271:LYS:HB3	1:B:272:PRO:HD3	1.88	0.55
1:D:1:MET:HB3	1:D:10:SER:OG	2.07	0.55
1:D:175:ASN:O	1:D:176:ASN:CB	2.56	0.54
1:A:107:LEU:HB3	1:D:265:THR:CG2	2.38	0.54
1:A:204:ASP:O	1:A:206:ILE:HD12	2.09	0.53
1:C:55[B]:ARG:CG	1:C:55[B]:ARG:NH1	2.63	0.53
1:B:102[B]:LEU:CD2	1:B:148:ASP:HB3	2.39	0.53
1:D:206:ILE:HD11	1:D:242:LEU:HG	1.91	0.53
1:D:163:THR:O	1:D:164:LYS:HB2	2.09	0.53
1:D:258:LEU:HD13	1:D:261:PHE:CE2	2.42	0.52
1:D:266:ALA:HB3	1:D:269:GLU:CG	2.38	0.52
1:D:14:LYS:CE	5:D:595:HOH:O	2.54	0.52
1:D:26:ARG:HD2	5:D:524:HOH:O	2.10	0.52
1:A:292:LYS:HE3	5:B:664:HOH:O	2.10	0.52
1:C:17:GLY:HA3	1:C:62:LYS:HD3	1.92	0.52
1:B:272:PRO:O	1:B:273:LYS:CB	2.58	0.52
1:D:55:ARG:HD3	5:D:501:HOH:O	2.09	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:236:ASN:HD21	1:D:287:THR:HG23	1.75	0.50
1:A:81:LYS:NZ	5:A:503:HOH:O	2.34	0.50
1:A:2[A]:ARG:HH21	1:A:2[A]:ARG:HG3	1.66	0.49
1:D:2:ARG:HH11	1:D:2:ARG:CB	2.22	0.49
1:A:275:ALA:HB1	1:A:278:TRP:HB2	1.94	0.49
1:D:2:ARG:HD3	5:D:642:HOH:O	2.13	0.49
1:D:265:THR:OG1	1:D:266:ALA:N	2.44	0.49
1:D:269:GLU:CD	1:D:269:GLU:O	2.57	0.48
1:B:265:THR:CG2	1:C:108:ASN:ND2	2.75	0.48
1:B:102[B]:LEU:HD23	1:B:148:ASP:HB3	1.95	0.48
1:D:271:LYS:N	1:D:272:PRO:HD3	2.28	0.48
1:C:55[A]:ARG:HH21	1:C:55[A]:ARG:CB	2.25	0.48
1:B:45:GLU:HA	1:B:260:THR:HG21	1.95	0.48
1:A:104:PHE:HA	1:A:107:LEU:HD13	1.96	0.48
1:C:270:TYR:O	1:C:271:LYS:CB	2.61	0.47
1:A:230:LEU:HD11	1:A:234:LYS:HE3	1.96	0.47
1:B:98:ILE:CD1	1:B:102[B]:LEU:HD22	2.44	0.47
1:B:110:SER:OG	1:B:113:GLU:HG2	2.14	0.47
1:A:107:LEU:CD1	5:A:653:HOH:O	2.62	0.47
1:B:17:GLY:HA3	1:B:62:LYS:HD2	1.97	0.47
1:A:48:ASN:CB	1:A:260:THR:HG22	2.29	0.47
1:A:286:ASP:OD1	1:A:286:ASP:C	2.58	0.47
1:B:137:KCX:OQ1	1:B:170:HIS:HB2	2.16	0.46
1:A:16[A]:ILE:HG22	1:A:19:THR:OG1	2.15	0.46
1:A:271:LYS:N	1:A:272:PRO:HD2	2.31	0.46
1:C:55[B]:ARG:NH1	1:C:55[B]:ARG:CB	2.79	0.46
1:D:264:GLY:O	1:D:265:THR:C	2.58	0.46
1:A:27:VAL:HG22	1:A:261:PHE:CB	2.46	0.46
1:A:107:LEU:HD12	5:A:653:HOH:O	2.16	0.46
1:D:271:LYS:HG2	1:D:274:LEU:HD13	1.98	0.46
1:A:67:PRO:HB2	1:A:137:KCX:HG2	1.97	0.46
1:A:2[B]:ARG:HH21	1:A:2[B]:ARG:HG2	1.64	0.45
1:B:138:ILE:HD12	1:B:153:ILE:HG12	1.98	0.45
1:A:292:LYS:CE	5:B:664:HOH:O	2.65	0.45
1:A:259:CYS:C	1:A:260:THR:HG23	2.42	0.45
1:A:42:GLU:HG2	5:A:502:HOH:O	2.15	0.45
1:C:33:ARG:HA	1:C:40:TYR:CE1	2.52	0.44
1:B:14:LYS:HA	1:B:310:LYS:HE2	2.00	0.44
1:D:303:THR:HA	1:D:307:GLU:HB3	2.00	0.44
1:C:2:ARG:HG2	5:C:631:HOH:O	2.17	0.44
1:B:44:GLU:HG3	5:B:674:HOH:O	2.18	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:261:PHE:HE1	1:D:263:ALA:HB2	1.83	0.44
1:A:138:ILE:HD12	1:A:153:ILE:HG12	2.00	0.43
1:A:271:LYS:N	1:A:272:PRO:CD	2.81	0.43
1:B:33:ARG:HA	1:B:40:TYR:CE1	2.53	0.43
1:B:307:GLU:OE2	5:B:501:HOH:O	2.22	0.43
1:A:160:ASN:ND2	1:A:190:VAL:HG13	2.34	0.43
1:C:308:ASN:HB2	1:C:309:PRO:HD3	2.00	0.43
1:C:297:ASN:ND2	1:C:299:GLU:H	2.14	0.43
1:D:288:ILE:HB	1:D:289:PRO:HD3	2.00	0.42
1:B:166:PRO:HB2	1:B:312:PHE:CZ	2.54	0.42
1:C:66:ASP:OD1	1:C:66:ASP:C	2.62	0.42
1:D:252:MET:CE	1:D:309:PRO:HG3	2.50	0.42
1:B:154:ARG:NH1	1:B:188:GLU:OE2	2.45	0.42
1:C:29:SER:HB3	5:C:654:HOH:O	2.19	0.42
1:C:55[A]:ARG:HG3	1:C:55[A]:ARG:NH2	2.04	0.42
1:D:269:GLU:C	1:D:271:LYS:N	2.77	0.42
1:B:206:ILE:CG2	1:B:210:LYS:HE3	2.50	0.41
1:D:27:VAL:CG2	1:D:261:PHE:CD2	3.04	0.41
1:B:1:MET:HE2	5:B:587:HOH:O	2.21	0.41
1:D:27:VAL:HG21	1:D:261:PHE:CD2	2.56	0.41
1:D:261:PHE:HE1	1:D:263:ALA:CB	2.33	0.41
1:A:81:LYS:HE3	5:A:503:HOH:O	2.21	0.41
1:B:169:THR:O	1:B:198:GLY:HA3	2.21	0.41
1:D:269:GLU:C	1:D:271:LYS:H	2.29	0.41
1:C:142:GLU:N	1:C:143:PRO:CD	2.84	0.41
1:D:66:ASP:C	1:D:66:ASP:OD1	2.63	0.41
1:D:227:ASP:OD1	1:D:231:PRO:HA	2.20	0.41
1:A:257:TYR:CE2	1:A:259:CYS:HA	2.56	0.40
1:B:265:THR:HG23	1:C:108:ASN:HD22	1.84	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	302/314 (96%)	290 (96%)	10 (3%)	2 (1%)	18	14
1	B	312/314 (99%)	301 (96%)	10 (3%)	1 (0%)	36	35
1	C	307/314 (98%)	293 (95%)	12 (4%)	2 (1%)	18	14
1	D	311/314 (99%)	290 (93%)	17 (6%)	4 (1%)	9	5
All	All	1232/1256 (98%)	1174 (95%)	49 (4%)	9 (1%)	18	14

All (9) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	273	LYS
1	C	271	LYS
1	D	268	PRO
1	D	2	ARG
1	D	266	ALA
1	A	2[A]	ARG
1	A	2[B]	ARG
1	C	2	ARG
1	D	270	TYR

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	266/271 (98%)	256 (96%)	10 (4%)	29	29
1	B	272/271 (100%)	266 (98%)	6 (2%)	45	50
1	C	271/271 (100%)	264 (97%)	7 (3%)	40	44
1	D	271/271 (100%)	266 (98%)	5 (2%)	51	58
All	All	1080/1084 (100%)	1052 (97%)	28 (3%)	43	44

All (28) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1	MET
1	A	2[A]	ARG

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	2[B]	ARG
1	A	107	LEU
1	A	169	THR
1	A	186	THR
1	A	206	ILE
1	A	228	LEU
1	A	254	SER
1	A	273	LYS
1	B	113	GLU
1	B	206	ILE
1	B	228	LEU
1	B	254	SER
1	B	260	THR
1	B	273	LYS
1	C	1	MET
1	C	55[A]	ARG
1	C	55[B]	ARG
1	C	183	ARG
1	C	254	SER
1	C	260	THR
1	C	273	LYS
1	D	2	ARG
1	D	26	ARG
1	D	169	THR
1	D	254	SER
1	D	260	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (11) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	108	ASN
1	A	160	ASN
1	B	176	ASN
1	B	236	ASN
1	C	48	ASN
1	C	108	ASN
1	C	182	GLN
1	C	236	ASN
1	C	297	ASN
1	D	58	GLN
1	D	236	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
1	KCX	B	137	1,3,2	10,11,12	0.76	0	6,12,14	0.56	0
1	KCX	D	137	1,3,2	10,11,12	1.41	1 (10%)	6,12,14	2.19	2 (33%)
1	KCX	C	137	1,3,2	10,11,12	2.28	1 (10%)	6,12,14	2.20	1 (16%)
1	KCX	A	137	1,3,2	10,11,12	1.08	1 (10%)	6,12,14	1.09	1 (16%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	KCX	B	137	1,3,2	-	0/9/10/12	-
1	KCX	D	137	1,3,2	-	0/9/10/12	-
1	KCX	C	137	1,3,2	-	0/9/10/12	-
1	KCX	A	137	1,3,2	-	4/9/10/12	-

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	137	KCX	OQ1-CX	6.74	1.34	1.21
1	D	137	KCX	OQ1-CX	3.85	1.28	1.21
1	A	137	KCX	CB-CA	2.09	1.56	1.53

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	137	KCX	OQ1-CX-NZ	-5.15	117.09	124.92
1	D	137	KCX	OQ1-CX-NZ	-4.71	117.76	124.92
1	D	137	KCX	CE-NZ-CX	2.39	126.03	121.98
1	A	137	KCX	CE-NZ-CX	2.13	125.60	121.98

There are no chirality outliers.

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	A	137	KCX	N-CA-CB-CG
1	A	137	KCX	C-CA-CB-CG
1	A	137	KCX	CA-CB-CG-CD
1	A	137	KCX	CG-CD-CE-NZ

There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	B	137	KCX	1	0
1	A	137	KCX	1	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 16 ligands modelled in this entry, 8 are monoatomic - leaving 8 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	$\# Z > 2$
4	GOL	D	403	-	5,5,5	0.64	0	5,5,5	0.86	0
4	GOL	B	404	-	5,5,5	0.86	0	5,5,5	1.09	0
4	GOL	A	404	-	5,5,5	0.79	0	5,5,5	0.59	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	GOL	C	403	-	5,5,5	0.39	0	5,5,5	0.95	0
4	GOL	C	404	3,2	5,5,5	0.78	0	5,5,5	1.20	1 (20%)
4	GOL	A	405	-	5,5,5	1.04	0	5,5,5	0.76	0
4	GOL	A	403	-	5,5,5	1.15	0	5,5,5	2.20	3 (60%)
4	GOL	B	403	-	5,5,5	0.50	0	5,5,5	0.51	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	GOL	D	403	-	-	4/4/4/4	-
4	GOL	B	404	-	-	2/4/4/4	-
4	GOL	A	404	-	-	2/4/4/4	-
4	GOL	C	403	-	-	0/4/4/4	-
4	GOL	C	404	3,2	-	0/4/4/4	-
4	GOL	A	405	-	-	4/4/4/4	-
4	GOL	A	403	-	-	4/4/4/4	-
4	GOL	B	403	-	-	1/4/4/4	-

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	403	GOL	O2-C2-C1	2.94	121.34	109.18
4	A	403	GOL	O3-C3-C2	-2.42	99.50	110.38
4	A	403	GOL	C3-C2-C1	-2.18	103.82	111.80
4	C	404	GOL	C3-C2-C1	-2.14	103.94	111.80

There are no chirality outliers.

All (17) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	403	GOL	C1-C2-C3-O3
4	A	405	GOL	C1-C2-C3-O3
4	B	404	GOL	O1-C1-C2-C3
4	D	403	GOL	O1-C1-C2-C3
4	D	403	GOL	C1-C2-C3-O3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
4	A	403	GOL	O2-C2-C3-O3
4	A	405	GOL	O1-C1-C2-O2
4	D	403	GOL	O1-C1-C2-O2
4	A	404	GOL	O1-C1-C2-C3
4	A	405	GOL	O1-C1-C2-C3
4	B	403	GOL	C1-C2-C3-O3
4	A	405	GOL	O2-C2-C3-O3
4	A	404	GOL	O1-C1-C2-O2
4	B	404	GOL	O1-C1-C2-O2
4	D	403	GOL	O2-C2-C3-O3
4	A	403	GOL	O1-C1-C2-O2
4	A	403	GOL	O1-C1-C2-C3

There are no ring outliers.

No monomer is involved in short contacts.

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	304/314 (96%)	-0.31	8 (2%) 57 56	11, 24, 42, 94	2 (0%)
1	B	313/314 (99%)	-0.34	10 (3%) 50 49	13, 23, 48, 84	1 (0%)
1	C	309/314 (98%)	-0.22	11 (3%) 46 45	17, 25, 50, 116	2 (0%)
1	D	313/314 (99%)	-0.03	14 (4%) 38 37	16, 29, 54, 161	0
All	All	1239/1256 (98%)	-0.23	43 (3%) 47 46	11, 25, 51, 161	5 (0%)

All (43) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	261	PHE	5.4
1	D	260	THR	5.2
1	D	272	PRO	5.2
1	C	268	PRO	5.2
1	C	263	ALA	4.9
1	A	272	PRO	4.9
1	D	265	THR	4.8
1	D	268	PRO	4.7
1	A	261	PHE	4.5
1	A	260	THR	4.3
1	A	1	MET	4.1
1	D	266	ALA	4.0
1	C	261	PHE	4.0
1	D	270	TYR	3.9
1	C	1	MET	3.9
1	C	270	TYR	3.7
1	B	266	ALA	3.6
1	D	1	MET	3.5
1	D	271	LYS	3.5
1	B	263	ALA	3.4
1	D	267	LYS	3.4

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	C	260	THR	3.3
1	D	263	ALA	3.3
1	B	268	PRO	3.2
1	C	262	ASP	3.2
1	B	261	PHE	3.2
1	C	272	PRO	3.1
1	B	1	MET	3.1
1	B	272	PRO	3.0
1	D	259	CYS	2.7
1	D	264	GLY	2.7
1	A	258	LEU	2.6
1	B	265	THR	2.6
1	C	271	LYS	2.5
1	D	273	LYS	2.5
1	B	270	TYR	2.4
1	C	274	LEU	2.3
1	A	273	LYS	2.3
1	B	260	THR	2.3
1	A	259	CYS	2.3
1	C	273	LYS	2.2
1	B	269	GLU	2.1
1	A	274	LEU	2.0

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

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
1	KCX	A	137	12/13	0.97	0.06	15,16,20,21	0
1	KCX	C	137	12/13	0.97	0.05	16,17,18,19	0
1	KCX	D	137	12/13	0.97	0.05	17,19,20,23	0
1	KCX	B	137	12/13	0.98	0.04	13,15,16,18	0

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands

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
4	GOL	A	405	6/6	0.83	0.16	47,52,62,63	0
4	GOL	A	403	6/6	0.90	0.11	31,33,34,41	0
4	GOL	C	404	6/6	0.91	0.12	35,41,54,61	0
4	GOL	B	403	6/6	0.92	0.09	27,32,42,49	0
4	GOL	D	403	6/6	0.92	0.10	35,41,43,48	0
4	GOL	A	404	6/6	0.94	0.11	23,30,43,43	0
4	GOL	C	403	6/6	0.94	0.07	27,30,34,35	0
4	GOL	B	404	6/6	0.95	0.07	27,32,36,41	0
3	CO	D	402	1/1	0.99	0.03	24,24,24,24	0
2	FE2	C	401	1/1	1.00	0.01	16,16,16,16	0
2	FE2	D	401	1/1	1.00	0.03	19,19,19,19	0
3	CO	A	402	1/1	1.00	0.02	19,19,19,19	0
3	CO	B	402	1/1	1.00	0.01	20,20,20,20	0
3	CO	C	402	1/1	1.00	0.01	20,20,20,20	0
2	FE2	A	401	1/1	1.00	0.01	15,15,15,15	0
2	FE2	B	401	1/1	1.00	0.02	14,14,14,14	0

6.5 Other polymers

There are no such residues in this entry.