

# Full wwPDB X-ray Structure Validation Report (i)

#### Jan 29, 2024 - 08:12 pm GMT

:	8CBB
:	Structure of homodimeric luciferase from Enhygromyxa salina
:	Yudenko, A.; Remeeva, A.; Gushchin, I.
:	2023-01-25
:	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 (i) 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 (1)) were used in the production of this report:

MolProbity	:	4.02b-467
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
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)	:	2.36

# 1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:  $X\text{-}RAY \, DIFFRACTION$ 

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	Similar resolution
	$(\# { m Entries})$	$(\# { m Entries},  { m resolution}  { m range}({ m \AA}))$
$R_{free}$	130704	3359(2.74-2.70)
Clashscore	141614	3686 (2.74-2.70)
Ramachandran outliers	138981	3622(2.74-2.70)
Sidechain outliers	138945	3623 (2.74-2.70)
RSRZ outliers	127900	3276 (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 <=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	А	371	73%	16%	•• 8%
1	В	371	.% 73%	19%	• 6%
1	С	371	.% <b>74</b> %	20%	
1	D	371	74%	18%	• 8%



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# 2 Entry composition (i)

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.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace	
1	Δ	249	Total	С	Ν	0	S	0	0	0
	A	342	2694	1709	472	497	16	0		0
1	Р	247	Total	С	Ν	0	S	0	1	0
	D	347	2713	1722	475	500	16	0	1	U
1	C	256	Total	С	Ν	0	S	0	1	0
	U	- 200	2815	1788	495	515	17	0		0
1	Л	3/1	Total	С	Ν	0	S	0	1	0
I D	341	2675	1705	461	493	16	0		0	

• Molecule 1 is a protein called Alkanal monooxygenase alpha chain.

There are 32 discrepancies between the modelled and reference sequences:

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



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Chain	Residue	Modelled	Actual	Comment	Reference
С	369	HIS	-	expression tag	UNP A0A2S9XZH0
С	370	HIS	-	expression tag	UNP A0A2S9XZH0
С	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



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	А	1	$\begin{array}{c cc} Total & O & S \\ 5 & 4 & 1 \end{array}$	0	0
			Total O S		
2	В	1	5 4 1	0	0
2	С	1	Total O S	0	0
		-	5 4 1	Ŭ	Ŭ
2	D	1	Total O S	0	0
_		-	5 4 1	Ŭ	Ŭ

• Molecule 3 is water.



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	А	35	$\begin{array}{cc} \text{Total} & \text{O} \\ 35 & 35 \end{array}$	0	0
3	В	41	Total         O           41         41	0	0
3	С	56	Total         O           56         56	0	0
3	D	33	Total         O           33         33	0	0



# 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: Alkanal monooxygenase alpha chain





• Molecule 1: Alkanal monooxygenase alpha chain





# 4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1	Depositor
Cell constants	51.82Å 73.37Å 93.97Å	Deperitor
a, b, c, $\alpha$ , $\beta$ , $\gamma$	$88.72^{\circ}$ $77.93^{\circ}$ $87.10^{\circ}$	Depositor
$\mathbf{P}_{\text{acclution}}(\hat{\mathbf{A}})$	91.89 - 2.71	Depositor
Resolution (A)	91.89 - 2.71	EDS
% Data completeness	97.1 (91.89-2.71)	Depositor
(in resolution range)	97.1 (91.89-2.71)	EDS
R <sub>merge</sub>	0.07	Depositor
R <sub>sym</sub>	(Not available)	Depositor
$< I/\sigma(I) > 1$	$1.90 (at 2.73 \text{\AA})$	Xtriage
Refinement program	REFMAC 5.8.0352	Depositor
B B.	0.191 , $0.269$	Depositor
$\Pi, \Pi_{free}$	0.197 , $0.269$	DCC
$R_{free}$ test set	1743 reflections $(4.90%)$	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 , $36.9$	EDS
L-test for twinning <sup>2</sup>	$<  L  > = 0.50, < L^2 > = 0.34$	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.

<sup>&</sup>lt;sup>2</sup>Theoretical 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.



<sup>&</sup>lt;sup>1</sup>Intensities estimated from amplitudes.

# 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

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).

Mal	Chain	Bond	lengths	Bond angles		
	Chain	RMSZ	# Z  > 5	RMSZ	# Z  > 5	
1	А	0.26	0/2758	0.40	0/3743	
1	В	0.27	0/2779	0.39	0/3775	
1	С	0.26	0/2888	0.39	0/3923	
1	D	0.27	0/2744	0.39	0/3727	
All	All	0.26	0/11169	0.39	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	А	0	9
1	В	0	9
1	С	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	А	113	ARG	Sidechain
1	А	214	ARG	Sidechain
1	А	24	ARG	Sidechain
1	А	241	ARG	Sidechain
1	А	243	ARG	Sidechain



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

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## 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	А	2694	0	2607	45	0
1	В	2713	0	2606	49	0
1	С	2815	0	2718	42	0
1	D	2675	0	2568	40	0
2	А	5	0	0	0	0



Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	В	5	0	0	0	0
2	С	5	0	0	0	0
2	D	5	0	0	0	0
3	А	35	0	0	1	0
3	В	41	0	0	0	0
3	С	56	0	0	0	0
3	D	33	0	0	0	0
All	All	11082	0	10499	169	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 (169) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom 1	Atom 2	Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
1:A:11:MET:HE2	1:A:37:ALA:HB2	1.54	0.87
1:B:13:LEU:HD12	1:B:47:MET:HE1	1.60	0.82
1:B:13:LEU:HD12	1:B:47:MET:CE	2.12	0.78
1:C:13:LEU:HD12	1:C:47:MET:CE	2.19	0.73
1:A:152:SER:O	1:A:158:ASN:HA	1.94	0.68
1:B:92:LEU:HG	1:B:141:MET:HE3	1.75	0.67
1:C:274:VAL:HG22	1:C:275:GLU:H	1.58	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: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:A:311:PRO:O	1:A:315:ILE:HG13	1.99	0.63
1:B:14:ASN:HB2	1:B:335:GLU:CD	2.19	0.62
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:B:292:ASP:O	1:B:293:THR:OG1	2.11	0.60
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
1:D:152:SER:O	1:D:158:ASN:HA	2.03	0.59
1:B:241:ARG:HH11	1:B:313:ASP:CG	2.06	0.58
1:C:13:LEU:HD12	1:C:47:MET:HE1	1.85	0.58
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



A 4 1	A t arra 0	Interatomic	Clash
Atom-1	Atom-2	distance $(\text{\AA})$	overlap (Å)
1:D:311:PRO:O	1:D:315:ILE:HG13	2.03	0.58
1:A:113:ARG:NH1	1:A:130:THR:OG1	2.29	0.57
1:B:44:SER:HA	1:B:76:LYS:O	2.05	0.56
1:C:11:MET:HE3	1:C:33:TYR:HB3	1.87	0.56
1:B:84:LEU:N	1:B:85:PRO:CD	2.68	0.56
1:A:11:MET:HE1	1:A:33:TYR:O	2.05	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: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:D:12:PHE:CD2	1:D:331:VAL:HG12	2.44	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:81:ILE:HD13	1:A:112:GLY:HA3	1.92	0.51
1:B:92:LEU:CG	1:B:141:MET:HE3	2.40	0.51
1:A:230:THR:HG23	1:A:329:ARG:CG	2.40	0.51
1:C:13:LEU:HD12	1:C:47:MET:HE2	1.93	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
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: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

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A 4 arra 1		Interatomic	Clash
Atom-1	Atom-2	distance $(\text{\AA})$	overlap (Å)
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:C:92:LEU:HG	1:C:141:MET:HE1	1.95	0.48
1:A:24:ARG:NH2	1:B:101:GLN:O	2.46	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: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:C:11:MET:HE1	1:C:37:ALA:HB2	1.98	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:C:11:MET:HE1	1:C:33:TYR:O	2.16	0.45
1:B:13:LEU:HB2	1:B:47:MET:CE	2.46	0.45
1:A:155:PRO:HG2	1:A:156:PHE:CD2	2.52	0.45
1:B:13:LEU:CD1	1:B:47:MET:HE1	2.40	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:B:45:ALA:O	1:B:77:VAL:HA	2.16	0.45
1:B:88:HIS:ND1	1:B:89:PRO:HD2	2.32	0.44



		Interatomic	Clash
Atom-1	Atom-2	distance $(\text{\AA})$	overlap (Å)
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:A:47:MET:CE	1:A:77:VAL:HG13	2.48	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:B:11:MET:HE3	1:B:334:PHE:CE2	2.52	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: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:A:11:MET:HE3	1:A:33:TYR:HB3	2.00	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: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: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
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



Atom 1	Atom 2	Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
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:B:321:VAL:O	1:B:325:THR:OG1	2.25	0.41
1:B:13:LEU:HD12	1:B:47:MET:HE2	1.97	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:B:79:THR:HG1	1:B:110:GLY:H	1.69	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:11:MET:CE	1:A:33:TYR:HB3	2.51	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	Perce	entiles
1	А	338/371~(91%)	328~(97%)	10 (3%)	0	100	100
1	В	342/371~(92%)	332~(97%)	9~(3%)	1 (0%)	41	65
1	С	355/371~(96%)	343~(97%)	9~(2%)	3~(1%)	19	41
1	D	338/371~(91%)	330~(98%)	8 (2%)	0	100	100
All	All	1373/1484~(92%)	1333 (97%)	36 (3%)	4 (0%)	41	65





All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	В	52	PHE
1	С	293	THR
1	С	115	PHE
1	С	52	PHE

#### 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	А	281/316~(89%)	267~(95%)	14~(5%)	24 49		
1	В	280/316~(89%)	272~(97%)	8(3%)	42 70		
1	С	293/316~(93%)	277 (94%)	16 (6%)	21 44		
1	D	275/316~(87%)	268~(98%)	7 (2%)	47 75		
All	All	1129/1264~(89%)	1084 (96%)	45~(4%)	31 58		

All (45) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	А	24	ARG
1	А	38	GLU
1	А	47	MET
1	А	55	TYR
1	А	66	SER
1	А	84	LEU
1	А	115	PHE
1	А	131	ARG
1	А	208	SER
1	А	245	ARG
1	А	281	LEU
1	А	328	LYS
1	А	329	ARG
1	А	341	ASP
1	В	11	MET
1	В	24	ARG



Mol	Chain	Res	Type
1	В	47	MET
1	В	53	THR
1	В	204	ASN
1	В	205	GLU
1	В	241	ARG
1	В	267	ASP
1	С	6	ASP
1	С	24	ARG
1	С	47	MET
1	С	53	THR
1	С	63	VAL
1	С	117	ASP
1	С	153	ASP
1	С	183	SER
1	С	208	SER
1	С	237	VAL
1	С	242	GLU
1	С	266	ILE
1	С	283	LYS
1	С	335	GLU
1	С	341	ASP
1	С	349	LEU
1	D	6	ASP
1	D	11	MET
1	D	25	ARG
1	D	55	TYR
1	D	149	VAL
1	D	183	SER
1	D	340	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (17) such sidechains are listed below:

Mol	Chain	$\operatorname{Res}$	Type
1	А	50	HIS
1	А	82	ASN
1	А	203	HIS
1	А	263	GLN
1	В	82	ASN
1	В	203	HIS
1	В	263	GLN
1	С	50	HIS
1	С	82	ASN



Mol	Chain	Res	Type
1	С	203	HIS
1	С	263	GLN
1	С	320	HIS
1	D	50	HIS
1	D	82	ASN
1	D	158	ASN
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 monosaccharides 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).

Mal	Turne	pe Chain Res	Chain Res	Dec Link	Bond lengths			Bond angles		
INIOI	туре			I nes	nes		Counts	RMSZ	# Z >2	Counts
2	SO4	А	401	-	4,4,4	0.39	0	$6,\!6,\!6$	0.05	0
2	SO4	С	401	-	4,4,4	0.38	0	6,6,6	0.05	0
2	SO4	D	401	-	4,4,4	0.36	0	6,6,6	0.06	0
2	SO4	В	401	-	4,4,4	0.36	0	$6,\!6,\!6$	0.05	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 (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,  $95^{th}$  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	< <b>RSRZ</b> >	#RSRZ>2	$OWAB(Å^2)$	Q<0.9
1	А	342/371~(92%)	-0.27	1 (0%) 94 95	21, 40, 71, 102	0
1	В	347/371~(93%)	-0.26	5 (1%) 75 77	21, 35, 79, 105	0
1	С	356/371~(95%)	-0.35	2 (0%) 89 90	19, 32, 59, 109	1 (0%)
1	D	341/371~(91%)	-0.26	1 (0%) 94 95	24, 40, 87, 104	0
All	All	1386/1484~(93%)	-0.29	9 (0%) 89 90	19, 36, 75, 109	1 (0%)

All (9) RSRZ outliers are listed below:

Mol	Chain	$\mathbf{Res}$	Type	RSRZ
1	А	115	PHE	3.6
1	В	268	ILE	2.9
1	В	291	GLY	2.9
1	С	289	ILE	2.7
1	В	272	HIS	2.4
1	С	291	GLY	2.2
1	В	117	ASP	2.2
1	В	266	ILE	2.2
1	D	361	ALA	2.1

## 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,  $95^{th}$  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	$\mathbf{B} ext{-factors}(\mathrm{\AA}^2)$	Q<0.9
2	SO4	D	401	5/5	0.92	0.15	70,74,82,83	0
2	SO4	В	401	5/5	0.93	0.15	51,62,69,70	0
2	SO4	С	401	5/5	0.94	0.15	52,63,63,67	0
2	SO4	А	401	5/5	0.95	0.16	57,57,63,64	0

### 6.5 Other polymers (i)

There are no such residues in this entry.

