



Full wwPDB X-ray Structure Validation Report ⓘ

Jan 17, 2023 – 06:44 PM EST

PDB ID : 2QYV
Title : Crystal structure of putative Xaa-His dipeptidase (YP_718209.1) from Haemophilus somnus 129PT at 2.11 Å resolution
Authors : Joint Center for Structural Genomics (JCSG)
Deposited on : 2007-08-15
Resolution : 2.11 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 : 2.31.2
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) : 2.31.2

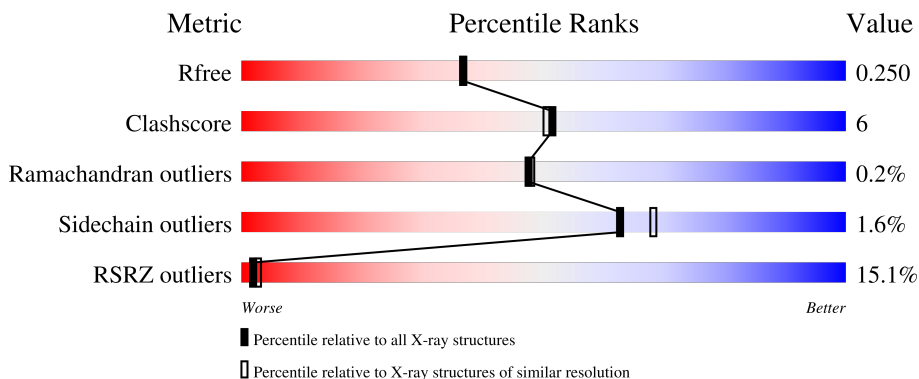
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.11 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	6241 (2.14-2.10)
Clashscore	141614	6778 (2.14-2.10)
Ramachandran outliers	138981	6705 (2.14-2.10)
Sidechain outliers	138945	6706 (2.14-2.10)
RSRZ outliers	127900	6112 (2.14-2.10)

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	487	
1	B	487	

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	SO4	B	511	-	-	-	X
4	GOL	A	512	-	-	-	X
4	GOL	B	514	-	-	-	X
4	GOL	B	519	-	-	-	X

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 7920 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 Xaa-His dipeptidase.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
			Total	C	N	O	S	Se			
1	A	472	3631	2309	619	690	6	7	0	3	0
1	B	470	3615	2300	616	686	6	7	0	4	0

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	0	GLY	-	expression tag	UNP Q0I1B9
B	0	GLY	-	expression tag	UNP Q0I1B9

- Molecule 2 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	2	Total	Zn	0	0
			2	2		
2	B	2	Total	Zn	0	0
			2	2		

- Molecule 3 is SULFATE ION (three-letter code: SO4) (formula: O₄S).



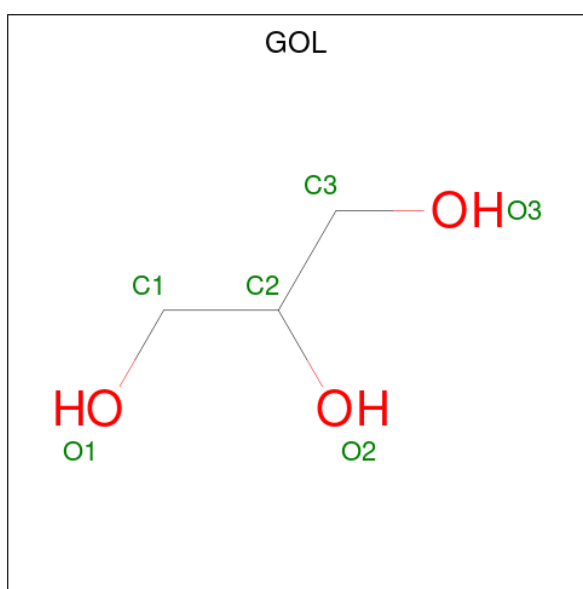
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	O	S	0	0
			5	4	1		
3	A	1	Total	O	S	0	0
			5	4	1		
3	A	1	Total	O	S	0	0
			5	4	1		
3	A	1	Total	O	S	0	0
			5	4	1		
3	A	1	Total	O	S	0	0
			5	4	1		
3	A	1	Total	O	S	0	0
			5	4	1		
3	A	1	Total	O	S	0	0
			5	4	1		
3	B	1	Total	O	S	0	0
			5	4	1		
3	B	1	Total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

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

- Molecule 4 is GLYCEROL (three-letter code: GOL) (formula: C₃H₈O₃).



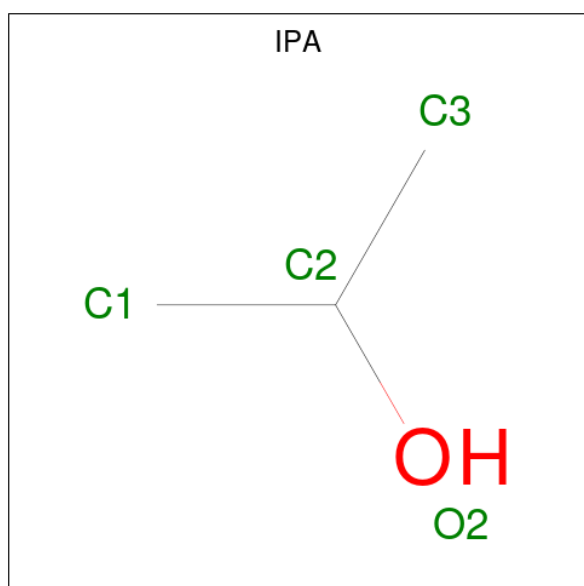
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			6	3	3		
4	A	1	Total	C	O	0	0
			6	3	3		
4	A	1	Total	C	O	0	0
			6	3	3		
4	A	1	Total	C	O	0	0
			6	3	3		
4	A	1	Total	C	O	0	0
			6	3	3		
4	A	1	Total	C	O	0	0
			6	3	3		
4	A	1	Total	C	O	0	0
			6	3	3		

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

- Molecule 5 is ISOPROPYL ALCOHOL (three-letter code: IPA) (formula: C₃H₈O).



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

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

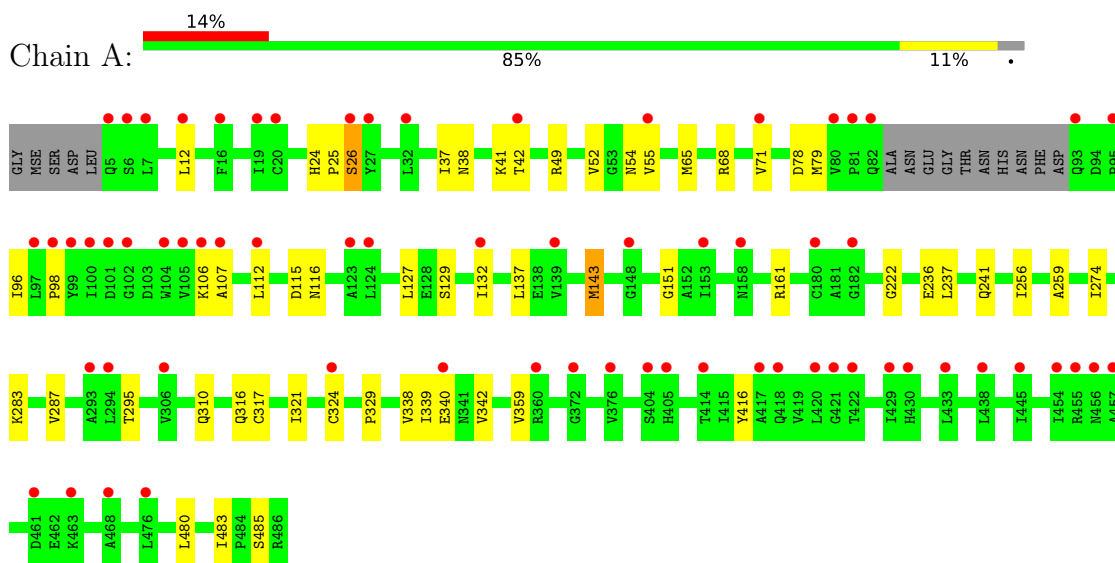
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	243	Total	O	0	0
			243	243		
6	B	223	Total	O	0	0
			223	223		

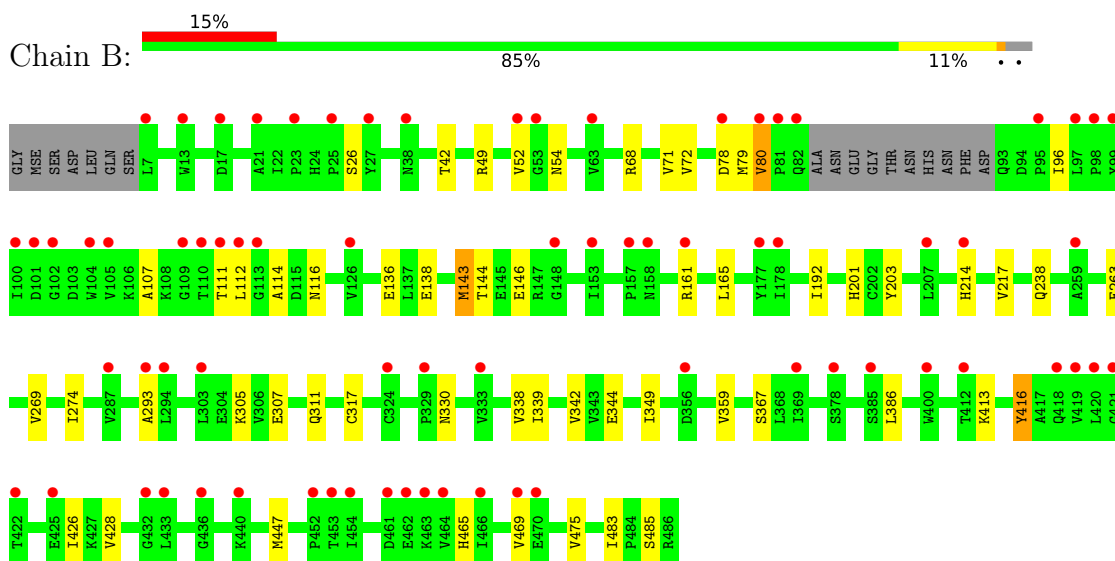
3 Residue-property plots [i](#)

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: Xaa-His dipeptidase



- Molecule 1: Xaa-His dipeptidase



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, α , β , γ	173.92Å 84.29Å 123.20Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	47.84 – 2.11 47.82 – 2.11	Depositor EDS
% Data completeness (in resolution range)	97.7 (47.84-2.11) 97.7 (47.82-2.11)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	0.09	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.83 (at 2.10Å)	Xtrriage
Refinement program	REFMAC 5.2.0019, PHENIX	Depositor
R, R_{free}	0.220 , 0.244 0.227 , 0.250	Depositor DCC
R_{free} test set	5107 reflections (4.99%)	wwPDB-VP
Wilson B-factor (Å ²)	31.1	Xtrriage
Anisotropy	0.464	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 59.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.46$, $\langle L^2 \rangle = 0.29$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	7920	wwPDB-VP
Average B, all atoms (Å ²)	60.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 66.29 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 6.1844e-06. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

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 [i](#)

5.1 Standard geometry [i](#)

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

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	0.51	2/3705 (0.1%)	0.62	0/5033
1	B	0.52	2/3692 (0.1%)	0.63	0/5019
All	All	0.52	4/7397 (0.1%)	0.63	0/10052

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	143	MSE	SE-CE	5.75	2.29	1.95
1	B	317	CYS	CB-SG	-5.50	1.72	1.81
1	B	143	MSE	SE-CE	5.42	2.27	1.95
1	A	317	CYS	CB-SG	-5.29	1.73	1.81

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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	3631	0	3599	37	0
1	B	3615	0	3578	48	0
2	A	2	0	0	0	0
2	B	2	0	0	0	0
3	A	40	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	B	50	0	0	0	0
4	A	48	0	64	4	0
4	B	54	0	72	2	0
5	A	8	0	16	0	0
5	B	4	0	8	2	0
6	A	243	0	0	3	0
6	B	223	0	0	1	0
All	All	7920	0	7337	83	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 6.

All (83) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:143:MSE:CE	1:B:143:MSE:SE	2.27	1.33
1:A:143:MSE:CE	1:A:143:MSE:SE	2.29	1.31
1:A:71:VAL:HG21	1:A:483:ILE:HD13	1.38	1.04
1:B:71:VAL:HG21	1:B:483:ILE:HD13	1.39	1.04
1:B:71:VAL:HG21	1:B:483:ILE:CD1	2.04	0.86
1:B:80:VAL:HG23	1:B:146:GLU:HG2	1.57	0.84
1:B:71:VAL:CG2	1:B:483:ILE:HD13	2.13	0.78
1:A:79:MSE:SE	1:A:96:ILE:HD11	2.34	0.77
1:B:338:VAL:HG23	1:B:339:ILE:HG13	1.69	0.73
1:A:71:VAL:HG21	1:A:483:ILE:CD1	2.18	0.72
1:A:222:GLY:O	1:A:295:THR:HG21	1.89	0.72
1:B:80:VAL:HG23	1:B:146:GLU:CG	2.20	0.72
1:A:237:LEU:HD12	1:A:241:GLN:HG3	1.75	0.69
1:A:71:VAL:CG2	1:A:483:ILE:HD13	2.20	0.68
1:A:329:PRO:HA	4:A:517:GOL:H2	1.74	0.68
1:B:79:MSE:SE	1:B:96:ILE:HD11	2.44	0.68
1:A:338:VAL:HG23	1:A:339:ILE:HG13	1.77	0.66
1:A:41:LYS:NZ	6:A:721:HOH:O	2.29	0.66
1:B:68:ARG:HD3	1:B:483:ILE:O	1.96	0.65
1:B:238:GLN:HE21	4:B:521:GOL:H31	1.63	0.63
1:A:324:CYS:HA	1:B:386:LEU:HD11	1.79	0.63
1:B:107:ALA:HB2	1:B:112:LEU:HA	1.81	0.63
1:A:26:SER:HA	1:A:78:ASP:HB2	1.83	0.61
1:B:339:ILE:HD13	1:B:428:VAL:HG11	1.85	0.57
1:B:26:SER:HA	1:B:78:ASP:HB2	1.86	0.57
1:A:324:CYS:N	1:B:386:LEU:HD11	2.21	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:38:ASN:O	1:A:42:THR:HG23	2.06	0.55
1:A:236:GLU:HG3	4:A:511:GOL:H12	1.89	0.54
4:A:517:GOL:H11	6:A:751:HOH:O	2.08	0.53
1:A:324:CYS:CA	1:B:386:LEU:HD11	2.40	0.52
1:B:307:GLU:HG3	5:B:522:IPA:H32	1.92	0.51
1:B:339:ILE:HD13	1:B:428:VAL:CG1	2.40	0.51
1:A:340:GLU:O	1:A:342:VAL:HG23	2.11	0.51
1:A:79:MSE:SE	1:A:96:ILE:CD1	3.09	0.50
1:B:238:GLN:HE21	4:B:521:GOL:C3	2.25	0.50
1:B:274:ILE:HD12	6:B:699:HOH:O	2.10	0.49
1:B:339:ILE:CG2	1:B:342:VAL:HG21	2.41	0.49
1:A:49:ARG:HA	1:A:54:ASN:O	2.13	0.48
1:A:12:LEU:C	1:A:12:LEU:HD23	2.34	0.48
1:B:165:LEU:HB3	1:B:447:MSE:HG2	1.96	0.48
1:A:37:ILE:HD11	1:A:55:VAL:HG13	1.95	0.47
1:B:330:ASN:OD1	1:B:349:ILE:HG22	2.15	0.47
1:A:24:HIS:N	1:A:25:PRO:CD	2.77	0.47
1:B:79:MSE:SE	1:B:96:ILE:CD1	3.12	0.47
1:B:416:TYR:CD1	1:B:475:VAL:HG21	2.50	0.47
1:A:129:SER:CB	1:A:132:ILE:HD12	2.45	0.47
1:A:321:ILE:HD13	1:A:359:VAL:HG21	1.98	0.46
1:B:339:ILE:HG21	1:B:342:VAL:HG21	1.96	0.46
1:B:79:MSE:CE	1:B:96:ILE:HD11	2.46	0.46
1:A:222:GLY:C	1:A:295:THR:HG21	2.37	0.45
1:B:144:THR:HG22	1:B:144:THR:O	2.17	0.45
4:A:517:GOL:C1	6:A:751:HOH:O	2.64	0.45
1:B:413:LYS:CE	1:B:426:ILE:HD11	2.47	0.45
1:A:52:VAL:HG11	1:A:151:GLY:HA2	1.99	0.45
1:B:138:GLU:OE2	1:B:161[B]:ARG:HG3	2.18	0.44
1:B:214:HIS:HB3	1:B:217:VAL:HG22	2.00	0.44
1:A:256:ILE:HG22	1:A:259:ALA:HB3	2.00	0.43
1:A:68:ARG:HD3	1:A:483:ILE:O	2.18	0.43
1:B:413:LYS:CD	1:B:426:ILE:HD11	2.48	0.43
1:B:307:GLU:CG	5:B:522:IPA:H32	2.48	0.43
1:B:214:HIS:ND1	1:B:217:VAL:HG22	2.34	0.43
1:B:201:HIS:O	1:B:269:VAL:HA	2.19	0.42
1:B:203:TYR:CE2	1:B:305:LYS:HB2	2.54	0.42
1:A:480:LEU:HA	1:A:483:ILE:HD12	2.01	0.42
1:A:115:ASP:HA	1:A:116:ASN:HA	1.85	0.42
1:B:136:GLU:OE2	1:B:161[B]:ARG:NH1	2.52	0.42
1:B:79:MSE:HE1	1:B:111:THR:O	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:79:MSE:HE1	1:B:96:ILE:HD11	2.00	0.42
1:A:65:MSE:SE	1:A:68:ARG:HD2	2.68	0.42
1:A:274:ILE:H	1:A:274:ILE:HD12	1.85	0.42
1:B:72:VAL:HA	1:B:138:GLU:O	2.20	0.41
1:B:192:ILE:HD11	1:B:359:VAL:HG23	2.01	0.41
1:B:465:HIS:O	1:B:469:VAL:HG23	2.21	0.41
1:A:98:PRO:HA	1:A:106:LYS:O	2.21	0.41
1:A:324:CYS:HA	1:B:386:LEU:CD1	2.50	0.41
1:B:49:ARG:HA	1:B:54:ASN:O	2.21	0.41
1:B:342:VAL:HG11	1:B:428:VAL:HG22	2.02	0.41
1:A:107:ALA:HB2	1:A:112:LEU:HA	2.03	0.40
1:B:112:LEU:HD23	1:B:114:ALA:HB2	2.03	0.40
1:A:283:LYS:O	1:A:287:VAL:HG23	2.22	0.40
1:B:344:GLU:O	1:B:367:SER:HA	2.22	0.40
1:A:127:LEU:HD23	1:A:137:LEU:HD23	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	471/487 (97%)	454 (96%)	16 (3%)	1 (0%)	47	48
1	B	470/487 (96%)	456 (97%)	13 (3%)	1 (0%)	47	48
All	All	941/974 (97%)	910 (97%)	29 (3%)	2 (0%)	47	48

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	293	ALA
1	A	26	SER

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	391/409 (96%)	386 (99%)	5 (1%)	69	74
1	B	389/409 (95%)	381 (98%)	8 (2%)	53	57
All	All	780/818 (95%)	767 (98%)	13 (2%)	62	66

All (13) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	161	ARG
1	A	310	GLN
1	A	316	GLN
1	A	416	TYR
1	A	485	SER
1	B	52	VAL
1	B	80	VAL
1	B	116	ASN
1	B	263[A]	GLU
1	B	263[B]	GLU
1	B	311	GLN
1	B	416	TYR
1	B	485	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

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 monosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 42 ligands modelled in this entry, 4 are monoatomic - leaving 38 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	SO4	A	507	-	4,4,4	0.17	0	6,6,6	0.21	0
3	SO4	A	508	-	4,4,4	0.14	0	6,6,6	0.36	0
3	SO4	B	510	-	4,4,4	0.17	0	6,6,6	0.11	0
4	GOL	B	516	-	5,5,5	0.33	0	5,5,5	0.52	0
4	GOL	B	515	-	5,5,5	0.44	0	5,5,5	0.34	0
3	SO4	A	503	-	4,4,4	0.09	0	6,6,6	0.78	0
3	SO4	B	505	-	4,4,4	0.14	0	6,6,6	0.22	0
3	SO4	B	506	-	4,4,4	0.09	0	6,6,6	0.51	0
4	GOL	A	513	-	5,5,5	0.46	0	5,5,5	0.24	0
3	SO4	A	510	-	4,4,4	0.14	0	6,6,6	0.07	0
4	GOL	A	515	-	5,5,5	0.41	0	5,5,5	0.26	0
4	GOL	B	514	-	5,5,5	0.34	0	5,5,5	0.36	0
5	IPA	B	522	-	3,3,3	0.59	0	3,3,3	0.35	0
4	GOL	B	519	-	5,5,5	0.43	0	5,5,5	0.33	0
3	SO4	A	506	-	4,4,4	0.20	0	6,6,6	0.38	0
4	GOL	A	511	-	5,5,5	0.45	0	5,5,5	0.67	0
3	SO4	A	505	-	4,4,4	0.17	0	6,6,6	0.37	0
4	GOL	A	516	-	5,5,5	0.33	0	5,5,5	0.40	0
3	SO4	B	503	-	4,4,4	0.13	0	6,6,6	0.91	0
3	SO4	A	509	-	4,4,4	0.16	0	6,6,6	0.19	0
4	GOL	A	514	-	5,5,5	0.33	0	5,5,5	0.21	0
4	GOL	B	521	-	5,5,5	0.23	0	5,5,5	0.62	0
4	GOL	B	518	-	5,5,5	0.36	0	5,5,5	0.63	0
4	GOL	B	520	-	5,5,5	0.36	0	5,5,5	0.23	0
5	IPA	A	519	-	3,3,3	0.58	0	3,3,3	0.30	0
3	SO4	B	512	-	4,4,4	0.15	0	6,6,6	0.17	0
4	GOL	A	518	-	5,5,5	0.47	0	5,5,5	0.82	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	GOL	B	517	-	5,5,5	0.38	0	5,5,5	0.25	0
3	SO4	B	511	-	4,4,4	0.14	0	6,6,6	0.28	0
4	GOL	B	513	-	5,5,5	0.21	0	5,5,5	0.64	0
3	SO4	B	509	-	4,4,4	0.15	0	6,6,6	0.25	0
5	IPA	A	520	-	3,3,3	0.56	0	3,3,3	0.24	0
4	GOL	A	512	-	5,5,5	0.42	0	5,5,5	0.12	0
3	SO4	B	504	-	4,4,4	0.10	0	6,6,6	0.10	0
4	GOL	A	517	-	5,5,5	0.37	0	5,5,5	0.56	0
3	SO4	A	504	-	4,4,4	0.14	0	6,6,6	0.17	0
3	SO4	B	507	-	4,4,4	0.16	0	6,6,6	0.30	0
3	SO4	B	508	-	4,4,4	0.12	0	6,6,6	0.27	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	A	512	-	-	4/4/4/4	-
4	GOL	A	515	-	-	4/4/4/4	-
4	GOL	A	513	-	-	2/4/4/4	-
4	GOL	B	520	-	-	2/4/4/4	-
4	GOL	B	514	-	-	4/4/4/4	-
4	GOL	A	518	-	-	2/4/4/4	-
4	GOL	B	516	-	-	2/4/4/4	-
4	GOL	A	511	-	-	2/4/4/4	-
4	GOL	B	519	-	-	2/4/4/4	-
4	GOL	A	516	-	-	3/4/4/4	-
4	GOL	A	517	-	-	3/4/4/4	-
4	GOL	B	517	-	-	2/4/4/4	-
4	GOL	A	514	-	-	4/4/4/4	-
4	GOL	B	513	-	-	2/4/4/4	-
4	GOL	B	515	-	-	2/4/4/4	-
4	GOL	B	521	-	-	0/4/4/4	-
4	GOL	B	518	-	-	2/4/4/4	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (42) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	512	GOL	O1-C1-C2-C3
4	A	514	GOL	O1-C1-C2-C3
4	A	515	GOL	O1-C1-C2-O2
4	A	515	GOL	O1-C1-C2-C3
4	A	518	GOL	C1-C2-C3-O3
4	B	513	GOL	C1-C2-C3-O3
4	B	514	GOL	O1-C1-C2-C3
4	B	515	GOL	C1-C2-C3-O3
4	B	516	GOL	O1-C1-C2-O2
4	B	516	GOL	O1-C1-C2-C3
4	B	518	GOL	C1-C2-C3-O3
4	B	518	GOL	O2-C2-C3-O3
4	B	520	GOL	O2-C2-C3-O3
4	A	511	GOL	O1-C1-C2-C3
4	A	514	GOL	C1-C2-C3-O3
4	A	515	GOL	C1-C2-C3-O3
4	A	516	GOL	O1-C1-C2-C3
4	A	517	GOL	O1-C1-C2-C3
4	B	514	GOL	C1-C2-C3-O3
4	B	519	GOL	O1-C1-C2-C3
4	B	520	GOL	C1-C2-C3-O3
4	A	512	GOL	O1-C1-C2-O2
4	A	514	GOL	O2-C2-C3-O3
4	A	515	GOL	O2-C2-C3-O3
4	A	516	GOL	O1-C1-C2-O2
4	A	517	GOL	O1-C1-C2-O2
4	B	513	GOL	O2-C2-C3-O3
4	B	514	GOL	O2-C2-C3-O3
4	A	518	GOL	O2-C2-C3-O3
4	B	514	GOL	O1-C1-C2-O2
4	A	511	GOL	O1-C1-C2-O2
4	A	513	GOL	O2-C2-C3-O3
4	B	517	GOL	O2-C2-C3-O3
4	B	515	GOL	O2-C2-C3-O3
4	B	519	GOL	O1-C1-C2-O2
4	A	512	GOL	C1-C2-C3-O3
4	A	514	GOL	O1-C1-C2-O2
4	A	513	GOL	C1-C2-C3-O3
4	A	512	GOL	O2-C2-C3-O3
4	A	517	GOL	O2-C2-C3-O3

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Mol	Chain	Res	Type	Atoms
4	A	516	GOL	C1-C2-C3-O3
4	B	517	GOL	C1-C2-C3-O3

There are no ring outliers.

4 monomers are involved in 8 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	B	522	IPA	2	0
4	A	511	GOL	1	0
4	B	521	GOL	2	0
4	A	517	GOL	3	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 [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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	465/487 (95%)	1.18	67 (14%) 2 3	29, 59, 86, 99	0
1	B	463/487 (95%)	1.25	73 (15%) 2 2	29, 59, 86, 99	0
All	All	928/974 (95%)	1.21	140 (15%) 2 3	29, 59, 86, 99	0

All (140) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	99	TYR	9.0
1	A	99	TYR	7.1
1	B	100	ILE	7.1
1	A	417	ALA	6.1
1	B	27	TYR	5.9
1	A	468	ALA	5.8
1	B	102	GLY	5.7
1	B	112	LEU	5.7
1	B	101	ASP	5.7
1	A	80	VAL	5.2
1	B	80	VAL	5.1
1	B	97	LEU	5.1
1	A	107	ALA	5.1
1	A	153	ILE	4.9
1	B	466	ILE	4.9
1	B	461	ASP	4.9
1	A	100	ILE	4.8
1	A	294	LEU	4.7
1	B	454	ILE	4.6
1	A	7	LEU	4.6
1	A	461	ASP	4.5
1	A	101	ASP	4.5
1	B	104	TRP	4.5
1	A	97	LEU	4.5

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Mol	Chain	Res	Type	RSRZ
1	B	23	PRO	4.5
1	B	420	LEU	4.4
1	B	81	PRO	4.3
1	B	294	LEU	4.2
1	A	104	TRP	4.0
1	B	422	THR	4.0
1	A	158	ASN	4.0
1	A	404	SER	3.9
1	B	38[A]	ASN	3.9
1	B	105	VAL	3.7
1	A	5	GLN	3.7
1	B	109	GLY	3.7
1	A	421	GLY	3.6
1	B	214	HIS	3.5
1	A	102	GLY	3.5
1	B	158	ASN	3.5
1	A	422	THR	3.5
1	B	7	LEU	3.4
1	A	454	ILE	3.4
1	A	20	CYS	3.4
1	B	287	VAL	3.3
1	A	414	THR	3.2
1	A	98	PRO	3.1
1	A	112	LEU	3.1
1	A	95	PRO	3.1
1	B	13	TRP	3.0
1	B	53	GLY	3.0
1	A	438	LEU	2.9
1	B	462	GLU	2.9
1	B	464	VAL	2.9
1	B	111	THR	2.9
1	A	420	LEU	2.9
1	B	25	PRO	2.9
1	A	19	ILE	2.9
1	A	418	GLN	2.9
1	B	95	PRO	2.9
1	A	306	VAL	2.8
1	B	369	ILE	2.8
1	A	32	LEU	2.8
1	B	52	VAL	2.7
1	A	42	THR	2.7
1	A	6	SER	2.7

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Mol	Chain	Res	Type	RSRZ
1	B	110	THR	2.7
1	B	469	VAL	2.7
1	A	376	VAL	2.6
1	A	139	VAL	2.6
1	B	148	GLY	2.6
1	B	98	PRO	2.6
1	A	324	CYS	2.6
1	A	93	GLN	2.6
1	A	16	PHE	2.6
1	B	425	GLU	2.5
1	A	463	LYS	2.5
1	B	400	TRP	2.5
1	B	17	ASP	2.5
1	B	126	VAL	2.5
1	A	105	VAL	2.4
1	B	153	ILE	2.4
1	A	124	LEU	2.4
1	B	177	TYR	2.4
1	A	26	SER	2.4
1	B	433	LEU	2.4
1	A	455	ARG	2.4
1	B	324	CYS	2.4
1	A	433	LEU	2.4
1	B	82	GLN	2.4
1	A	12	LEU	2.3
1	B	63	VAL	2.3
1	B	293	ALA	2.3
1	B	432	GLY	2.3
1	B	178	ILE	2.3
1	A	55	VAL	2.3
1	A	429	ILE	2.3
1	B	303	LEU	2.3
1	A	182	GLY	2.3
1	B	412	THR	2.3
1	B	436	GLY	2.3
1	B	259	ALA	2.3
1	B	463	LYS	2.3
1	A	445	ILE	2.3
1	A	293	ALA	2.2
1	B	78	ASP	2.2
1	B	453	THR	2.2
1	A	81	PRO	2.2

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Mol	Chain	Res	Type	RSRZ
1	B	440	LYS	2.2
1	B	21	ALA	2.2
1	B	207	LEU	2.2
1	A	82	GLN	2.2
1	B	161[A]	ARG	2.2
1	B	113	GLY	2.2
1	B	419	VAL	2.2
1	A	405	HIS	2.2
1	A	430	HIS	2.2
1	A	123	ALA	2.2
1	B	470	GLU	2.2
1	B	452	PRO	2.2
1	A	132	ILE	2.1
1	A	340	GLU	2.1
1	A	360	ARG	2.1
1	B	329	PRO	2.1
1	A	27	TYR	2.1
1	A	148	GLY	2.1
1	A	457	ALA	2.1
1	A	372	GLY	2.1
1	B	333	VAL	2.1
1	B	157	PRO	2.1
1	B	418	GLN	2.1
1	A	71	VAL	2.1
1	B	378	SER	2.0
1	A	476	LEU	2.0
1	A	456	ASN	2.0
1	A	106	LYS	2.0
1	B	385[A]	SER	2.0
1	A	180	CYS	2.0
1	B	356	ASP	2.0
1	B	421	GLY	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
4	GOL	A	512	6/6	0.36	0.42	97,99,99,99	0
4	GOL	B	519	6/6	0.44	0.57	94,97,98,98	0
4	GOL	A	516	6/6	0.56	0.27	85,88,88,89	0
4	GOL	B	516	6/6	0.57	0.30	67,71,73,75	0
4	GOL	B	521	6/6	0.64	0.36	76,78,79,80	0
4	GOL	B	515	6/6	0.67	0.24	86,87,88,88	0
3	SO4	A	509	5/5	0.69	0.36	100,100,102,103	0
3	SO4	B	509	5/5	0.69	0.28	113,115,116,117	0
5	IPA	A	520	4/4	0.70	0.28	74,76,76,77	0
2	ZN	B	502	1/1	0.71	0.19	117,117,117,117	0
3	SO4	B	511	5/5	0.75	0.40	119,120,120,120	0
2	ZN	B	501	1/1	0.76	0.08	95,95,95,95	0
4	GOL	B	514	6/6	0.77	0.41	75,79,81,81	0
3	SO4	B	504	5/5	0.77	0.28	134,135,135,135	0
4	GOL	A	517	6/6	0.77	0.21	65,65,66,67	0
4	GOL	A	514	6/6	0.78	0.32	71,75,76,78	0
3	SO4	B	505	5/5	0.79	0.37	91,95,96,97	0
5	IPA	B	522	4/4	0.79	0.39	68,69,71,71	0
3	SO4	B	512	5/5	0.82	0.32	123,125,126,126	0
3	SO4	B	508	5/5	0.82	0.31	107,107,109,109	0
4	GOL	B	520	6/6	0.83	0.17	66,70,71,74	0
5	IPA	A	519	4/4	0.83	0.19	68,68,70,72	0
2	ZN	A	502	1/1	0.84	0.13	131,131,131,131	0
4	GOL	A	518	6/6	0.86	0.17	61,69,72,73	0
4	GOL	A	515	6/6	0.86	0.26	57,64,68,71	0
4	GOL	B	517	6/6	0.86	0.19	78,80,80,82	0
3	SO4	A	507	5/5	0.87	0.30	96,98,99,100	0
3	SO4	A	505	5/5	0.87	0.28	98,101,101,102	0
3	SO4	A	504	5/5	0.88	0.26	111,111,112,113	0
3	SO4	B	507	5/5	0.88	0.29	84,86,87,88	0
4	GOL	B	518	6/6	0.88	0.22	70,72,75,77	0
3	SO4	B	506	5/5	0.89	0.31	85,87,91,93	0
3	SO4	A	506	5/5	0.89	0.30	79,83,85,87	0
3	SO4	B	510	5/5	0.89	0.26	106,107,108,108	0
4	GOL	A	513	6/6	0.89	0.13	82,82,84,84	0
3	SO4	A	508	5/5	0.90	0.28	82,82,84,85	0
3	SO4	B	503	5/5	0.91	0.14	58,62,64,65	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
3	SO4	A	510	5/5	0.91	0.16	121,122,122,122	0
4	GOL	B	513	6/6	0.94	0.14	41,44,45,45	0
4	GOL	A	511	6/6	0.94	0.10	33,37,40,42	0
3	SO4	A	503	5/5	0.95	0.14	46,58,62,62	0
2	ZN	A	501	1/1	0.99	0.13	73,73,73,73	0

6.5 Other polymers [i](#)

There are no such residues in this entry.