



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 06:38 PM UTC

PDB ID : 2QYV / pdb_00002qyv
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	:	4-5-2 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

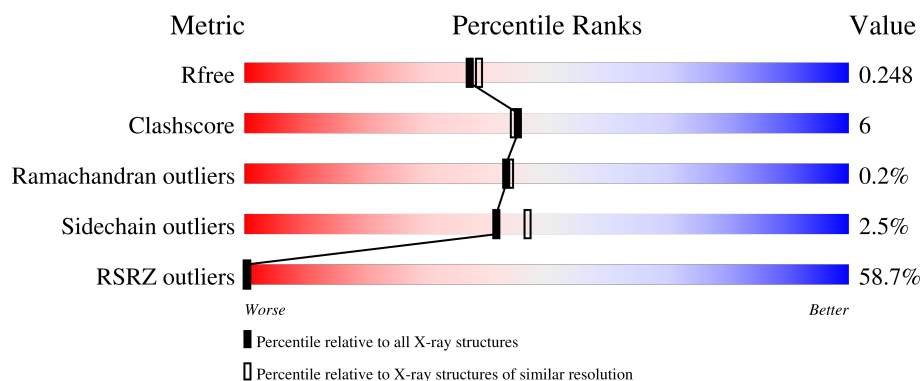
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.11 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}	180053	8290 (2.14-2.10)
Clashscore	190562	8817 (2.14-2.10)
Ramachandran outliers	187476	8738 (2.14-2.10)
Sidechain outliers	187428	8739 (2.14-2.10)
RSRZ outliers	180081	8294 (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	52% 84%12%..
1	B	487	60% 84%11%..

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			

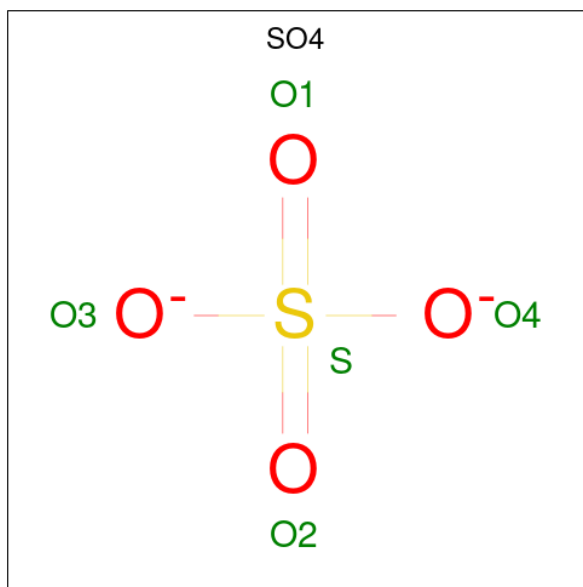
There are 2 discrepancies between the modelled and reference sequences:

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

- Molecule 2 is ZINC ION (CCD ID: 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 (CCD ID: 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 (CCD ID: GOL) (formula: $C_3H_8O_3$).



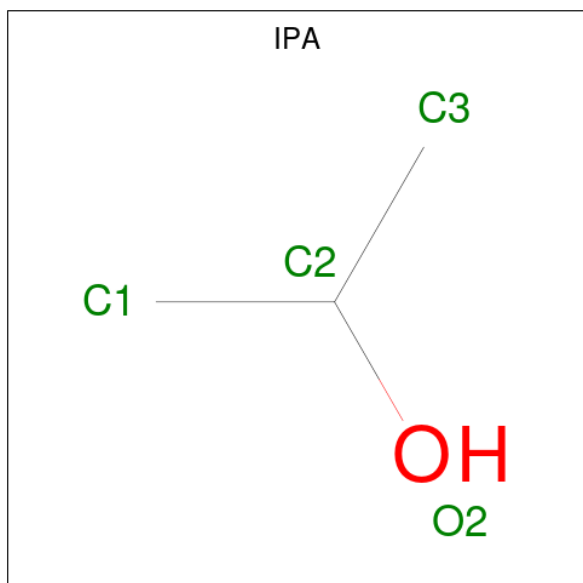
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			6	3	3		
4	A	1	Total	C	O	0	0
			6	3	3		
4	A	1	Total	C	O	0	0
			6	3	3		
4	A	1	Total	C	O	0	0
			6	3	3		
4	A	1	Total	C	O	0	0
			6	3	3		
4	A	1	Total	C	O	0	0
			6	3	3		
4	A	1	Total	C	O	0	0
			6	3	3		

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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 (CCD ID: IPA) (formula: C_3H_8O).



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		

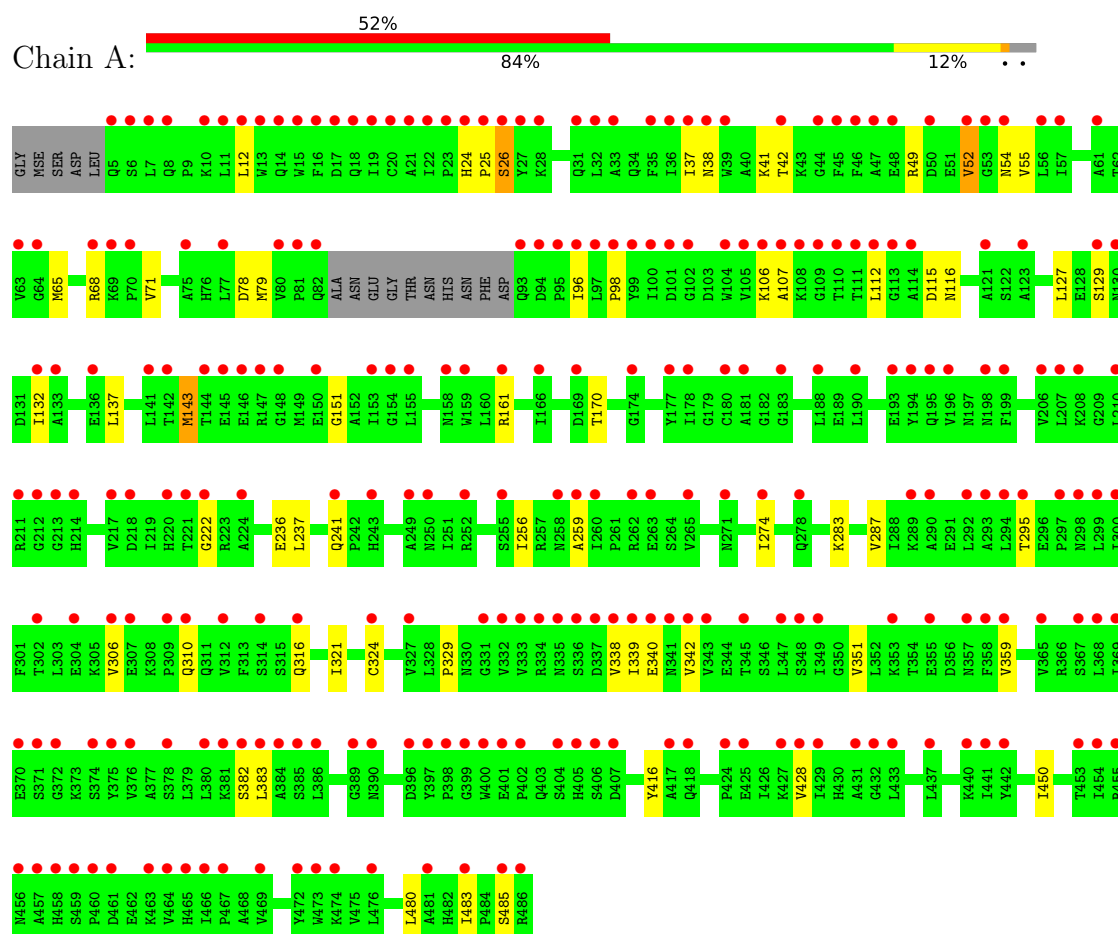
- Molecule 6 is water.

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

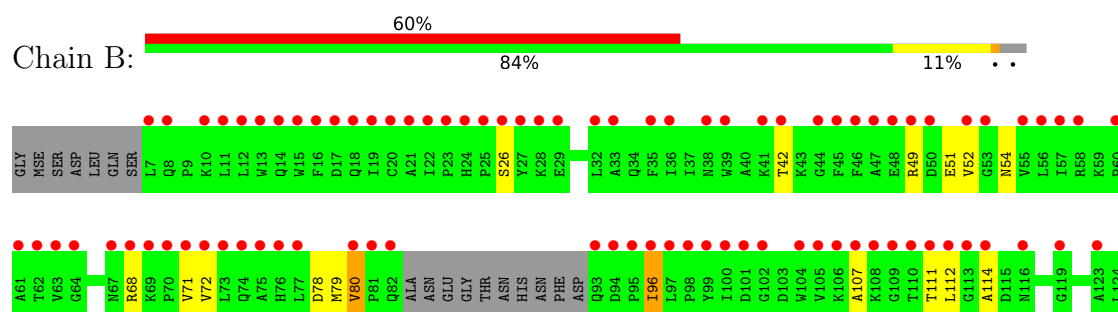
3 Residue-property plots [i](#)

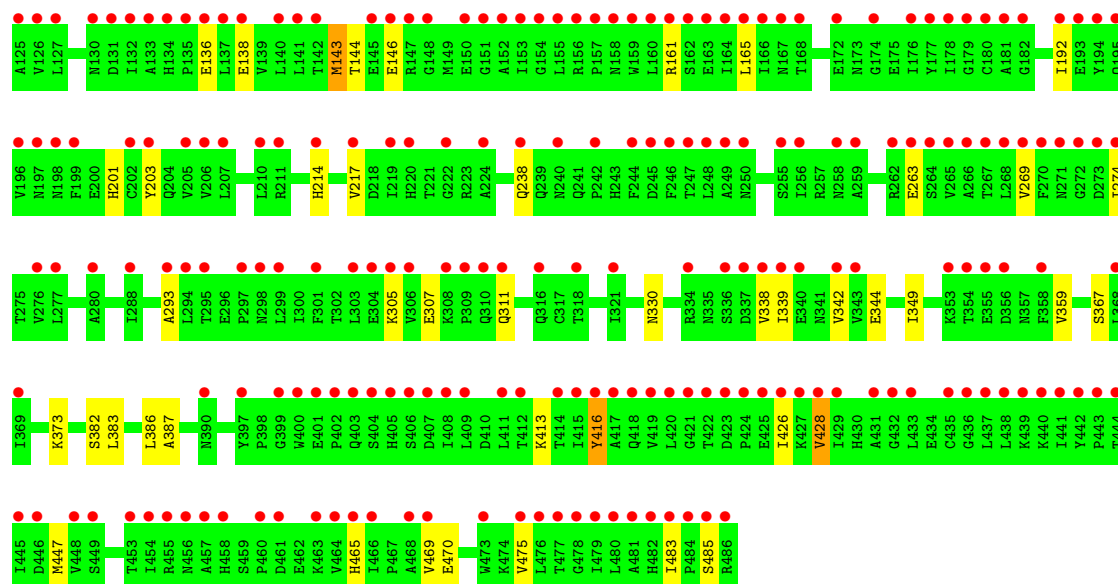
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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 2 ₁ 2 ₁ 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 47.84 – 2.11	Depositor EDS
% Data completeness (in resolution range)	97.7 (47.84-2.11) 97.7 (47.84-2.11)	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, PHENIX	Depositor
R, R_{free}	0.220 , 0.244 0.225 , 0.248	Depositor DCC
R_{free} test set	5107 reflections (4.88%)	wwPDB-VP
Wilson B-factor (Å ²)	31.1	Xtriage
Anisotropy	0.464	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 60.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.46$, $\langle L^2 \rangle = 0.29$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.92	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.*

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, IPA, ZN, GOL

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.69	1/3705 (0.0%)	0.83	0/5033
1	B	0.70	2/3692 (0.1%)	0.85	0/5019
All	All	0.70	3/7397 (0.0%)	0.84	0/10052

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	143	MSE	SE-CE	11.30	2.29	1.95
1	B	143	MSE	SE-CE	10.66	2.27	1.95
1	B	387	ALA	CA-CB	-5.11	1.44	1.53

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	39	0
1	B	3615	0	3578	50	0
2	A	2	0	0	0	0
2	B	2	0	0	0	0
3	A	40	0	0	0	0
3	B	50	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
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	87	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 (87) 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: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:A:41:LYS:NZ	6:A:721:HOH:O	2.29	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
1:A:38:ASN:O	1:A:42:THR:HG23	2.06	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:12:LEU:C	1:A:12:LEU:HD23	2.34	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:A:222:GLY:C	1:A:295:THR:HG21	2.37	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: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: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:A:382:SER:O	1:A:383:LEU:C	2.61	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:96:ILE:HD11	2.00	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:79:MSE:HE1	1:B:111:THR:O	2.19	0.42
1:B:382:SER:O	1:B:383:LEU:C	2.61	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:A:170:THR:HB	1:A:450:ILE:C	2.44	0.41
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:B:51:GLU:CD	1:B:51:GLU:H	2.29	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%)	43	44
1	B	470/487 (96%)	456 (97%)	13 (3%)	1 (0%)	43	44
All	All	941/974 (97%)	910 (97%)	29 (3%)	2 (0%)	43	44

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%)	382 (98%)	9 (2%)	44	50
1	B	389/409 (95%)	378 (97%)	11 (3%)	38	42
All	All	780/818 (95%)	760 (97%)	20 (3%)	42	45

All (20) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	52	VAL
1	A	161	ARG
1	A	306	VAL
1	A	310	GLN
1	A	316	GLN
1	A	351	VAL
1	A	416	TYR
1	A	428	VAL
1	A	485	SER
1	B	52	VAL
1	B	80	VAL
1	B	96	ILE
1	B	263[A]	GLU
1	B	263[B]	GLU
1	B	311	GLN
1	B	373	LYS
1	B	416	TYR
1	B	428	VAL
1	B	470	GLU
1	B	485	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (9) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	185	ASN
1	A	310	GLN
1	A	320	ASN
1	B	31	GLN
1	B	204	GLN
1	B	238	GLN
1	B	250	ASN
1	B	320	ASN
1	B	335	ASN

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 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	$\# Z > 2$
4	GOL	A	517	-	5,5,5	0.38	0	5,5,5	0.58	0
4	GOL	B	513	-	5,5,5	0.22	0	5,5,5	0.68	0
4	GOL	B	521	-	5,5,5	0.23	0	5,5,5	0.66	0
3	SO4	B	504	-	4,4,4	0.21	0	6,6,6	0.09	0
4	GOL	A	512	-	5,5,5	0.44	0	5,5,5	0.10	0
3	SO4	B	510	-	4,4,4	0.28	0	6,6,6	0.08	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	SO4	B	508	-	4,4,4	0.23	0	6,6,6	0.27	0
5	IPA	A	519	-	3,3,3	0.57	0	3,3,3	0.30	0
4	GOL	A	514	-	5,5,5	0.34	0	5,5,5	0.21	0
3	SO4	A	510	-	4,4,4	0.25	0	6,6,6	0.09	0
3	SO4	B	506	-	4,4,4	0.20	0	6,6,6	0.47	0
4	GOL	A	518	-	5,5,5	0.50	0	5,5,5	0.85	0
3	SO4	A	509	-	4,4,4	0.28	0	6,6,6	0.21	0
4	GOL	B	518	-	5,5,5	0.37	0	5,5,5	0.65	0
5	IPA	A	520	-	3,3,3	0.56	0	3,3,3	0.24	0
3	SO4	B	511	-	4,4,4	0.25	0	6,6,6	0.20	0
3	SO4	B	507	-	4,4,4	0.27	0	6,6,6	0.31	0
3	SO4	B	512	-	4,4,4	0.26	0	6,6,6	0.19	0
3	SO4	A	508	-	4,4,4	0.26	0	6,6,6	0.37	0
3	SO4	B	509	-	4,4,4	0.25	0	6,6,6	0.27	0
4	GOL	B	520	-	5,5,5	0.36	0	5,5,5	0.23	0
4	GOL	A	511	-	5,5,5	0.46	0	5,5,5	0.71	0
4	GOL	A	516	-	5,5,5	0.33	0	5,5,5	0.44	0
3	SO4	B	505	-	4,4,4	0.25	0	6,6,6	0.22	0
3	SO4	A	507	-	4,4,4	0.28	0	6,6,6	0.25	0
4	GOL	A	515	-	5,5,5	0.42	0	5,5,5	0.26	0
3	SO4	A	505	-	4,4,4	0.26	0	6,6,6	0.40	0
4	GOL	B	516	-	5,5,5	0.35	0	5,5,5	0.53	0
3	SO4	B	503	-	4,4,4	0.24	0	6,6,6	0.87	0
3	SO4	A	506	-	4,4,4	0.31	0	6,6,6	0.42	0
4	GOL	B	515	-	5,5,5	0.44	0	5,5,5	0.36	0
4	GOL	A	513	-	5,5,5	0.46	0	5,5,5	0.25	0
4	GOL	B	519	-	5,5,5	0.45	0	5,5,5	0.33	0
3	SO4	A	504	-	4,4,4	0.25	0	6,6,6	0.12	0
4	GOL	B	517	-	5,5,5	0.39	0	5,5,5	0.27	0
4	GOL	B	514	-	5,5,5	0.36	0	5,5,5	0.37	0
3	SO4	A	503	-	4,4,4	0.20	0	6,6,6	0.70	0
5	IPA	B	522	-	3,3,3	0.59	0	3,3,3	0.36	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	516	-	-	2/4/4/4	-
4	GOL	A	517	-	-	3/4/4/4	-
4	GOL	B	513	-	-	2/4/4/4	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	GOL	B	515	-	-	2/4/4/4	-
4	GOL	B	517	-	-	1/4/4/4	-
4	GOL	B	521	-	-	0/4/4/4	-
4	GOL	A	512	-	-	4/4/4/4	-
4	GOL	A	513	-	-	1/4/4/4	-
4	GOL	B	519	-	-	2/4/4/4	-
4	GOL	A	514	-	-	4/4/4/4	-
4	GOL	A	515	-	-	4/4/4/4	-
4	GOL	A	518	-	-	2/4/4/4	-
4	GOL	B	514	-	-	4/4/4/4	-
4	GOL	B	520	-	-	2/4/4/4	-
4	GOL	B	516	-	-	2/4/4/4	-
4	GOL	A	511	-	-	2/4/4/4	-
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 (39) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	512	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	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	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

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Mol	Chain	Res	Type	Atoms
4	B	514	GOL	C1-C2-C3-O3
4	B	515	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	514	GOL	O1-C1-C2-O2
4	A	512	GOL	O2-C2-C3-O3
4	A	517	GOL	O2-C2-C3-O3
4	A	512	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
4	A	517	GOL	3	0
4	B	521	GOL	2	0
4	A	511	GOL	1	0
5	B	522	IPA	2	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	465/487 (95%)	2.22	252 (54%) 0 0	25, 59, 86, 99	3 (0%)
1	B	463/487 (95%)	2.54	293 (63%) 0 0	25, 59, 86, 99	4 (0%)
All	All	928/974 (95%)	2.38	545 (58%) 0 0	25, 59, 86, 99	7 (0%)

All (545) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	93	GLN	9.2
1	B	93	GLN	8.0
1	A	294	LEU	7.9
1	B	7	LEU	6.5
1	B	294	LEU	5.9
1	B	105	VAL	5.9
1	B	21	ALA	5.8
1	B	94	ASP	5.7
1	A	5	GLN	5.7
1	A	94	ASP	5.6
1	B	70	PRO	5.5
1	B	13	TRP	5.5
1	A	99	TYR	5.5
1	B	63	VAL	5.5
1	B	95	PRO	5.4
1	B	99	TYR	5.4
1	A	339	ILE	5.4
1	B	161[A]	ARG	5.4
1	B	464	VAL	5.3
1	B	429	ILE	5.3
1	B	485	SER	5.3
1	A	217	VAL	5.2
1	A	7	LEU	5.1
1	B	465	HIS	5.0

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Mol	Chain	Res	Type	RSRZ
1	A	100	ILE	5.0
1	B	26	SER	5.0
1	B	342	VAL	4.9
1	B	178	ILE	4.9
1	B	109	GLY	4.8
1	B	442	TYR	4.8
1	A	82	GLN	4.8
1	B	82	GLN	4.8
1	B	217	VAL	4.8
1	B	108	LYS	4.8
1	A	21	ALA	4.8
1	B	96	ILE	4.7
1	B	255	SER	4.6
1	B	338	VAL	4.6
1	B	159	TRP	4.6
1	B	106	LYS	4.6
1	B	463	LYS	4.6
1	A	148	GLY	4.6
1	A	338	VAL	4.6
1	B	46	PHE	4.6
1	B	177	TYR	4.5
1	A	6	SER	4.5
1	B	80	VAL	4.5
1	B	12	LEU	4.5
1	B	53	GLY	4.4
1	B	67	ASN	4.4
1	B	160	LEU	4.4
1	A	105	VAL	4.3
1	B	337	ASP	4.3
1	B	163	GLU	4.3
1	A	96	ILE	4.3
1	B	484	PRO	4.3
1	B	97	LEU	4.3
1	B	486	ARG	4.3
1	A	298	ASN	4.3
1	B	424	PRO	4.3
1	A	292	LEU	4.3
1	B	11	LEU	4.3
1	B	409	LEU	4.3
1	A	293	ALA	4.2
1	B	33	ALA	4.2
1	B	38[A]	ASN	4.2

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Mol	Chain	Res	Type	RSRZ
1	A	108	LYS	4.2
1	B	460	PRO	4.2
1	B	20	CYS	4.2
1	A	454	ILE	4.2
1	B	100	ILE	4.2
1	B	402	PRO	4.2
1	B	16	PHE	4.2
1	B	81	PRO	4.2
1	B	454	ILE	4.1
1	A	107	ALA	4.1
1	B	15	TRP	4.1
1	B	400	TRP	4.1
1	B	426	ILE	4.1
1	A	16	PHE	4.1
1	B	306	VAL	4.1
1	B	164	ILE	4.1
1	B	214	HIS	4.1
1	B	404	SER	4.1
1	B	60	PRO	4.1
1	B	132	ILE	4.1
1	A	104	TRP	4.0
1	A	433	LEU	4.0
1	B	483	ILE	4.0
1	B	272	GLY	4.0
1	B	412	THR	4.0
1	A	81	PRO	4.0
1	B	441	ILE	4.0
1	A	429	ILE	4.0
1	A	464	VAL	3.9
1	A	24	HIS	3.9
1	B	428	VAL	3.9
1	B	153	ILE	3.9
1	A	112	LEU	3.9
1	B	64	GLY	3.8
1	A	97	LEU	3.8
1	B	140	LEU	3.8
1	B	155	LEU	3.8
1	B	461	ASP	3.8
1	A	132	ILE	3.8
1	B	274	ILE	3.8
1	B	479	ILE	3.8
1	B	249	ALA	3.8

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Mol	Chain	Res	Type	RSRZ
1	B	448	VAL	3.8
1	B	68	ARG	3.8
1	B	77	LEU	3.8
1	B	263[A]	GLU	3.8
1	B	182	GLY	3.8
1	B	19	ILE	3.7
1	A	11	LEU	3.7
1	B	420	LEU	3.7
1	A	455	ARG	3.7
1	B	340	GLU	3.7
1	A	334	ARG	3.7
1	B	433	LEU	3.7
1	A	222	GLY	3.7
1	B	445	ILE	3.7
1	B	271	ASN	3.6
1	B	425	GLU	3.6
1	B	339	ILE	3.6
1	B	422	THR	3.6
1	B	436	GLY	3.6
1	B	110	THR	3.6
1	B	401	GLU	3.6
1	A	337	ASP	3.6
1	B	71	VAL	3.6
1	A	42	THR	3.6
1	B	107	ALA	3.6
1	B	411	LEU	3.6
1	B	418	GLN	3.6
1	B	198	ASN	3.5
1	A	53	GLY	3.5
1	B	136	GLU	3.5
1	B	405	HIS	3.5
1	A	38	ASN	3.5
1	A	212	GLY	3.5
1	B	162	SER	3.5
1	A	263	GLU	3.5
1	A	342	VAL	3.5
1	B	458	HIS	3.5
1	A	14	GLN	3.5
1	B	316	GLN	3.5
1	B	113	GLY	3.5
1	A	343	VAL	3.5
1	A	95	PRO	3.4

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Mol	Chain	Res	Type	RSRZ
1	B	166	ILE	3.4
1	A	340	GLU	3.4
1	B	17	ASP	3.4
1	B	41	LYS	3.4
1	A	20	CYS	3.4
1	B	24	HIS	3.4
1	A	390	ASN	3.4
1	B	416	TYR	3.4
1	A	428	VAL	3.4
1	B	135	PRO	3.4
1	B	152	ALA	3.4
1	B	310	GLN	3.4
1	B	403	GLN	3.4
1	A	211	ARG	3.4
1	B	148	GLY	3.4
1	B	431	ALA	3.4
1	A	316	GLN	3.4
1	A	405	HIS	3.3
1	B	69	LYS	3.3
1	A	109	GLY	3.3
1	A	332	VAL	3.3
1	A	385[A]	SER	3.3
1	A	22	ILE	3.3
1	A	155	LEU	3.3
1	A	380	LEU	3.3
1	A	295	THR	3.3
1	A	52	VAL	3.3
1	B	52	VAL	3.3
1	B	133	ALA	3.3
1	B	268	LEU	3.3
1	A	341	ASN	3.3
1	A	13	TRP	3.3
1	B	61	ALA	3.3
1	B	408	ILE	3.3
1	A	110	THR	3.2
1	B	55	VAL	3.2
1	B	32	LEU	3.2
1	B	154	GLY	3.2
1	A	63	VAL	3.2
1	A	28	LYS	3.2
1	B	10	LYS	3.2
1	B	250	ASN	3.2

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Mol	Chain	Res	Type	RSRZ
1	B	298	ASN	3.2
1	A	27	TYR	3.2
1	A	369	ILE	3.2
1	B	165	LEU	3.2
1	B	45	PHE	3.2
1	A	485	SER	3.2
1	A	432	GLY	3.2
1	A	402	PRO	3.2
1	A	159	TRP	3.2
1	B	457	ALA	3.2
1	B	137	LEU	3.2
1	A	371	SER	3.2
1	A	221	THR	3.2
1	B	98	PRO	3.2
1	A	368	LEU	3.1
1	A	304	GLU	3.1
1	B	270	PHE	3.1
1	B	421	GLY	3.1
1	A	23	PRO	3.1
1	A	98	PRO	3.1
1	B	112	LEU	3.1
1	B	256	ILE	3.1
1	A	106	LYS	3.1
1	A	113	GLY	3.1
1	B	222	GLY	3.1
1	A	158	ASN	3.1
1	A	310	GLN	3.1
1	B	14	GLN	3.1
1	A	32	LEU	3.1
1	A	77	LEU	3.1
1	A	39	TRP	3.1
1	A	463	LYS	3.1
1	B	104	TRP	3.1
1	A	255[A]	SER	3.1
1	B	336	SER	3.1
1	A	297	PRO	3.1
1	A	460	PRO	3.1
1	B	435	CYS	3.1
1	A	374	SER	3.1
1	B	297	PRO	3.0
1	A	458	HIS	3.0
1	A	259	ALA	3.0

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Mol	Chain	Res	Type	RSRZ
1	A	437	LEU	3.0
1	A	130	ASN	3.0
1	A	161	ARG	3.0
1	A	213	GLY	3.0
1	B	455	ARG	3.0
1	B	39	TRP	3.0
1	B	111	THR	3.0
1	B	354	THR	3.0
1	B	414	THR	3.0
1	A	145	GLU	3.0
1	A	47	ALA	3.0
1	B	181	ALA	3.0
1	A	466	ILE	3.0
1	B	62	THR	3.0
1	B	25	PRO	3.0
1	A	214	HIS	3.0
1	B	76	HIS	3.0
1	A	75	ALA	3.0
1	B	293	ALA	3.0
1	B	196	VAL	3.0
1	B	157	PRO	3.0
1	A	35	PHE	3.0
1	B	301	PHE	3.0
1	A	150	GLU	2.9
1	B	116	ASN	2.9
1	B	399	GLY	2.9
1	B	318	THR	2.9
1	A	194	TYR	2.9
1	B	27	TYR	2.9
1	A	473	TRP	2.9
1	A	355	GLU	2.9
1	A	336	SER	2.9
1	A	224	ALA	2.9
1	B	437	LEU	2.9
1	A	306	VAL	2.9
1	B	8	GLN	2.9
1	A	367	SER	2.9
1	B	406	SER	2.9
1	A	250	ASN	2.9
1	A	372	GLY	2.9
1	B	438	LEU	2.9
1	B	205	VAL	2.9

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Mol	Chain	Res	Type	RSRZ
1	B	355	GLU	2.9
1	A	181	ALA	2.9
1	B	280	ALA	2.9
1	A	207	LEU	2.8
1	A	80	VAL	2.8
1	B	415	ILE	2.8
1	B	167	ASN	2.8
1	A	218	ASP	2.8
1	A	457	ALA	2.8
1	B	174	GLY	2.8
1	A	324	CYS	2.8
1	A	198	ASN	2.8
1	B	240	ASN	2.8
1	B	131	ASP	2.8
1	A	183	GLY	2.8
1	A	146	GLU	2.8
1	A	307	GLU	2.8
1	B	123	ALA	2.8
1	A	19	ILE	2.8
1	A	456	ASN	2.8
1	B	18	GLN	2.8
1	A	442	TYR	2.8
1	A	10	LYS	2.8
1	A	111	THR	2.8
1	B	308	LYS	2.8
1	A	312	VAL	2.8
1	B	57	ILE	2.8
1	A	486	ARG	2.7
1	B	50	ASP	2.7
1	B	150	GLU	2.7
1	B	407	ASP	2.7
1	B	478	GLY	2.7
1	B	477	THR	2.7
1	B	211	ARG	2.7
1	B	130	ASN	2.7
1	B	180	CYS	2.7
1	B	288	ILE	2.7
1	B	220	HIS	2.7
1	A	102	GLY	2.7
1	B	439	LYS	2.7
1	A	33	ALA	2.7
1	B	368	LEU	2.7

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Mol	Chain	Res	Type	RSRZ
1	B	311	GLN	2.7
1	A	37	ILE	2.7
1	B	417	ALA	2.7
1	A	383	LEU	2.7
1	A	398	PRO	2.7
1	B	194	TYR	2.7
1	A	289	LYS	2.7
1	A	389	GLY	2.7
1	B	172	GLU	2.6
1	B	193	GLU	2.6
1	B	358	PHE	2.6
1	A	188	LEU	2.6
1	B	127	LEU	2.6
1	B	277	LEU	2.6
1	B	264	SER	2.6
1	A	427	LYS	2.6
1	A	260	ILE	2.6
1	B	269	VAL	2.6
1	B	343	VAL	2.6
1	B	432	GLY	2.6
1	A	8	GLN	2.6
1	B	480	LEU	2.6
1	A	68	ARG	2.6
1	A	153	ILE	2.6
1	B	419	VAL	2.6
1	B	179	GLY	2.6
1	B	145	GLU	2.6
1	B	295	THR	2.6
1	A	25	PRO	2.6
1	A	69	LYS	2.6
1	B	299	LEU	2.6
1	A	147	ARG	2.6
1	B	156	ARG	2.6
1	A	300	ILE	2.6
1	A	333	VAL	2.6
1	A	441	ILE	2.6
1	B	72	VAL	2.6
1	B	102	GLY	2.6
1	B	151	GLY	2.6
1	A	465	HIS	2.6
1	B	440	LYS	2.6
1	A	123	ALA	2.6

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Mol	Chain	Res	Type	RSRZ
1	B	444	THR	2.6
1	A	467	PRO	2.6
1	A	335	ASN	2.5
1	B	353	LYS	2.5
1	B	147	ARG	2.5
1	B	242	PRO	2.5
1	B	195	GLN	2.5
1	B	246	PHE	2.5
1	A	36	ILE	2.5
1	A	154	GLY	2.5
1	A	220	HIS	2.5
1	A	375	TYR	2.5
1	A	180	CYS	2.5
1	A	169	ASP	2.5
1	A	309	PRO	2.5
1	A	314	SER	2.5
1	A	370	GLU	2.5
1	A	481	ALA	2.5
1	B	468	ALA	2.5
1	A	386	LEU	2.5
1	B	248	LEU	2.5
1	A	199	PHE	2.5
1	A	359	VAL	2.5
1	B	22	ILE	2.5
1	B	126	VAL	2.5
1	B	202	CYS	2.5
1	B	203	TYR	2.5
1	A	48	GLU	2.5
1	B	449	SER	2.5
1	A	417	ALA	2.5
1	A	190	LEU	2.5
1	B	141	LEU	2.5
1	A	46	PHE	2.5
1	B	427	LYS	2.5
1	B	262	ARG	2.5
1	A	64	GLY	2.5
1	A	15	TRP	2.5
1	B	473	TRP	2.5
1	A	166	ILE	2.5
1	B	369	ILE	2.5
1	B	469	VAL	2.4
1	B	125	ALA	2.4

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Mol	Chain	Res	Type	RSRZ
1	B	481	ALA	2.4
1	A	381	LYS	2.4
1	B	56	LEU	2.4
1	B	334	ARG	2.4
1	B	219	ILE	2.4
1	B	304	GLU	2.4
1	B	265	VAL	2.4
1	A	382	SER	2.4
1	A	397	TYR	2.4
1	A	12	LEU	2.4
1	A	54	ASN	2.4
1	A	425	GLU	2.4
1	A	50	ASP	2.4
1	A	469	VAL	2.4
1	B	397	TYR	2.4
1	A	243	HIS	2.4
1	A	299	LEU	2.4
1	B	210	LEU	2.4
1	B	138	GLU	2.4
1	A	101	ASP	2.4
1	B	199	PHE	2.4
1	A	483	ILE	2.4
1	B	466	ILE	2.4
1	A	262	ARG	2.4
1	A	384	ALA	2.3
1	A	399	GLY	2.3
1	B	356	ASP	2.3
1	B	244	PHE	2.3
1	A	196	VAL	2.3
1	B	206	VAL	2.3
1	B	276	VAL	2.3
1	B	23	PRO	2.3
1	B	42	THR	2.3
1	A	31	GLN	2.3
1	A	431	ALA	2.3
1	B	259	ALA	2.3
1	A	174	GLY	2.3
1	A	17	ASP	2.3
1	B	273	ASP	2.3
1	A	440	LYS	2.3
1	B	28	LYS	2.3
1	A	358	PHE	2.3

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Mol	Chain	Res	Type	RSRZ
1	A	26	SER	2.3
1	A	57	ILE	2.3
1	B	192	ILE	2.3
1	A	142	THR	2.3
1	A	302	THR	2.3
1	A	56	LEU	2.3
1	A	472	TYR	2.3
1	A	208	LYS	2.3
1	B	35	PHE	2.3
1	B	238	GLN	2.3
1	A	327	VAL	2.3
1	A	70	PRO	2.3
1	B	247	THR	2.3
1	A	133	ALA	2.3
1	B	446	ASP	2.3
1	B	207	LEU	2.3
1	B	476	LEU	2.3
1	A	400	TRP	2.3
1	B	48	GLU	2.2
1	B	146	GLU	2.2
1	A	404	SER	2.2
1	A	459	SER	2.2
1	A	178	ILE	2.2
1	A	345	THR	2.2
1	B	142	THR	2.2
1	B	309	PRO	2.2
1	B	453	THR	2.2
1	A	258	ASN	2.2
1	A	271	ASN	2.2
1	B	101	ASP	2.2
1	B	423	ASP	2.2
1	A	290	ALA	2.2
1	B	224	ALA	2.2
1	A	136	GLU	2.2
1	B	267	THR	2.2
1	B	443	PRO	2.2
1	A	396	ASP	2.2
1	B	29	GLU	2.2
1	A	210	LEU	2.2
1	A	476	LEU	2.2
1	A	274	ILE	2.2
1	B	36	ILE	2.2

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Mol	Chain	Res	Type	RSRZ
1	A	365	VAL	2.2
1	A	401	GLU	2.2
1	A	61	ALA	2.2
1	A	121	ALA	2.2
1	A	418	GLN	2.2
1	B	75	ALA	2.2
1	B	134	HIS	2.2
1	B	49	ARG	2.2
1	A	357	ASN	2.2
1	A	331	GLY	2.1
1	A	141	LEU	2.1
1	A	406	SER	2.1
1	A	474	LYS	2.1
1	B	390	ASN	2.1
1	A	407	ASP	2.1
1	A	195	GLN	2.1
1	A	45	PHE	2.1
1	A	376	VAL	2.1
1	B	44	GLY	2.1
1	B	482	HIS	2.1
1	A	252	ARG	2.1
1	A	353	LYS	2.1
1	B	303	LEU	2.1
1	B	305	LYS	2.1
1	A	193	GLU	2.1
1	B	197	ASN	2.1
1	A	461	ASP	2.1
1	A	241	GLN	2.1
1	B	58	ARG	2.1
1	A	114	ALA	2.1
1	B	114	ALA	2.1
1	A	378	SER	2.1
1	B	258	ASN	2.1
1	A	177	TYR	2.1
1	A	424	PRO	2.1
1	A	453	THR	2.1
1	A	44	GLY	2.1
1	A	349	ILE	2.1
1	A	265	VAL	2.1
1	B	475	VAL	2.1
1	A	348	SER	2.1
1	B	47	ALA	2.1

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Mol	Chain	Res	Type	RSRZ
1	B	266	ALA	2.1
1	A	18	GLN	2.0
1	A	144	THR	2.0
1	B	168	THR	2.0
1	B	119	GLY	2.0
1	B	176	ILE	2.0
1	B	321	ILE	2.0
1	A	206	VAL	2.0
1	A	129	SER	2.0
1	A	249	ALA	2.0
1	B	158	ASN	2.0
1	B	456	ASN	2.0
1	A	278	GLN	2.0
1	A	347	LEU	2.0
1	B	73	LEU	2.0
1	B	74	GLN	2.0
1	B	245	ASP	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	SO4	B	504	5/5	0.62	0.15	134,135,135,135	0
3	SO4	B	512	5/5	0.64	0.18	123,125,126,126	0
3	SO4	B	508	5/5	0.68	0.17	107,107,109,109	0
3	SO4	B	511	5/5	0.70	0.20	119,120,120,120	0
3	SO4	B	505	5/5	0.70	0.19	91,95,96,97	0
3	SO4	A	510	5/5	0.71	0.16	121,122,122,122	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
4	GOL	B	514	6/6	0.71	0.26	75,79,81,81	0
4	GOL	B	515	6/6	0.72	0.24	86,87,88,88	0
3	SO4	B	510	5/5	0.73	0.16	106,107,108,108	0
4	GOL	A	512	6/6	0.73	0.33	97,99,99,99	0
2	ZN	A	502	1/1	0.74	0.23	131,131,131,131	0
4	GOL	B	521	6/6	0.74	0.28	76,78,79,80	0
4	GOL	B	519	6/6	0.75	0.27	94,97,98,98	0
3	SO4	B	509	5/5	0.75	0.16	113,115,116,117	0
3	SO4	A	507	5/5	0.77	0.15	96,98,99,100	0
3	SO4	A	504	5/5	0.78	0.13	111,111,112,113	0
3	SO4	A	505	5/5	0.78	0.16	98,101,101,102	0
3	SO4	B	506	5/5	0.79	0.20	85,87,91,93	0
4	GOL	A	514	6/6	0.81	0.21	71,75,76,78	0
4	GOL	A	516	6/6	0.81	0.23	85,88,88,89	0
4	GOL	A	513	6/6	0.81	0.21	82,82,84,84	0
5	IPA	A	519	4/4	0.81	0.27	68,68,70,72	0
3	SO4	A	506	5/5	0.82	0.20	79,83,85,87	0
4	GOL	B	516	6/6	0.83	0.23	67,71,73,75	0
4	GOL	B	517	6/6	0.84	0.24	78,80,80,82	0
3	SO4	B	507	5/5	0.84	0.15	84,86,87,88	0
5	IPA	A	520	4/4	0.84	0.26	74,76,76,77	0
4	GOL	A	518	6/6	0.85	0.24	61,69,72,73	0
3	SO4	A	509	5/5	0.86	0.16	100,100,102,103	0
3	SO4	A	508	5/5	0.86	0.15	82,82,84,85	0
4	GOL	B	518	6/6	0.87	0.20	70,72,75,77	0
5	IPA	B	522	4/4	0.88	0.23	68,69,71,71	0
4	GOL	A	515	6/6	0.89	0.19	57,64,68,71	0
4	GOL	A	517	6/6	0.90	0.19	65,65,66,67	0
4	GOL	B	520	6/6	0.90	0.18	66,70,71,74	0
4	GOL	B	513	6/6	0.91	0.21	41,44,45,45	0
3	SO4	B	503	5/5	0.91	0.16	58,62,64,65	0
3	SO4	A	503	5/5	0.93	0.17	46,58,62,62	0
2	ZN	B	502	1/1	0.95	0.14	117,117,117,117	0
2	ZN	B	501	1/1	0.96	0.11	95,95,95,95	0
4	GOL	A	511	6/6	0.97	0.14	33,37,40,42	0
2	ZN	A	501	1/1	0.99	0.14	73,73,73,73	0

6.5 Other polymers [i](#)

There are no such residues in this entry.