



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 05:30 AM GMT

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
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix) : 1.9-1692
EDS : rb-20026688
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac : 5.8.0135
CCP4 : 6.5.0
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : trunk26865

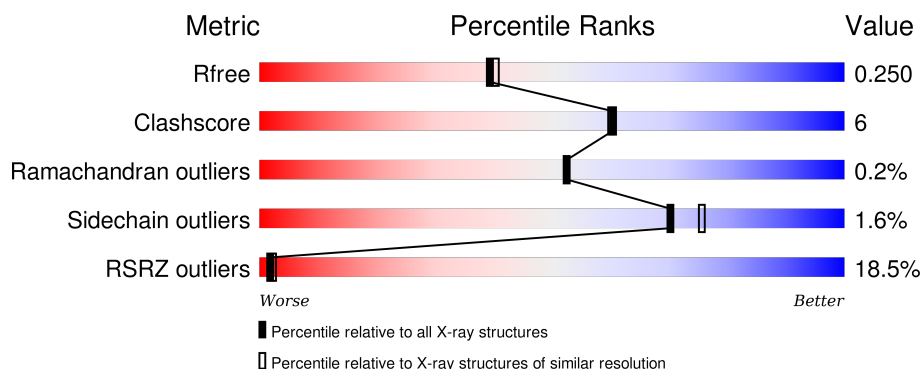
1 Overall quality at a glance ⓘ

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}	91344	4587 (2.14-2.10)
Clashscore	102246	5132 (2.14-2.10)
Ramachandran outliers	100387	5080 (2.14-2.10)
Sidechain outliers	100360	5081 (2.14-2.10)
RSRZ outliers	91569	4597 (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 on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. 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	<div> <div>17%</div> <div>85%</div> <div>11%</div> <div>.</div> </div>
1	B	487	<div> <div>19%</div> <div>85%</div> <div>11%</div> <div>..</div> </div>

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	A	506	-	-	-	X
3	SO4	A	509	-	-	-	X
3	SO4	B	506	-	-	-	X
3	SO4	B	508	-	-	-	X
3	SO4	B	511	-	-	-	X
3	SO4	B	512	-	-	-	X
4	GOL	A	512	-	-	-	X
4	GOL	A	514	-	-	-	X
4	GOL	A	515	-	-	-	X
4	GOL	A	516	-	-	-	X
4	GOL	B	515	-	-	-	X
4	GOL	B	516	-	-	-	X
4	GOL	B	521	-	-	-	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
1	A	472	Total	C	N	O	S	Se	0	3	0
			3631	2309	619	690	6	7			
1	B	470	Total	C	N	O	S	Se	0	4	0
			3615	2300	616	686	6	7			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	0	GLY	-	LEADER SEQUENCE	UNP Q0I1B9
B	0	GLY	-	LEADER SEQUENCE	UNP Q0I1B9

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

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



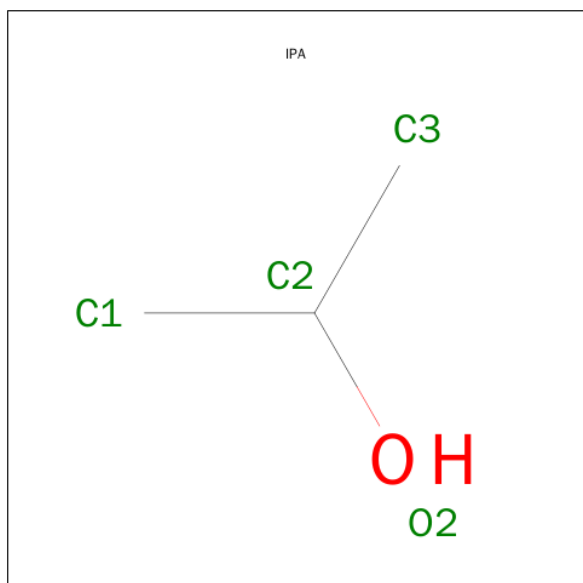
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			6	3	3		
4	B	1	Total	C	O	0	0
			6	3	3		
4	A	1	Total	C	O	0	0
			6	3	3		
4	B	1	Total	C	O	0	0
			6	3	3		
4	B	1	Total	C	O	0	0
			6	3	3		
4	B	1	Total	C	O	0	0
			6	3	3		
4	B	1	Total	C	O	0	0
			6	3	3		

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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	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	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		

- 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		

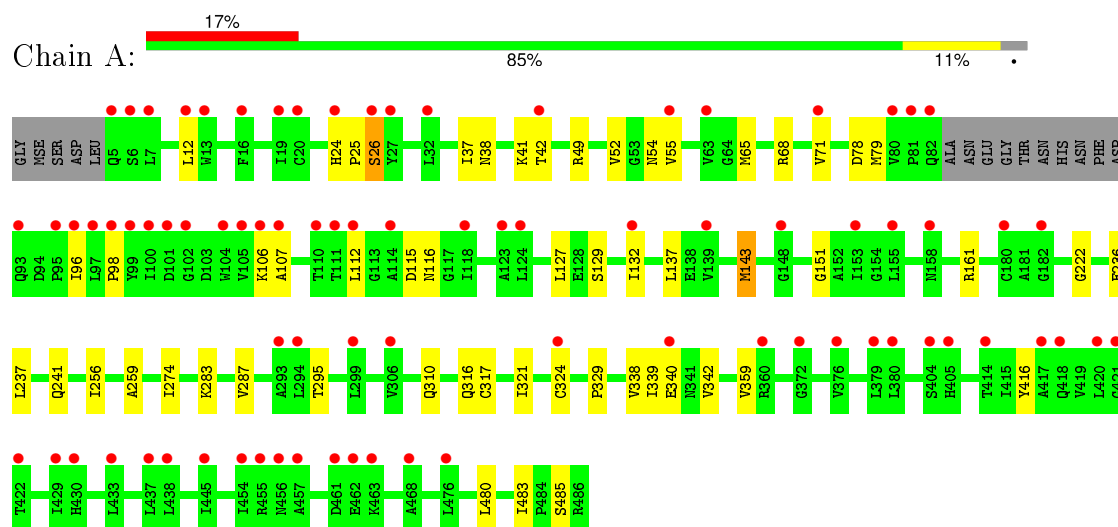
- Molecule 6 is water.

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

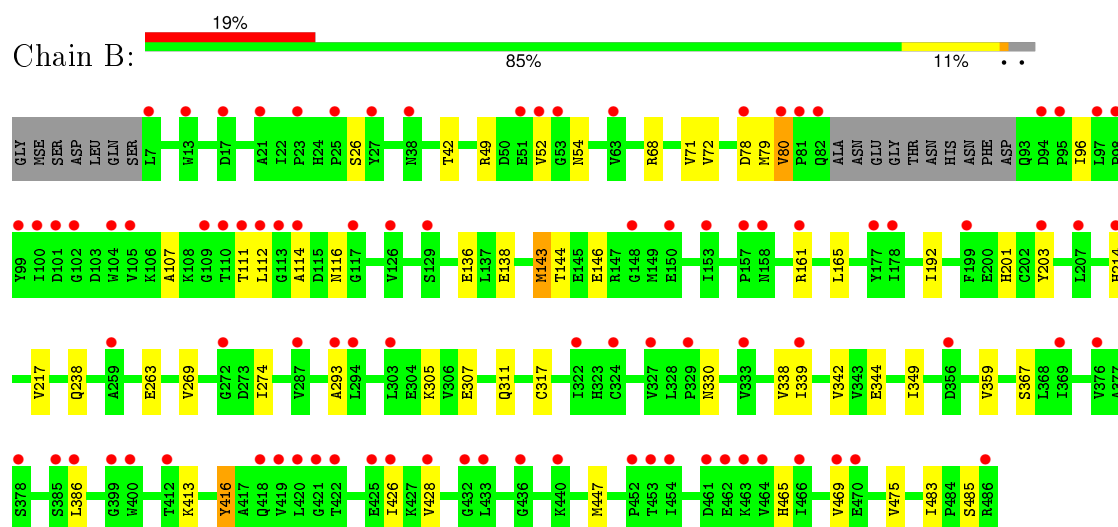
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.220 , 0.244 0.227 , 0.250	Depositor DCC
R_{free} test set	5107 reflections (5.25%)	DCC
Wilson B-factor (Å ²)	31.1	Xtriage
Anisotropy	0.464	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 59.7	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.46$, $\langle L^2 \rangle = 0.29$	Xtriage
Outliers	1 of 102315 reflections (0.001%)	Xtriage
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

Xtriage'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.*

¹ Intensities estimated from amplitudes.

² Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 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: GOL, ZN, IPA, 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	0.51	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:SE	1:A:143:MSE:CE	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:B:330:ASN:OD1	1:B:349:ILE:HG22	2.15	0.47
1:A:37:ILE:HD11	1:A:55:VAL:HG13	1.95	0.47
1:B:79:MSE:SE	1:B:96:ILE:CD1	3.12	0.47
1:A:24:HIS:N	1:A:25:PRO:CD	2.77	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:B:339:ILE:HG21	1:B:342:VAL:HG21	1.96	0.46
1:A:321:ILE:HD13	1:A:359:VAL:HG21	1.98	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:B:136:GLU:OE2	1:B:161[B]:ARG:NH1	2.52	0.42
1:A:115:ASP:HA	1:A:116:ASN:HA	1.85	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:B:342:VAL:HG11	1:B:428:VAL:HG22	2.02	0.41
1:A:324:CYS:HA	1:B:386:LEU:CD1	2.50	0.41
1:A:98:PRO:HA	1:A:106:LYS:O	2.21	0.41
1:B:49:ARG:HA	1:B:54:ASN:O	2.21	0.41
1:B:112:LEU:HD23	1:B:114:ALA:HB2	2.03	0.40
1:A:107:ALA:HB2	1:A:112:LEU:HA	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%)	52	52
1	B	470/487 (96%)	456 (97%)	13 (3%)	1 (0%)	52	52
All	All	941/974 (97%)	910 (97%)	29 (3%)	2 (0%)	52	52

All (2) Ramachandran outliers are listed below:

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

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	391/409 (96%)	386 (99%)	5 (1%)	76	81
1	B	389/409 (95%)	381 (98%)	8 (2%)	61	65
All	All	780/818 (95%)	767 (98%)	13 (2%)	70	73

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

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

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates

There are no carbohydrates in this entry.

5.6 Ligand geometry

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	503	-	4,4,4	0.19	0	6,6,6	0.77	0
3	SO4	A	504	-	4,4,4	0.15	0	6,6,6	0.16	0
3	SO4	A	505	-	4,4,4	0.23	0	6,6,6	0.52	0
3	SO4	A	506	-	4,4,4	0.14	0	6,6,6	0.53	0
3	SO4	A	507	-	4,4,4	0.21	0	6,6,6	0.37	0
3	SO4	A	508	-	4,4,4	0.15	0	6,6,6	0.28	0
3	SO4	A	509	-	4,4,4	0.12	0	6,6,6	0.15	0
3	SO4	A	510	-	4,4,4	0.17	0	6,6,6	0.09	0
4	GOL	A	511	-	5,5,5	0.42	0	5,5,5	0.67	0
4	GOL	A	512	-	5,5,5	0.38	0	5,5,5	0.16	0
4	GOL	A	513	-	5,5,5	0.44	0	5,5,5	0.21	0
4	GOL	A	514	-	5,5,5	0.29	0	5,5,5	0.26	0
4	GOL	A	515	-	5,5,5	0.38	0	5,5,5	0.30	0
4	GOL	A	516	-	5,5,5	0.30	0	5,5,5	0.39	0
4	GOL	A	517	-	5,5,5	0.33	0	5,5,5	0.58	0
4	GOL	A	518	-	5,5,5	0.42	0	5,5,5	0.81	0
5	IPA	A	519	-	3,3,3	0.59	0	3,3,3	0.29	0
5	IPA	A	520	-	3,3,3	0.57	0	3,3,3	0.24	0
3	SO4	B	503	-	4,4,4	0.15	0	6,6,6	1.04	0
3	SO4	B	504	-	4,4,4	0.17	0	6,6,6	0.17	0
3	SO4	B	505	-	4,4,4	0.19	0	6,6,6	0.21	0
3	SO4	B	506	-	4,4,4	0.18	0	6,6,6	0.53	0
3	SO4	B	507	-	4,4,4	0.14	0	6,6,6	0.22	0
3	SO4	B	508	-	4,4,4	0.12	0	6,6,6	0.22	0
3	SO4	B	509	-	4,4,4	0.22	0	6,6,6	0.19	0
3	SO4	B	510	-	4,4,4	0.13	0	6,6,6	0.08	0
3	SO4	B	511	-	4,4,4	0.18	0	6,6,6	0.30	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	SO4	B	512	-	4,4,4	0.17	0	6,6,6	0.17	0
4	GOL	B	513	-	5,5,5	0.19	0	5,5,5	0.67	0
4	GOL	B	514	-	5,5,5	0.29	0	5,5,5	0.39	0
4	GOL	B	515	-	5,5,5	0.42	0	5,5,5	0.31	0
4	GOL	B	516	-	5,5,5	0.27	0	5,5,5	0.52	0
4	GOL	B	517	-	5,5,5	0.36	0	5,5,5	0.25	0
4	GOL	B	518	-	5,5,5	0.31	0	5,5,5	0.59	0
4	GOL	B	519	-	5,5,5	0.39	0	5,5,5	0.39	0
4	GOL	B	520	-	5,5,5	0.33	0	5,5,5	0.21	0
4	GOL	B	521	-	5,5,5	0.18	0	5,5,5	0.59	0
5	IPA	B	522	-	3,3,3	0.60	0	3,3,3	0.34	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	SO4	A	503	-	-	0/0/0/0	0/0/0/0
3	SO4	A	504	-	-	0/0/0/0	0/0/0/0
3	SO4	A	505	-	-	0/0/0/0	0/0/0/0
3	SO4	A	506	-	-	0/0/0/0	0/0/0/0
3	SO4	A	507	-	-	0/0/0/0	0/0/0/0
3	SO4	A	508	-	-	0/0/0/0	0/0/0/0
3	SO4	A	509	-	-	0/0/0/0	0/0/0/0
3	SO4	A	510	-	-	0/0/0/0	0/0/0/0
4	GOL	A	511	-	-	0/4/4/4	0/0/0/0
4	GOL	A	512	-	-	0/4/4/4	0/0/0/0
4	GOL	A	513	-	-	0/4/4/4	0/0/0/0
4	GOL	A	514	-	-	0/4/4/4	0/0/0/0
4	GOL	A	515	-	-	0/4/4/4	0/0/0/0
4	GOL	A	516	-	-	0/4/4/4	0/0/0/0
4	GOL	A	517	-	-	0/4/4/4	0/0/0/0
4	GOL	A	518	-	-	0/4/4/4	0/0/0/0
5	IPA	A	519	-	-	0/0/0/0	0/0/0/0
5	IPA	A	520	-	-	0/0/0/0	0/0/0/0
3	SO4	B	503	-	-	0/0/0/0	0/0/0/0
3	SO4	B	504	-	-	0/0/0/0	0/0/0/0
3	SO4	B	505	-	-	0/0/0/0	0/0/0/0
3	SO4	B	506	-	-	0/0/0/0	0/0/0/0
3	SO4	B	507	-	-	0/0/0/0	0/0/0/0
3	SO4	B	508	-	-	0/0/0/0	0/0/0/0
3	SO4	B	509	-	-	0/0/0/0	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	SO4	B	510	-	-	0/0/0/0	0/0/0/0
3	SO4	B	511	-	-	0/0/0/0	0/0/0/0
3	SO4	B	512	-	-	0/0/0/0	0/0/0/0
4	GOL	B	513	-	-	0/4/4/4	0/0/0/0
4	GOL	B	514	-	-	0/4/4/4	0/0/0/0
4	GOL	B	515	-	-	0/4/4/4	0/0/0/0
4	GOL	B	516	-	-	0/4/4/4	0/0/0/0
4	GOL	B	517	-	-	0/4/4/4	0/0/0/0
4	GOL	B	518	-	-	0/4/4/4	0/0/0/0
4	GOL	B	519	-	-	0/4/4/4	0/0/0/0
4	GOL	B	520	-	-	0/4/4/4	0/0/0/0
4	GOL	B	521	-	-	0/4/4/4	0/0/0/0
5	IPA	B	522	-	-	0/0/0/0	0/0/0/0

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

4 monomers are involved in 8 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	511	GOL	1	0
4	A	517	GOL	3	0
4	B	521	GOL	2	0
5	B	522	IPA	2	0

5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

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	465/487 (95%)	1.29	81 (17%) 2 3	29, 59, 86, 99	0
1	B	463/487 (95%)	1.35	91 (19%) 1 2	29, 59, 86, 99	0
All	All	928/974 (95%)	1.32	172 (18%) 2 2	29, 59, 86, 99	0

All (172) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	99	TYR	9.2
1	B	100	ILE	7.5
1	A	99	TYR	7.3
1	A	417	ALA	6.2
1	B	27	TYR	6.2
1	B	102	GLY	6.1
1	A	468	ALA	6.0
1	B	112	LEU	5.9
1	B	101	ASP	5.8
1	A	80	VAL	5.5
1	B	80	VAL	5.5
1	B	97	LEU	5.4
1	A	153	ILE	5.3
1	A	107	ALA	5.2
1	B	466	ILE	5.1
1	B	461	ASP	5.1
1	A	100	ILE	5.0
1	A	7	LEU	4.9
1	B	454	ILE	4.9
1	A	294	LEU	4.9
1	A	97	LEU	4.8
1	A	461	ASP	4.7
1	B	104	TRP	4.7
1	B	23	PRO	4.7

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Mol	Chain	Res	Type	RSRZ
1	B	420	LEU	4.6
1	A	101	ASP	4.6
1	B	81	PRO	4.6
1	B	294	LEU	4.6
1	B	422	THR	4.3
1	A	104	TRP	4.2
1	A	158	ASN	4.2
1	A	404	SER	4.2
1	B	105	VAL	4.0
1	B	38[A]	ASN	4.0
1	B	109	GLY	4.0
1	A	421	GLY	3.8
1	A	102	GLY	3.8
1	A	422	THR	3.7
1	A	5	GLN	3.7
1	B	158	ASN	3.7
1	A	454	ILE	3.7
1	B	7	LEU	3.7
1	B	214	HIS	3.6
1	B	287	VAL	3.6
1	A	20	CYS	3.5
1	A	414	THR	3.4
1	A	98	PRO	3.3
1	A	112	LEU	3.3
1	A	95	PRO	3.2
1	B	13	TRP	3.2
1	B	53	GLY	3.2
1	B	464	VAL	3.2
1	A	438	LEU	3.1
1	B	25	PRO	3.1
1	A	306	VAL	3.1
1	B	111	THR	3.1
1	B	462	GLU	3.1
1	A	19	ILE	3.0
1	B	52	VAL	3.0
1	A	32	LEU	3.0
1	A	420	LEU	3.0
1	B	95	PRO	3.0
1	A	418	GLN	3.0
1	B	369	ILE	2.9
1	B	469	VAL	2.9
1	A	42	THR	2.9

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Mol	Chain	Res	Type	RSRZ
1	A	6	SER	2.9
1	A	376	VAL	2.8
1	A	139	VAL	2.8
1	B	110	THR	2.8
1	B	148	GLY	2.8
1	A	16	PHE	2.8
1	A	324	CYS	2.8
1	B	98	PRO	2.7
1	A	93	GLN	2.7
1	A	105	VAL	2.7
1	B	126	VAL	2.7
1	B	153	ILE	2.7
1	B	400	TRP	2.7
1	A	463	LYS	2.6
1	B	17	ASP	2.6
1	B	177	TYR	2.6
1	B	425	GLU	2.6
1	A	55	VAL	2.6
1	B	433	LEU	2.6
1	B	63	VAL	2.6
1	A	124	LEU	2.5
1	A	433	LEU	2.5
1	B	293	ALA	2.5
1	B	178	ILE	2.5
1	B	303	LEU	2.5
1	B	324	CYS	2.5
1	A	455	ARG	2.5
1	A	182	GLY	2.5
1	A	429	ILE	2.5
1	A	445	ILE	2.5
1	A	12	LEU	2.5
1	B	432	GLY	2.5
1	B	419	VAL	2.5
1	B	82	GLN	2.5
1	B	412	THR	2.4
1	B	453	THR	2.4
1	A	293	ALA	2.4
1	B	78	ASP	2.4
1	B	207	LEU	2.4
1	B	21	ALA	2.4
1	B	259	ALA	2.4
1	A	405	HIS	2.4

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Mol	Chain	Res	Type	RSRZ
1	B	113	GLY	2.4
1	B	436	GLY	2.4
1	A	123	ALA	2.4
1	A	26	SER	2.4
1	A	81	PRO	2.4
1	A	132	ILE	2.4
1	B	440	LYS	2.4
1	A	82	GLN	2.3
1	B	161[A]	ARG	2.3
1	B	452	PRO	2.3
1	B	463	LYS	2.3
1	A	430	HIS	2.3
1	A	71	VAL	2.3
1	B	333	VAL	2.3
1	B	470	GLU	2.3
1	A	148	GLY	2.3
1	A	360	ARG	2.3
1	A	457	ALA	2.3
1	A	372	GLY	2.2
1	B	329	PRO	2.2
1	A	476	LEU	2.2
1	A	27	TYR	2.2
1	A	340	GLU	2.2
1	A	63	VAL	2.2
1	B	339	ILE	2.2
1	B	418	GLN	2.2
1	A	155	LEU	2.2
1	B	378	SER	2.2
1	B	199	PHE	2.2
1	A	114	ALA	2.2
1	A	456	ASN	2.2
1	B	426	ILE	2.2
1	B	157	PRO	2.2
1	B	356	ASP	2.1
1	B	385[A]	SER	2.1
1	A	106	LYS	2.1
1	B	51	GLU	2.1
1	A	24	HIS	2.1
1	B	129	SER	2.1
1	A	180	CYS	2.1
1	B	421	GLY	2.1
1	B	322	ILE	2.1

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Mol	Chain	Res	Type	RSRZ
1	A	380	LEU	2.1
1	B	150	GLU	2.1
1	B	203	TYR	2.1
1	B	376	VAL	2.1
1	A	118	ILE	2.1
1	B	94	ASP	2.1
1	B	386	LEU	2.1
1	B	114	ALA	2.1
1	A	462	GLU	2.0
1	A	96	ILE	2.0
1	B	486	ARG	2.0
1	B	272	GLY	2.0
1	A	13	TRP	2.0
1	B	399	GLY	2.0
1	A	299	LEU	2.0
1	A	379	LEU	2.0
1	A	437	LEU	2.0
1	A	110	THR	2.0
1	A	111	THR	2.0
1	B	327	VAL	2.0
1	B	428	VAL	2.0
1	B	117	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 carbohydrates 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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. 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	LLDF	B-factors(\AA^2)	Q<0.9
3	SO4	A	509	5/5	0.69	0.36	8.77	100,100,102,103	0
4	GOL	B	521	6/6	0.63	0.37	8.64	76,78,79,80	0
4	GOL	A	516	6/6	0.56	0.27	8.45	85,88,88,89	0
4	GOL	A	512	6/6	0.35	0.42	7.33	97,99,99,99	0
4	GOL	A	514	6/6	0.78	0.32	6.98	71,75,76,78	0
4	GOL	B	515	6/6	0.66	0.24	5.58	86,87,88,88	0
3	SO4	B	511	5/5	0.75	0.40	4.89	119,120,120,120	0
3	SO4	B	512	5/5	0.82	0.31	4.83	123,125,126,126	0
3	SO4	A	506	5/5	0.89	0.30	4.14	79,83,85,87	0
4	GOL	B	516	6/6	0.57	0.29	3.66	67,71,73,75	0
3	SO4	B	506	5/5	0.88	0.31	3.56	85,87,91,93	0
4	GOL	A	515	6/6	0.86	0.26	2.65	57,64,68,71	0
3	SO4	B	508	5/5	0.82	0.31	2.64	107,107,109,109	0
4	GOL	A	517	6/6	0.77	0.21	1.17	65,65,66,67	0
5	IPA	A	519	4/4	0.82	0.19	0.39	68,68,70,72	0
4	GOL	B	518	6/6	0.87	0.22	0.19	70,72,75,77	0
4	GOL	B	520	6/6	0.83	0.17	-0.12	66,70,71,74	0
4	GOL	B	517	6/6	0.86	0.19	-0.28	78,80,80,82	0
4	GOL	A	518	6/6	0.86	0.17	-0.37	61,69,72,73	0
2	ZN	B	502	1/1	0.71	0.19	-0.49	117,117,117,117	0
2	ZN	A	502	1/1	0.84	0.13	-0.90	131,131,131,131	0
3	SO4	B	503	5/5	0.91	0.14	-1.01	58,62,64,65	0
2	ZN	A	501	1/1	0.99	0.13	-1.08	73,73,73,73	0
4	GOL	A	513	6/6	0.89	0.13	-1.85	82,82,84,84	0
4	GOL	B	513	6/6	0.94	0.15	-2.00	41,44,45,45	0
3	SO4	A	503	5/5	0.94	0.14	-2.04	46,58,62,62	0
4	GOL	A	511	6/6	0.94	0.10	-2.93	33,37,40,42	0
2	ZN	B	501	1/1	0.75	0.08	-4.11	95,95,95,95	0
5	IPA	A	520	4/4	0.70	0.28	-	74,76,76,77	0
3	SO4	A	510	5/5	0.90	0.16	-	121,122,122,122	0
3	SO4	A	504	5/5	0.88	0.26	-	111,111,112,113	0
3	SO4	A	505	5/5	0.87	0.28	-	98,101,101,102	0
3	SO4	A	508	5/5	0.90	0.28	-	82,82,84,85	0
3	SO4	B	507	5/5	0.88	0.30	-	84,86,87,88	0
4	GOL	B	514	6/6	0.78	0.40	-	75,79,81,81	0
3	SO4	B	510	5/5	0.89	0.26	-	106,107,108,108	0
4	GOL	B	519	6/6	0.43	0.57	-	94,97,98,98	0
5	IPA	B	522	4/4	0.78	0.39	-	68,69,71,71	0
3	SO4	B	505	5/5	0.78	0.36	-	91,95,96,97	0
3	SO4	A	507	5/5	0.87	0.29	-	96,98,99,100	0
3	SO4	B	504	5/5	0.77	0.28	-	134,135,135,135	0
3	SO4	B	509	5/5	0.68	0.28	-	113,115,116,117	0

6.5 Other polymers [i](#)

There are no such residues in this entry.