



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 01:12 PM UTC

PDB ID : 8CBB / pdb_00008cbb
Title : Structure of homodimeric luciferase from *Enhygromyxa salina*
Authors : Yudenko, A.; Remeeva, A.; Gushchin, I.
Deposited on : 2023-01-25
Resolution : 2.71 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

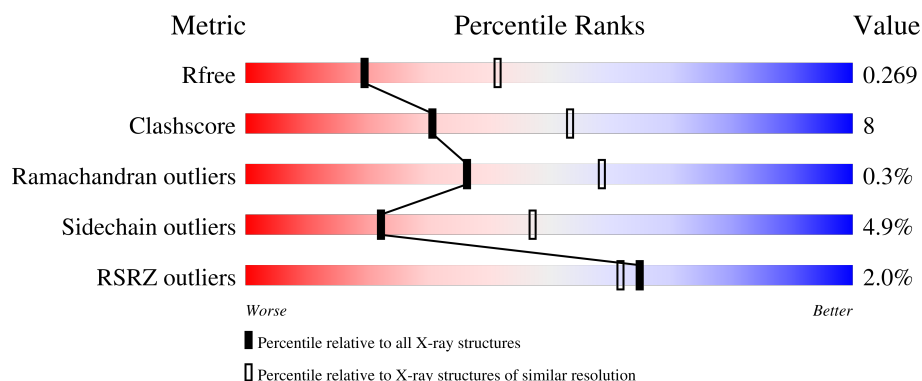
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

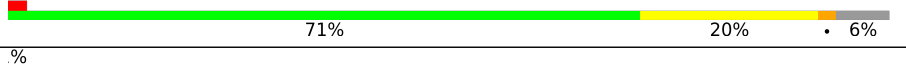
The reported resolution of this entry is 2.71 Å.

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	4348 (2.74-2.70)
Clashscore	190562	4665 (2.74-2.70)
Ramachandran outliers	187476	4584 (2.74-2.70)
Sidechain outliers	187428	4585 (2.74-2.70)
RSRZ outliers	180081	4348 (2.74-2.70)

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	371	 2% 73% 17% 8%
1	B	371	 2% 71% 20% 6%
1	C	371	 % 74% 20% . .
1	D	371	 2% 72% 18% 8%

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 11082 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 Alkanal monooxygenase alpha chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	342	Total	C	N	O	S	0	0	0
			2694	1709	472	497	16			
1	B	347	Total	C	N	O	S	0	1	0
			2713	1722	475	500	16			
1	C	356	Total	C	N	O	S	0	1	0
			2815	1788	495	515	17			
1	D	341	Total	C	N	O	S	0	1	0
			2675	1705	461	493	16			

There are 32 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	364	GLY	-	expression tag	UNP A0A2S9XZH0
A	365	SER	-	expression tag	UNP A0A2S9XZH0
A	366	HIS	-	expression tag	UNP A0A2S9XZH0
A	367	HIS	-	expression tag	UNP A0A2S9XZH0
A	368	HIS	-	expression tag	UNP A0A2S9XZH0
A	369	HIS	-	expression tag	UNP A0A2S9XZH0
A	370	HIS	-	expression tag	UNP A0A2S9XZH0
A	371	HIS	-	expression tag	UNP A0A2S9XZH0
B	364	GLY	-	expression tag	UNP A0A2S9XZH0
B	365	SER	-	expression tag	UNP A0A2S9XZH0
B	366	HIS	-	expression tag	UNP A0A2S9XZH0
B	367	HIS	-	expression tag	UNP A0A2S9XZH0
B	368	HIS	-	expression tag	UNP A0A2S9XZH0
B	369	HIS	-	expression tag	UNP A0A2S9XZH0
B	370	HIS	-	expression tag	UNP A0A2S9XZH0
B	371	HIS	-	expression tag	UNP A0A2S9XZH0
C	364	GLY	-	expression tag	UNP A0A2S9XZH0
C	365	SER	-	expression tag	UNP A0A2S9XZH0
C	366	HIS	-	expression tag	UNP A0A2S9XZH0
C	367	HIS	-	expression tag	UNP A0A2S9XZH0
C	368	HIS	-	expression tag	UNP A0A2S9XZH0

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Chain	Residue	Modelled	Actual	Comment	Reference
C	369	HIS	-	expression tag	UNP A0A2S9XZH0
C	370	HIS	-	expression tag	UNP A0A2S9XZH0
C	371	HIS	-	expression tag	UNP A0A2S9XZH0
D	364	GLY	-	expression tag	UNP A0A2S9XZH0
D	365	SER	-	expression tag	UNP A0A2S9XZH0
D	366	HIS	-	expression tag	UNP A0A2S9XZH0
D	367	HIS	-	expression tag	UNP A0A2S9XZH0
D	368	HIS	-	expression tag	UNP A0A2S9XZH0
D	369	HIS	-	expression tag	UNP A0A2S9XZH0
D	370	HIS	-	expression tag	UNP A0A2S9XZH0
D	371	HIS	-	expression tag	UNP A0A2S9XZH0

- Molecule 2 is SULFATE ION (CCD ID: SO4) (formula: O₄S).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	O	S	0	0
			5	4	1		
2	B	1	Total	O	S	0	0
			5	4	1		
2	C	1	Total	O	S	0	0
			5	4	1		
2	D	1	Total	O	S	0	0
			5	4	1		

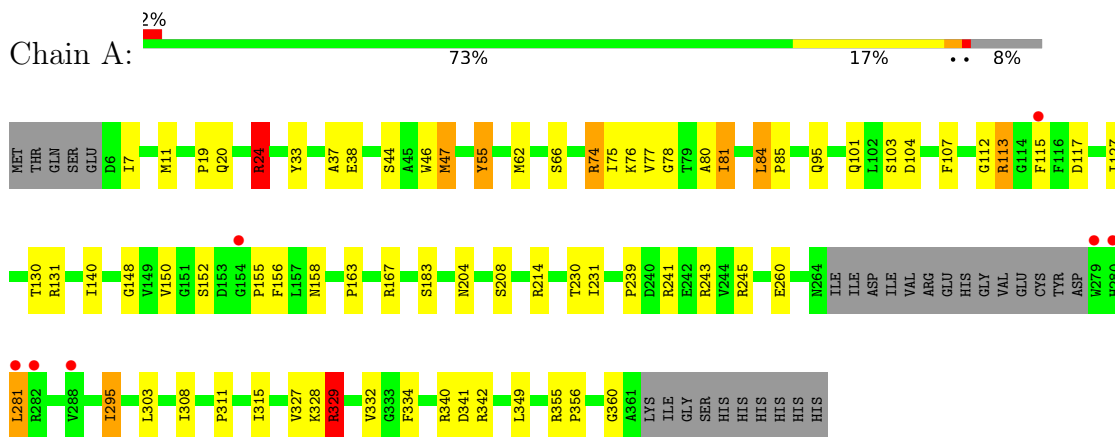
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	35	Total 35	O 35	0	0
3	B	41	Total 41	O 41	0	0
3	C	56	Total 56	O 56	0	0
3	D	33	Total 33	O 33	0	0

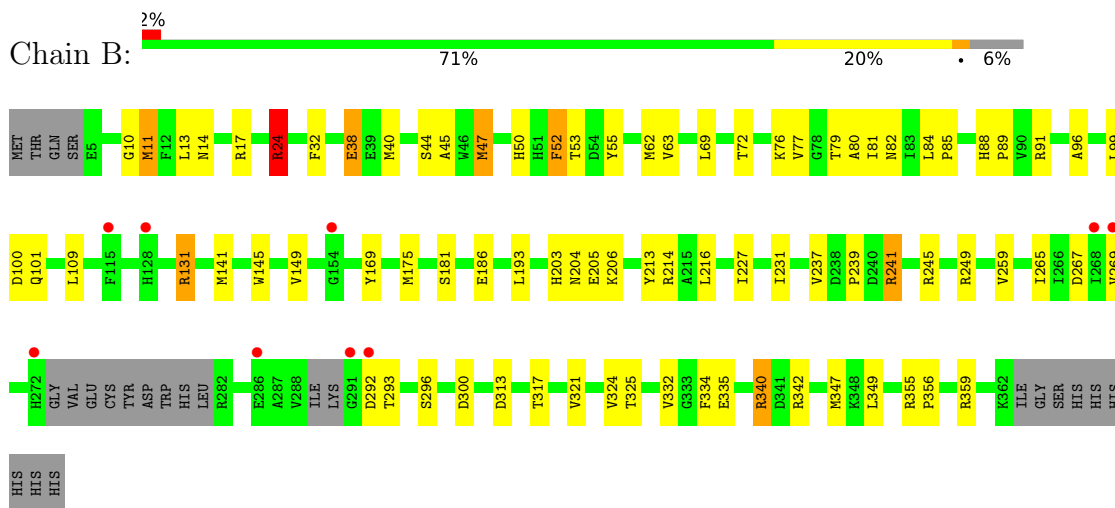
3 Residue-property plots

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.

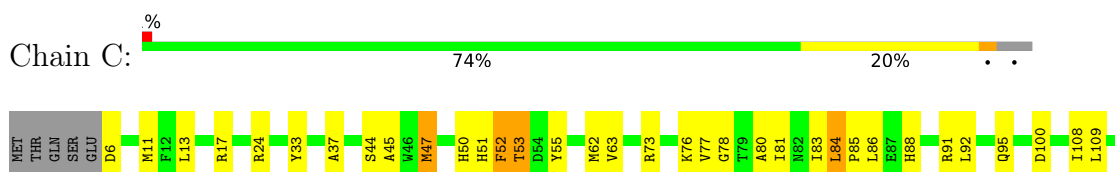
• Molecule 1: Alkanal monooxygenase alpha chain

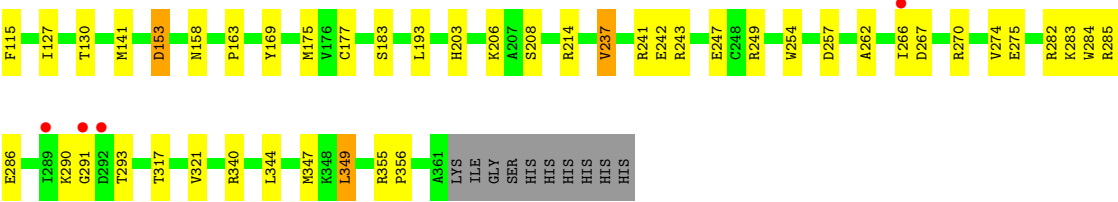


• Molecule 1: Alkanal monooxygenase alpha chain

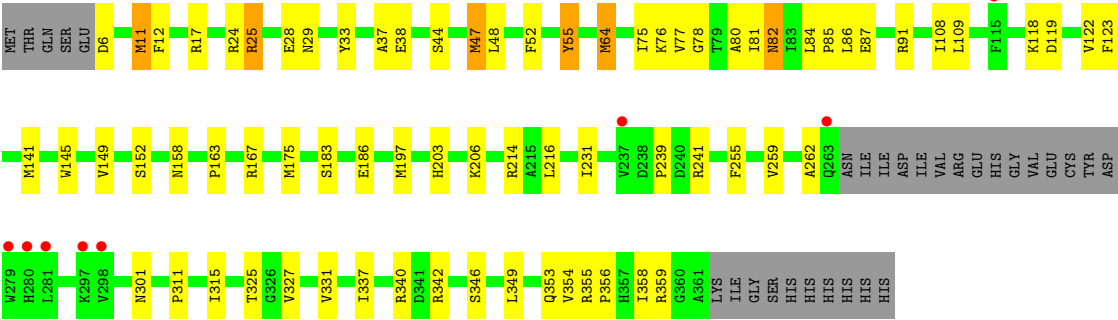


• Molecule 1: Alkanal monooxygenase alpha chain





● Molecule 1: Alkanal monooxygenase alpha chain



4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	51.82Å 73.37Å 93.97Å 88.72° 77.93° 87.10°	Depositor
Resolution (Å)	91.89 – 2.71 91.89 – 2.71	Depositor EDS
% Data completeness (in resolution range)	97.1 (91.89-2.71) 97.1 (91.89-2.71)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.90 (at 2.73Å)	Xtriage
Refinement program	REFMAC 5.8.0352	Depositor
R, R_{free}	0.191 , 0.269 0.197 , 0.269	Depositor DCC
R_{free} test set	1743 reflections (4.76%)	wwPDB-VP
Wilson B-factor (Å ²)	38.1	Xtriage
Anisotropy	0.029	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 36.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	0.107 for -h,k,-l	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	11082	wwPDB-VP
Average B, all atoms (Å ²)	41.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.80% 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: 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	0/2758	0.83	0/3743
1	B	0.51	0/2779	0.82	0/3775
1	C	0.51	0/2888	0.82	0/3923
1	D	0.51	0/2744	0.84	0/3727
All	All	0.51	0/11169	0.83	0/15168

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	9
1	B	0	9
1	C	0	9
1	D	0	6
All	All	0	33

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (33) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	113	ARG	Sidechain
1	A	214	ARG	Sidechain
1	A	24	ARG	Sidechain
1	A	241	ARG	Sidechain
1	A	243	ARG	Sidechain

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Mol	Chain	Res	Type	Group
1	A	329	ARG	Sidechain
1	A	340	ARG	Sidechain
1	A	342	ARG	Sidechain
1	A	74	ARG	Sidechain
1	B	131	ARG	Sidechain
1	B	17	ARG	Sidechain
1	B	214	ARG	Sidechain
1	B	24	ARG	Sidechain
1	B	245	ARG	Sidechain
1	B	340	ARG	Sidechain
1	B	342	ARG	Sidechain
1	B	91[A]	ARG	Sidechain
1	B	91[B]	ARG	Sidechain
1	C	17	ARG	Sidechain
1	C	214	ARG	Sidechain
1	C	241	ARG	Sidechain
1	C	249	ARG	Sidechain
1	C	285	ARG	Sidechain
1	C	290	LYS	Peptide
1	C	291	GLY	Peptide
1	C	51	HIS	Peptide
1	C	73	ARG	Sidechain
1	D	17	ARG	Sidechain
1	D	214	ARG	Sidechain
1	D	241	ARG	Sidechain
1	D	25	ARG	Sidechain
1	D	342	ARG	Sidechain
1	D	359	ARG	Sidechain

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	2694	0	2607	46	0
1	B	2713	0	2606	49	0
1	C	2815	0	2718	44	0
1	D	2675	0	2568	45	0
2	A	5	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	B	5	0	0	0	0
2	C	5	0	0	0	0
2	D	5	0	0	0	0
3	A	35	0	0	1	0
3	B	41	0	0	0	0
3	C	56	0	0	0	0
3	D	33	0	0	0	0
All	All	11082	0	10499	177	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 8.

All (177) 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:11:MET:HE2	1:A:37:ALA:HB2	1.60	0.84
1:A:47:MET:HE3	1:A:77:VAL:HG13	1.61	0.82
1:B:13:LEU:HD12	1:B:47:MET:CE	2.12	0.80
1:C:11:MET:HE2	1:C:37:ALA:HB2	1.71	0.73
1:C:13:LEU:HD12	1:C:47:MET:CE	2.19	0.73
1:D:109:LEU:HD23	1:D:175:MET:HE3	1.71	0.73
1:B:13:LEU:HD12	1:B:47:MET:HE1	1.71	0.71
1:A:152:SER:O	1:A:158:ASN:HA	1.94	0.68
1:C:274:VAL:HG22	1:C:275:GLU:H	1.58	0.67
1:B:14:ASN:HB2	1:B:335:GLU:CD	2.19	0.67
1:B:206:LYS:HE2	1:B:231:ILE:HD11	1.75	0.66
1:A:11:MET:CE	1:A:33:TYR:O	2.44	0.66
1:D:186:GLU:HA	1:D:216:LEU:HD13	1.77	0.66
1:B:11:MET:HE1	1:B:347:MET:HE3	1.78	0.66
1:A:80:ALA:HA	1:A:81:ILE:HG23	1.79	0.65
1:B:10:GLY:O	1:B:332:VAL:HG22	1.97	0.64
1:B:292:ASP:O	1:B:293:THR:OG1	2.11	0.63
1:B:241:ARG:HH11	1:B:313:ASP:CG	2.06	0.63
1:C:13:LEU:HD12	1:C:47:MET:HE2	1.80	0.63
1:A:311:PRO:O	1:A:315:ILE:HG13	1.99	0.63
1:C:52:PHE:O	1:D:163:PRO:HG2	2.01	0.61
1:B:355:ARG:N	1:B:356:PRO:CD	2.64	0.61
1:C:50:HIS:CE1	1:C:55:TYR:HB3	2.36	0.61
1:D:87:GLU:OE2	1:D:91[B]:ARG:NH1	2.32	0.60
1:D:12:PHE:CD1	1:D:48:LEU:HD11	2.37	0.59
1:B:317:THR:O	1:B:321:VAL:HG23	2.02	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:152:SER:O	1:D:158:ASN:HA	2.03	0.59
1:A:11:MET:HE1	1:A:33:TYR:O	2.03	0.59
1:B:13:LEU:HD12	1:B:47:MET:HE2	1.85	0.59
1:C:88:HIS:HB3	1:C:91:ARG:HG3	1.86	0.58
1:B:237:VAL:HG12	1:B:349:LEU:HD13	1.86	0.58
1:D:311:PRO:O	1:D:315:ILE:HG13	2.03	0.58
1:D:47:MET:HE3	1:D:77:VAL:HG13	1.86	0.58
1:A:11:MET:HE3	1:A:33:TYR:HB3	1.85	0.57
1:A:113:ARG:NH1	1:A:130:THR:OG1	2.29	0.57
1:A:62:MET:HE2	1:A:95:GLN:HB3	1.85	0.57
1:B:44:SER:HA	1:B:76:LYS:O	2.05	0.56
1:B:84:LEU:N	1:B:85:PRO:CD	2.68	0.56
1:C:84:LEU:N	1:C:85:PRO:CD	2.69	0.56
1:D:118:LYS:HE2	1:D:262:ALA:HB1	1.88	0.56
1:C:243:ARG:O	1:C:247:GLU:HG2	2.06	0.55
1:A:231:ILE:CG2	1:A:327:VAL:HG21	2.36	0.55
1:C:11:MET:HE3	1:C:33:TYR:HB3	1.89	0.55
1:D:239:PRO:HD3	1:D:349:LEU:HD11	1.89	0.55
1:D:48:LEU:N	1:D:48:LEU:HD12	2.23	0.54
1:A:230:THR:HG23	1:A:329:ARG:HG2	1.89	0.54
1:B:141:MET:HE2	1:B:145:TRP:CH2	2.43	0.54
1:D:12:PHE:CD2	1:D:331:VAL:HG12	2.44	0.53
1:B:141:MET:HE2	1:B:145:TRP:CZ2	2.43	0.53
1:C:274:VAL:HG22	1:C:275:GLU:N	2.21	0.53
1:A:239:PRO:HD3	1:A:349:LEU:HD11	1.91	0.52
1:D:29:ASN:HB3	1:D:33:TYR:CE2	2.45	0.52
1:B:79:THR:HG21	1:B:82:ASN:HD21	1.74	0.52
1:A:101:GLN:O	1:B:24:ARG:NH2	2.43	0.52
1:D:44:SER:HA	1:D:76:LYS:O	2.10	0.52
1:A:44:SER:HA	1:A:76:LYS:O	2.09	0.51
1:B:213:TYR:OH	1:B:227:ILE:HD13	2.11	0.51
1:A:47:MET:HE3	1:A:77:VAL:CG1	2.38	0.51
1:A:81:ILE:HD13	1:A:112:GLY:HA3	1.92	0.51
1:A:230:THR:HG23	1:A:329:ARG:CG	2.40	0.51
1:A:230:THR:CG2	1:A:329:ARG:HG2	2.41	0.51
1:D:255:PHE:O	1:D:259:VAL:HG23	2.11	0.51
1:B:239:PRO:HD3	1:B:349:LEU:HD11	1.93	0.50
1:C:355:ARG:HB3	1:C:356:PRO:HD3	1.93	0.50
1:A:80:ALA:HA	1:A:81:ILE:CG2	2.40	0.50
1:A:107:PHE:HB3	3:A:502:HOH:O	2.11	0.50
1:B:40:MET:HG3	1:C:284:TRP:CZ2	2.46	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:80:ALA:HA	1:C:81:ILE:HG23	1.93	0.50
1:D:315:ILE:HD11	1:D:353:GLN:O	2.11	0.50
1:D:355:ARG:N	1:D:356:PRO:CD	2.75	0.50
1:B:265:ILE:O	1:B:269:VAL:HG23	2.12	0.50
1:C:45:ALA:O	1:C:77:VAL:HA	2.11	0.49
1:B:241:ARG:NH1	1:B:313:ASP:OD1	2.43	0.49
1:B:13:LEU:HB2	1:B:47:MET:HE3	1.94	0.49
1:A:84:LEU:N	1:A:85:PRO:CD	2.76	0.49
1:A:355:ARG:N	1:A:356:PRO:CD	2.75	0.49
1:B:50:HIS:CE1	1:B:55:TYR:HD2	2.31	0.49
1:A:231:ILE:HG22	1:A:327:VAL:HG21	1.95	0.48
1:A:24:ARG:NH2	1:B:101:GLN:O	2.46	0.48
1:C:11:MET:SD	1:C:347:MET:HE3	2.54	0.48
1:D:86:LEU:HD11	1:D:119:ASP:HB3	1.95	0.48
1:D:206:LYS:HE2	1:D:231:ILE:HD11	1.96	0.48
1:D:118:LYS:CE	1:D:262:ALA:HB1	2.44	0.48
1:B:293:THR:HA	1:B:296:SER:HB3	1.95	0.47
1:D:84:LEU:N	1:D:85:PRO:CD	2.77	0.47
1:D:38:GLU:HG3	1:D:75:ILE:HB	1.94	0.47
1:D:118:LYS:O	1:D:122:VAL:HG23	2.15	0.47
1:B:32:PHE:CD2	1:B:340:ARG:HD2	2.48	0.47
1:C:355:ARG:N	1:C:356:PRO:CD	2.77	0.47
1:C:80:ALA:HA	1:C:81:ILE:CG2	2.44	0.47
1:B:79:THR:OG1	1:B:82:ASN:ND2	2.48	0.47
1:B:324:VAL:HG23	1:B:325:THR:HG23	1.96	0.47
1:C:100:ASP:OD2	1:C:169:TYR:N	2.48	0.47
1:B:11:MET:CE	1:B:334:PHE:CD2	2.97	0.47
1:C:11:MET:HE1	1:C:33:TYR:O	2.15	0.47
1:A:62:MET:O	1:A:66:SER:HB2	2.15	0.47
1:C:237:VAL:CG1	1:C:349:LEU:HB3	2.45	0.47
1:D:47:MET:SD	1:D:64:MET:HG2	2.55	0.47
1:A:303:LEU:HD23	1:A:308:ILE:HD12	1.98	0.46
1:C:267:ASP:OD1	1:C:270:ARG:NH1	2.49	0.46
1:D:239:PRO:HD3	1:D:349:LEU:CD1	2.46	0.46
1:A:163:PRO:HG2	1:B:52:PHE:O	2.15	0.46
1:D:206:LYS:CE	1:D:231:ILE:HD11	2.46	0.46
1:A:260:GLU:OE2	1:A:295:ILE:HD11	2.16	0.46
1:C:177:CYS:HB2	1:C:193:LEU:HD23	1.97	0.46
1:C:203:HIS:HA	1:C:206:LYS:HE3	1.97	0.46
1:A:140:ILE:HG23	1:A:150:VAL:HG21	1.97	0.45
1:B:13:LEU:HB2	1:B:47:MET:CE	2.46	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:155:PRO:HG2	1:A:156:PHE:CD2	2.52	0.45
1:C:127:ILE:O	1:C:130:THR:HG23	2.16	0.45
1:D:24:ARG:O	1:D:28:GLU:HB2	2.17	0.45
1:C:109:LEU:O	1:C:175:MET:HA	2.17	0.45
1:C:163:PRO:O	1:D:52:PHE:HA	2.17	0.45
1:D:141:MET:HE2	1:D:145:TRP:CH2	2.51	0.45
1:B:45:ALA:O	1:B:77:VAL:HA	2.16	0.45
1:C:13:LEU:HD12	1:C:47:MET:HE1	1.98	0.44
1:B:88:HIS:ND1	1:B:89:PRO:HD2	2.32	0.44
1:C:254:TRP:O	1:C:257:ASP:HB3	2.17	0.44
1:D:354:VAL:O	1:D:358:ILE:HG12	2.17	0.44
1:B:186:GLU:HA	1:B:216:LEU:HD13	1.99	0.44
1:D:11:MET:HE3	1:D:37:ALA:HB2	2.00	0.44
1:C:52:PHE:C	1:C:53:THR:CG2	2.91	0.44
1:D:141:MET:CE	1:D:145:TRP:CH2	3.00	0.44
1:A:19:PRO:HD2	1:A:20:GLN:OE1	2.18	0.43
1:A:329:ARG:HG2	1:A:329:ARG:HH11	1.83	0.43
1:D:197:MET:HB2	1:D:231:ILE:HD12	2.00	0.43
1:D:84:LEU:HA	1:D:84:LEU:HD23	1.82	0.43
1:A:74:ARG:HG3	1:A:75:ILE:N	2.33	0.43
1:A:231:ILE:HG21	1:A:327:VAL:HG21	2.00	0.43
1:C:62:MET:HE2	1:C:95:GLN:HB3	2.00	0.43
1:D:82:ASN:N	1:D:82:ASN:HD22	2.17	0.43
1:B:193:LEU:HD12	1:B:193:LEU:HA	1.83	0.43
1:C:83:ILE:HG22	1:C:86:LEU:HD13	2.01	0.43
1:C:78:GLY:HA2	1:C:108:ILE:O	2.19	0.43
1:A:281:LEU:HD23	1:A:281:LEU:HA	1.87	0.43
1:C:44:SER:HA	1:C:76:LYS:O	2.18	0.42
1:A:332:VAL:HG23	1:A:334:PHE:CE2	2.54	0.42
1:A:7:ILE:HD11	1:A:360:GLY:HA2	2.01	0.42
1:B:62:MET:HE1	1:B:96:ALA:HA	2.02	0.42
1:D:337:ILE:HD13	1:D:346:SER:HB2	2.00	0.42
1:C:50:HIS:CD2	1:C:55:TYR:CD2	3.07	0.42
1:C:91:ARG:HG2	1:D:123:PHE:CE1	2.55	0.42
1:C:237:VAL:HG12	1:C:349:LEU:HB3	2.02	0.42
1:B:203:HIS:HD2	1:B:206:LYS:NZ	2.17	0.42
1:B:321:VAL:O	1:B:325:THR:OG1	2.25	0.42
1:B:69:LEU:HD12	1:B:99:LEU:HD11	2.02	0.42
1:B:249:ARG:NH1	1:B:300:ASP:OD1	2.45	0.42
1:D:78:GLY:HA2	1:D:108:ILE:O	2.20	0.42
1:D:80:ALA:HA	1:D:81:ILE:HG23	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:12:PHE:HD1	1:D:48:LEU:HD11	1.85	0.41
1:A:230:THR:OG1	1:A:329:ARG:HG2	2.20	0.41
1:B:100:ASP:OD2	1:B:169:TYR:N	2.53	0.41
1:B:131:ARG:NH2	1:B:181:SER:OG	2.53	0.41
1:D:325:THR:OG1	1:D:327:VAL:HG13	2.19	0.41
1:B:38:GLU:HG3	1:B:72:THR:HG22	2.03	0.41
1:C:11:MET:CE	1:C:33:TYR:O	2.68	0.41
1:A:46:TRP:CZ3	1:A:78:GLY:HA3	2.55	0.41
1:A:117:ASP:HA	1:A:127:ILE:HD12	2.03	0.41
1:A:103:SER:O	1:A:104:ASP:HB2	2.21	0.41
1:B:109:LEU:O	1:B:175:MET:HA	2.20	0.41
1:C:53:THR:HG21	1:C:262:ALA:HA	2.03	0.41
1:A:148:GLY:HA3	1:A:167:ARG:HH11	1.85	0.41
1:D:167:ARG:O	1:D:167:ARG:HG3	2.21	0.41
1:B:50:HIS:ND1	1:B:55:TYR:HD2	2.18	0.41
1:B:349:LEU:HD23	1:B:349:LEU:HA	1.89	0.41
1:C:317:THR:O	1:C:321:VAL:HG23	2.21	0.41
1:A:46:TRP:HA	1:A:78:GLY:O	2.21	0.41
1:A:84:LEU:N	1:A:85:PRO:HD2	2.36	0.41
1:C:92:LEU:HG	1:C:141:MET:CE	2.51	0.41
1:C:282:ARG:O	1:C:286:GLU:HG3	2.20	0.40
1:D:55:TYR:HD1	1:D:255:PHE:CE1	2.39	0.40
1:D:203:HIS:O	1:D:206:LYS:HB2	2.21	0.40
1:D:11:MET:HE2	1:D:11:MET:HB2	1.84	0.40
1:C:153:ASP:HA	1:C:158[A]:ASN:HD22	1.86	0.40
1:C:340:ARG:O	1:C:344:LEU:HG	2.21	0.40
1:A:55:TYR:O	1:A:55:TYR:CD1	2.74	0.40
1:B:80:ALA:HA	1:B:81:ILE:HG23	2.02	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	338/371 (91%)	328 (97%)	10 (3%)	0	100	100
1	B	342/371 (92%)	332 (97%)	9 (3%)	1 (0%)	36	59
1	C	355/371 (96%)	343 (97%)	9 (2%)	3 (1%)	16	35
1	D	338/371 (91%)	330 (98%)	8 (2%)	0	100	100
All	All	1373/1484 (92%)	1333 (97%)	36 (3%)	4 (0%)	36	59

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	52	PHE
1	C	293	THR
1	C	115	PHE
1	C	52	PHE

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	281/316 (89%)	264 (94%)	17 (6%)	17	39
1	B	280/316 (89%)	267 (95%)	13 (5%)	24	50
1	C	293/316 (93%)	279 (95%)	14 (5%)	23	48
1	D	275/316 (87%)	264 (96%)	11 (4%)	28	55
All	All	1129/1264 (89%)	1074 (95%)	55 (5%)	22	47

All (55) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	24	ARG
1	A	38	GLU
1	A	47	MET
1	A	55	TYR
1	A	81	ILE
1	A	84	LEU
1	A	115	PHE

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Mol	Chain	Res	Type
1	A	131	ARG
1	A	183	SER
1	A	204	ASN
1	A	208	SER
1	A	245	ARG
1	A	281	LEU
1	A	295	ILE
1	A	328	LYS
1	A	329	ARG
1	A	341	ASP
1	B	11	MET
1	B	24	ARG
1	B	38	GLU
1	B	47	MET
1	B	53	THR
1	B	63	VAL
1	B	149	VAL
1	B	204	ASN
1	B	205	GLU
1	B	241	ARG
1	B	259	VAL
1	B	267	ASP
1	B	359	ARG
1	C	6	ASP
1	C	24	ARG
1	C	47	MET
1	C	53	THR
1	C	63	VAL
1	C	84	LEU
1	C	153	ASP
1	C	183	SER
1	C	208	SER
1	C	237	VAL
1	C	242	GLU
1	C	266	ILE
1	C	283	LYS
1	C	349	LEU
1	D	6	ASP
1	D	11	MET
1	D	25	ARG
1	D	47	MET
1	D	55	TYR

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Mol	Chain	Res	Type
1	D	64	MET
1	D	82	ASN
1	D	149	VAL
1	D	183	SER
1	D	301	ASN
1	D	340	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (30) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	50	HIS
1	A	82	ASN
1	A	135	HIS
1	A	136	ASN
1	A	142	GLN
1	A	191	ASN
1	A	199	HIS
1	A	203	HIS
1	A	263	GLN
1	A	353	GLN
1	B	82	ASN
1	B	136	ASN
1	B	142	GLN
1	B	191	ASN
1	B	203	HIS
1	B	263	GLN
1	C	50	HIS
1	C	128	HIS
1	C	203	HIS
1	C	263	GLN
1	C	320	HIS
1	C	353	GLN
1	D	14	ASN
1	D	50	HIS
1	D	82	ASN
1	D	95	GLN
1	D	158	ASN
1	D	199	HIS
1	D	203	HIS
1	D	320	HIS

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

4 ligands 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	$\# Z > 2$
2	SO4	B	401	-	4,4,4	0.32	0	6,6,6	0.08	0
2	SO4	D	401	-	4,4,4	0.31	0	6,6,6	0.09	0
2	SO4	A	401	-	4,4,4	0.34	0	6,6,6	0.07	0
2	SO4	C	401	-	4,4,4	0.34	0	6,6,6	0.07	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.

No monomer is involved in short contacts.

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	342/371 (92%)	0.10	7 (2%) 65 62	21, 40, 71, 102	0
1	B	347/371 (93%)	0.03	9 (2%) 57 54	20, 35, 79, 105	1 (0%)
1	C	356/371 (95%)	-0.17	4 (1%) 78 76	19, 32, 59, 109	2 (0%)
1	D	341/371 (91%)	0.13	8 (2%) 61 58	18, 40, 87, 104	1 (0%)
All	All	1386/1484 (93%)	0.02	28 (2%) 65 62	18, 36, 75, 109	4 (0%)

All (28) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	279	TRP	5.0
1	A	280	HIS	4.0
1	B	291	GLY	3.7
1	D	279	TRP	3.5
1	C	292	ASP	3.2
1	A	115	PHE	3.1
1	B	268	ILE	3.0
1	D	280	HIS	3.0
1	C	291	GLY	3.0
1	B	115	PHE	2.9
1	B	272	HIS	2.8
1	B	154	GLY	2.7
1	D	237	VAL	2.7
1	D	297	LYS	2.5
1	D	115	PHE	2.5
1	D	263	GLN	2.5
1	B	286	GLU	2.4
1	A	281	LEU	2.4
1	C	266	ILE	2.4
1	A	154	GLY	2.3
1	B	292	ASP	2.3

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Mol	Chain	Res	Type	RSRZ
1	C	289	ILE	2.2
1	A	288	VAL	2.2
1	B	128	HIS	2.2
1	B	269	VAL	2.2
1	D	298	VAL	2.1
1	D	281	LEU	2.0
1	A	282	ARG	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($\text{\AA}^2$)	Q<0.9
2	SO4	D	401	5/5	0.68	0.16	70,74,82,83	0
2	SO4	B	401	5/5	0.79	0.16	51,62,69,70	0
2	SO4	C	401	5/5	0.84	0.14	52,63,63,67	0
2	SO4	A	401	5/5	0.87	0.12	57,57,63,64	0

6.5 Other polymers [i](#)

There are no such residues in this entry.