

Full wwPDB X-ray Structure Validation Report (i)

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PDB ID	:	6JHM
Title	:	Crystal structure of Flavin-dependent Monooxygenase HadA
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Deposited on	:	2019-02-18
Resolution	:	2.30 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
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 2.30 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	$egin{array}{c} { m Whole \ archive} \ (\#{ m Entries}) \end{array}$	${f Similar\ resolution}\ (\#{ m Entries,\ resolution\ range}({ m \AA}))$
R_{free}	130704	5042(2.30-2.30)
Clashscore	141614	5643 (2.30-2.30)
Ramachandran outliers	138981	5575(2.30-2.30)
Sidechain outliers	138945	5575 (2.30-2.30)
RSRZ outliers	127900	4938 (2.30-2.30)

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	517	% 	13%	•••		
1	В	517	4%	14%	• 5%		
1	С	517	2% 8 0%	14%	• 5%		
1	D	517	5%	15% •	10%		



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2 Entry composition (i)

There are 2 unique types of molecules in this entry. The entry contains 16409 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	Λ	404	Total	С	Ν	0	\mathbf{S}	0	0	0
	A	494	3953	2509	715	713	16	0		0
1	Р	401	Total	С	Ν	0	S	0	0	0
1	D	491	3924	2493	708	707	16	0	0	0
1	C	480	Total	С	Ν	0	S	0	0	0
1			3911	2485	706	704	16	0	0	0
1	Л	467	Total	С	Ν	0	S	0	0	0
	407	3751	2387	677	672	15	0	U	U	

• Molecule 1 is a protein called Chlorophenol monooxygenase.

• Molecule 2 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	А	271	Total O 271 271	0	0
2	В	218	Total O 218 218	0	0
2	С	227	Total O 227 227	0	0
2	D	154	Total O 154 154	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: Chlorophenol monooxygenase



R409 C204 P414 C204 P415 C204 P414 P22 R421 P222 R421 P222 R417 P222 R417 P223 R417 P223 R417 P223 R41 P223 R41 P223 R41 P223 R415 P224 R415 P223 R415 P224 R415 P223 R415 P223 R415 P223 R416 P223 R415 P223 R415 P223 R415 P321 R415 P321 R415 P323 R415 P321 R416 P321 R417 P321 R417 P321 R417 P321 R418 P321 R417 P331 R418

 \bullet Molecule 1: Chlorophenol monooxy genase





4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants	97.92Å 128.14Å 182.18Å	Depositor
a, b, c, α , β , γ	90.00° 90.00° 90.00°	Depositor
Bosolution(A)	20.69 - 2.30	Depositor
Resolution (A)	20.68 - 2.30	EDS
% Data completeness	99.7 (20.69-2.30)	Depositor
(in resolution range)	99.9 (20.68-2.30)	EDS
R_{merge}	0.12	Depositor
R _{sym}	(Not available)	Depositor
$< I/\sigma(I) > 1$	$2.58 (at 2.30 \text{\AA})$	Xtriage
Refinement program	REFMAC 5.8.0222	Depositor
P. P.	0.200 , 0.261	Depositor
n, n_{free}	0.200 , 0.257	DCC
R_{free} test set	5068 reflections (4.97%)	wwPDB-VP
Wilson B-factor $(Å^2)$	19.8	Xtriage
Anisotropy	0.617	Xtriage
Bulk solvent $k_{sol}(e/Å^3), B_{sol}(Å^2)$	0.34 , 37.7	EDS
L-test for $twinning^2$	$ < L >=0.50, < L^2>=0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	16409	wwPDB-VP
Average B, all atoms $(Å^2)$	24.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: The largest off-origin peak in the Patterson function is 3.62% of the height of the origin peak. No significant pseudotranslation is detected.

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.



¹Intensities estimated from amplitudes.

5 Model quality (i)

5.1 Standard geometry (i)

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		
	Unam	RMSZ	# Z > 5	RMSZ	# Z > 5	
1	А	0.64	0/4054	0.81	3/5494~(0.1%)	
1	В	0.61	0/4025	0.78	1/5456~(0.0%)	
1	С	0.61	0/4011	0.76	0/5435	
1	D	0.54	0/3850	0.71	0/5219	
All	All	0.60	0/15940	0.77	4/21604~(0.0%)	

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	8
1	С	0	8
1	D	0	4
All	All	0	29

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Ζ	$Observed(^{o})$	$\operatorname{Ideal}(^{o})$
1	А	367	ARG	NE-CZ-NH2	-6.11	117.24	120.30
1	А	367	ARG	NE-CZ-NH1	5.22	122.91	120.30
1	В	284	ARG	NE-CZ-NH1	-5.05	117.78	120.30
1	А	141	ARG	NE-CZ-NH1	5.03	122.82	120.30

There are no chirality outliers.

All (29) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	А	141	ARG	Sidechain
		<u> </u>		



Mol	Chain	Res	Type	Group
1	А	284	ARG	Sidechain
1	А	3	ARG	Sidechain
1	А	35	ARG	Sidechain
1	А	367	ARG	Sidechain
1	А	387	ARG	Sidechain
1	А	426	ARG	Sidechain
1	А	504	ARG	Sidechain
1	А	75	ARG	Sidechain
1	В	208	ARG	Sidechain
1	В	3	ARG	Sidechain
1	В	367	ARG	Sidechain
1	В	475	ARG	Sidechain
1	В	504	ARG	Sidechain
1	В	67	ARG	Sidechain
1	В	75	ARG	Sidechain
1	В	81	ARG	Sidechain
1	С	141	ARG	Sidechain
1	С	326	ARG	Sidechain
1	С	367	ARG	Sidechain
1	С	409	ARG	Sidechain
1	С	417	ARG	Sidechain
1	С	421	ARG	Sidechain
1	С	475	ARG	Sidechain
1	С	75	ARG	Sidechain
1	D	144	ARG	Sidechain
1	D	284	ARG	Sidechain
1	D	296	ARG	Sidechain
1	D	75	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	3953	0	3850	48	0
1	В	3924	0	3823	51	0
1	С	3911	0	3812	55	0
1	D	3751	0	3660	58	0
2	А	271	0	0	3	0



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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	В	218	0	0	3	0
2	С	227	0	0	7	0
2	D	154	0	0	3	0
All	All	16409	0	15145	192	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 (192) 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:342:ILE:HD13	1:B:347:LEU:HD11	1.51	0.89
1:C:342:ILE:HD13	1:D:347:LEU:HD11	1.58	0.85
1:A:157:PRO:HA	1:C:387:ARG:NH1	1.94	0.82
1:A:156:ASP:HB3	1:A:157:PRO:HD2	1.61	0.82
1:A:114:ILE:HD11	1:A:140:ILE:HG21	1.61	0.82
1:D:298:MET:HE2	1:D:338:LEU:HA	1.63	0.80
1:D:337:MET:HE2	1:D:370:TYR:HB2	1.66	0.78
1:C:109:VAL:HG22	1:C:285:VAL:O	1.84	0.77
1:C:337:MET:CE	1:C:370:TYR:HB2	2.18	0.73
1:A:157:PRO:HA	1:C:387:ARG:HH12	1.55	0.70
1:D:367:ARG:NH2	1:D:449:THR:O	2.26	0.69
1:C:337:MET:HE2	1:C:370:TYR:HB2	1.74	0.69
1:B:442:VAL:HG11	1:D:390:LEU:HD22	1.75	0.68
1:B:435:ASP:OD1	1:D:435:ASP:OD1	2.13	0.67
1:A:294:LEU:CD1	1:A:337:MET:HE3	2.24	0.66
1:B:254:ASP:HB2	1:D:391:ILE:HD11	1.78	0.66
1:C:481:ASP:OD1	1:C:481:ASP:C	2.35	0.65
1:B:57:MET:HE3	1:B:86:TYR:HE1	1.63	0.63
1:C:342:ILE:CD1	1:D:347:LEU:HD11	2.29	0.63
1:D:314:HIS:ND1	1:D:421:ARG:HD3	2.13	0.62
1:D:298:MET:CE	1:D:338:LEU:HA	2.30	0.61
1:A:393:ALA:HB2	1:A:407:PHE:CE1	2.36	0.60
1:A:417:ARG:HG2	1:A:418:PRO:HD2	1.84	0.60
1:A:177:GLU:HB2	1:A:184:VAL:HB	1.81	0.60
1:A:114:ILE:HD11	1:A:140:ILE:CG2	2.31	0.60
1:B:174:ARG:CZ	1:B:215:GLN:HE21	2.15	0.60
1:C:501:ASP:HB3	1:C:504:ARG:HB3	1.83	0.60
1:B:294:LEU:HD12	1:B:337:MET:CE	2.32	0.59
1:A:454:ILE:O	1:A:458:THR:OG1	2.20	0.59
1:A:156:ASP:HB3	1:A:157:PRO:CD	2.33	0.59



		Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
1:B:17:ASN:OD1	1:B:24:LYS:NZ	2.36	0.59
1:B:453:GLY:O	1:B:457:LEU:HG	2.02	0.59
1:B:442:VAL:CG1	1:D:390:LEU:HD22	2.33	0.58
1:D:230:ILE:HD13	1:D:257:THR:HG23	1.84	0.58
1:A:71:TRP:CG	1:A:144:ARG:HG3	2.39	0.58
1:D:440:LEU:HD21	2:D:739:HOH:O	2.04	0.58
1:A:294:LEU:CD1	1:A:337:MET:CE	2.81	0.58
1:C:297:GLN:HB3	1:C:337:MET:HE2	1.86	0.58
1:A:439:ARG:HH11	1:A:440:LEU:HD12	1.69	0.58
1:C:463:GLU:OE2	1:C:504:ARG:NH1	2.34	0.58
1:A:335:GLN:NE2	1:B:470:TYR:OH	2.29	0.58
1:A:463:GLU:HB2	1:A:511:LEU:HD22	1.85	0.58
1:D:337:MET:CE	1:D:370:TYR:HB2	2.32	0.57
1:A:435:ASP:OD1	1:C:435:ASP:OD1	2.22	0.57
1:A:461:ARG:HD2	1:A:504:ARG:NH1	2.19	0.57
1:A:254:ASP:HB2	1:C:391:ILE:HD11	1.87	0.56
1:B:314:HIS:ND1	1:B:421:ARG:HD3	2.20	0.56
1:A:223:VAL:HG13	1:A:230:ILE:HD11	1.86	0.56
1:B:57:MET:HE3	1:B:86:TYR:CE1	2.40	0.56
1:B:254:ASP:HB2	1:D:391:ILE:CD1	2.34	0.56
1:B:415:VAL:HG23	1:B:415:VAL:O	2.05	0.56
1:B:385:SER:OG	1:B:389:ALA:HB2	2.05	0.56
1:D:213:GLY:O	1:D:273:GLY:HA2	2.06	0.56
1:C:347:LEU:HD11	1:D:342:ILE:CD1	2.36	0.55
1:C:135:LYS:NZ	2:C:606:HOH:O	2.39	0.55
1:C:429:ARG:NH1	2:C:607:HOH:O	2.39	0.55
1:D:84:ARG:CD	1:D:341:LEU:HD21	2.36	0.55
1:B:201:ILE:HG22	1:B:203:ILE:HD13	1.88	0.55
1:D:361:LEU:HD11	1:D:464:PHE:CZ	2.41	0.55
1:A:463:GLU:HG3	1:A:511:LEU:HD22	1.88	0.55
1:C:19:TRP:CD1	1:C:24:LYS:HE3	2.42	0.55
1:D:296:ARG:NH1	1:D:444:GLU:OE1	2.37	0.54
1:D:393:ALA:HB2	1:D:407:PHE:CE1	2.43	0.54
1:C:236:LEU:HB2	1:C:251:ASP:OD2	2.07	0.54
1:D:438:SER:O	1:D:441:PHE:HB3	2.08	0.54
1:B:174:ARG:NH2	1:B:215:GLN:HE21	2.06	0.53
1:A:298:MET:SD	1:A:338:LEU:HD13	2.49	0.53
1:D:236:LEU:HD13	1:D:435:ASP:HB3	1.91	0.53
1:B:156:ASP:HB3	1:B:157:PRO:HD2	1.92	0.52
1:A:463:GLU:HB2	1:A:511:LEU:CD2	2.39	0.52
1:B:397:GLN:NE2	1:D:21:GLY:O	2.43	0.52



		Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
1:C:117:PRO:HB2	1:C:133:ALA:HB1	1.92	0.52
1:A:254:ASP:C	1:C:391:ILE:HD11	2.31	0.51
1:B:318:ASN:HD22	1:B:318:ASN:H	1.58	0.51
1:D:61:ASP:OD1	1:D:65:GLN:N	2.43	0.51
1:A:136:ILE:HG12	1:A:270:PHE:CD1	2.46	0.51
1:C:461:ARG:HD2	1:C:504:ARG:NH1	2.25	0.51
1:D:281:TYR:N	1:D:282:PRO:CD	2.74	0.51
1:C:105:VAL:HG22	1:C:292:HIS:CE1	2.45	0.51
1:C:456:MET:CE	2:C:675:HOH:O	2.59	0.51
1:D:59:TYR:CE1	1:D:67:ARG:HB3	2.45	0.51
1:D:390:LEU:HD23	1:D:390:LEU:H	1.75	0.51
1:C:71:TRP:CG	1:C:144:ARG:HG3	2.46	0.51
1:A:114:ILE:CD1	1:A:140:ILE:HG21	2.39	0.51
1:C:156:ASP:C	2:C:813:HOH:O	2.49	0.50
1:D:361:LEU:HD21	1:D:464:PHE:HZ	1.75	0.50
1:B:294:LEU:CD1	1:B:337:MET:CE	2.89	0.50
1:D:91:MET:HE1	1:D:296:ARG:HB2	1.92	0.50
1:D:109:VAL:HG22	1:D:285:VAL:O	2.11	0.50
1:A:443:PHE:CE2	1:A:447:ASN:HB2	2.47	0.50
1:B:84:ARG:HD2	1:B:341:LEU:HD21	1.93	0.50
1:A:360:ILE:HA	1:A:363:TYR:CE2	2.47	0.49
1:D:84:ARG:HD3	1:D:341:LEU:HD21	1.94	0.49
1:D:236:LEU:HD13	1:D:435:ASP:CB	2.42	0.49
1:B:294:LEU:HD12	1:B:337:MET:HE3	1.95	0.49
1:D:298:MET:HE2	1:D:338:LEU:CA	2.36	0.49
1:C:466:GLY:O	1:C:475:ARG:NH1	2.45	0.49
1:D:109:VAL:HG13	1:D:285:VAL:CG1	2.43	0.49
1:C:309:VAL:O	1:C:313:GLU:HB2	2.12	0.49
1:C:347:LEU:HD11	1:D:342:ILE:HD12	1.95	0.48
1:D:390:LEU:HG	1:D:391:ILE:N	2.28	0.48
1:A:318:ASN:HD22	1:A:318:ASN:H	1.62	0.48
1:C:321:PRO:O	1:C:325:THR:HG23	2.13	0.48
1:D:17:ASN:OD1	1:D:24:LYS:NZ	2.43	0.48
1:B:360:ILE:HA	1:B:363:TYR:CE2	2.48	0.47
1:C:342:ILE:HD13	1:D:347:LEU:CD1	2.38	0.47
1:D:109:VAL:HG13	1:D:285:VAL:HG13	1.95	0.47
1:A:254:ASP:OD2	1:C:390:LEU:HD21	2.15	0.47
1:B:71:TRP:CG	1:B:144:ARG:HG3	2.48	0.47
1:B:84:ARG:CD	1:B:341:LEU:HD21	2.44	0.47
1:B:100:PRO:HB3	1:B:296:ARG:NE	2.30	0.47
1:C:2:ILE:HG22	2:C:721:HOH:O	2.15	0.47



		Interatomic	Clash
Atom-1	Atom-2	distance (\AA)	overlap (Å)
1:B:109:VAL:HG22	1:B:285:VAL:O	2.15	0.46
2:A:779:HOH:O	1:B:329:LYS:HG3	2.15	0.46
1:C:200:TRP:CZ3	1:C:222:PRO:HD3	2.50	0.46
1:C:84:ARG:HD2	1:C:341:LEU:HD21	1.97	0.46
1:D:84:ARG:HD2	1:D:341:LEU:HD21	1.97	0.46
1:B:105:VAL:HG22	1:B:292:HIS:CE1	2.51	0.46
1:B:20:VAL:HG23	1:B:25:ILE:HG13	1.97	0.46
1:D:360:ILE:HA	1:D:363:TYR:CE2	2.51	0.46
1:B:180:GLU:HB2	2:B:785:HOH:O	2.16	0.45
1:B:294:LEU:CD1	1:B:337:MET:HE1	2.45	0.45
1:C:84:ARG:CD	1:C:341:LEU:HD21	2.46	0.45
1:B:91:MET:HB2	1:B:97:ALA:HA	1.98	0.45
1:A:294:LEU:HD12	1:A:337:MET:CE	2.45	0.45
1:C:2:ILE:CG2	2:C:721:HOH:O	2.64	0.45
1:B:174:ARG:NH2	1:B:215:GLN:NE2	2.64	0.45
1:A:315:ILE:HG22	1:A:317:THR:HG23	1.99	0.45
1:B:440:LEU:O	1:B:441:PHE:C	2.54	0.45
1:B:463:GLU:HG3	1:B:511:LEU:HD22	1.99	0.45
1:C:236:LEU:HG	1:C:435:ASP:HB2	1.99	0.45
1:B:281:TYR:N	1:B:282:PRO:CD	2.80	0.45
1:D:23:GLU:OE1	2:D:601:HOH:O	2.21	0.44
1:B:53:LEU:HB3	1:B:57:MET:HG2	1.98	0.44
1:C:154:PHE:CE1	1:C:204:GLY:HA3	2.53	0.44
1:C:351:THR:HB	1:C:352:PRO:HD2	2.00	0.44
1:A:290:HIS:CE1	1:A:449:THR:HG23	2.53	0.44
1:D:60:ILE:HD11	1:D:66:ARG:NH2	2.32	0.44
1:D:273:GLY:O	1:D:275:PRO:HD3	2.18	0.44
1:A:20:VAL:HB	1:A:25:ILE:HD11	2.00	0.44
1:D:200:TRP:CZ3	1:D:222:PRO:HD3	2.53	0.44
1:B:83:LYS:O	1:B:86:TYR:HB3	2.17	0.43
1:D:85:LYS:HA	2:D:646:HOH:O	2.18	0.43
1:C:19:TRP:CE2	1:C:24:LYS:HE3	2.54	0.43
1:C:19:TRP:NE1	1:C:24:LYS:HE3	2.32	0.43
1:B:507:GLU:O	2:B:601:HOH:O	2.21	0.43
1:A:84:ARG:HD2	1:A:341:LEU:HD21	2.00	0.43
1:B:71:TRP:CE2	1:B:144:ARG:HA	2.54	0.43
1:D:361:LEU:HD11	1:D:464:PHE:HZ	1.82	0.43
1:A:455:ARG:O	1:A:459:MET:HG2	2.18	0.43
1:B:118:ALA:HB3	1:B:119:PRO:HD3	2.01	0.43
1:D:455:ARG:O	1:D:459:MET:HG2	2.18	0.43
1:C:208:ARG:NH1	2:C:622:HOH:O	2.51	0.43



		Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
1:C:463:GLU:CD	1:C:504:ARG:HH12	2.19	0.43
1:C:451:LEU:HD11	1:C:455:ARG:CZ	2.49	0.42
1:D:390:LEU:HG	1:D:391:ILE:HD13	2.01	0.42
1:A:194:GLY:HA3	2:A:628:HOH:O	2.19	0.42
1:B:297:GLN:HB3	1:B:337:MET:HE2	2.01	0.42
1:C:154:PHE:CD1	1:C:204:GLY:HA3	2.53	0.42
1:A:397:GLN:NE2	1:C:21:GLY:O	2.50	0.42
1:C:141:ARG:HH21	1:C:144:ARG:HH22	1.66	0.42
1:D:457:LEU:HD12	1:D:457:LEU:C	2.39	0.42
1:B:69:MET:HB2	1:B:86:TYR:CD1	2.55	0.42
1:B:501:ASP:HB3	1:B:504:ARG:HB3	2.00	0.42
1:D:118:ALA:HB3	1:D:119:PRO:HD3	2.00	0.42
1:A:84:ARG:CD	1:A:341:LEU:HD21	2.50	0.42
1:C:293:ALA:O	1:C:297:GLN:HG3	2.19	0.42
1:C:338:LEU:HG	1:C:342:ILE:HD12	2.01	0.42
1:D:351:THR:HB	1:D:352:PRO:HD2	2.01	0.42
1:B:350:HIS:HA	1:B:355:HIS:O	2.20	0.41
1:B:417:ARG:HG2	1:B:418:PRO:HD2	2.02	0.41
1:C:137:VAL:O	1:C:141:ARG:HG2	2.19	0.41
1:C:393:ALA:HB2	1:C:407:PHE:CE1	2.55	0.41
1:C:464:PHE:CZ	1:C:511:LEU:HD13	2.54	0.41
1:A:300:ARG:NH1	2:A:613:HOH:O	2.44	0.41
1:D:203:ILE:HD11	1:D:259:PHE:CZ	2.55	0.41
1:A:205:VAL:HG11	1:A:216:VAL:HA	2.02	0.41
1:D:318:ASN:H	1:D:318:ASN:HD22	1.67	0.41
1:A:153:GLN:O	1:A:189:LYS:HE2	2.20	0.41
1:D:290:HIS:O	1:D:293:ALA:HB3	2.20	0.41
1:C:469:PRO:HB2	1:C:515:MET:HG2	2.03	0.41
1:A:360:ILE:HA	1:A:363:TYR:CZ	2.55	0.41
1:B:294:LEU:CD1	1:B:337:MET:HE3	2.51	0.41
1:C:311:ILE:HD12	1:C:311:ILE:HA	1.96	0.41
1:A:448:GLY:O	1:A:449:THR:C	2.59	0.41
1:D:3:ARG:HB2	1:D:147:ASP:HB2	2.03	0.41
1:A:329:LYS:HD3	2:B:690:HOH:O	2.21	0.40
1:A:473:LEU:O	1:A:477:VAL:HG23	2.21	0.40
1:A:458:THR:HG22	1:A:464:PHE:CE2	2.56	0.40
1:B:515:MET:HE3	1:B:515:MET:HB2	1.93	0.40
1:D:139:PHE:O	1:D:142:TYR:HB3	2.21	0.40
1:C:24:LYS:HE2	1:C:24:LYS:HA	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	ntiles
1	А	488/517~(94%)	476 (98%)	12 (2%)	0	100	100
1	В	485/517~(94%)	477~(98%)	8 (2%)	0	100	100
1	С	483/517~(93%)	473~(98%)	10 (2%)	0	100	100
1	D	463/517~(90%)	454 (98%)	9~(2%)	0	100	100
All	All	1919/2068~(93%)	1880 (98%)	39~(2%)	0	100	100

There are no Ramachandran outliers to report.

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	412/432~(95%)	384~(93%)	28 (7%)	16 21
1	В	409/432~(95%)	391~(96%)	18 (4%)	28 39
1	С	407/432~(94%)	393~(97%)	14 (3%)	37 51
1	D	394/432~(91%)	368~(93%)	26~(7%)	16 22
All	All	1622/1728~(94%)	1536 (95%)	86 (5%)	22 31

All (86) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	А	54	GLN
1	А	62	GLU



Mol	Chain	Res	Type
1	А	75	ARG
1	А	78	GLU
1	А	91	MET
1	А	109	VAL
1	А	168	GLU
1	А	208	ARG
1	А	284	ARG
1	А	318	ASN
1	А	329	LYS
1	А	363	TYR
1	А	376	GLN
1	А	387	ARG
1	А	417	ARG
1	А	435	ASP
1	А	439	ARG
1	А	440	LEU
1	А	441	PHE
1	А	449	THR
1	А	452	GLN
1	А	456	MET
1	А	458	THR
1	А	460	GLN
1	А	476	GLN
1	А	481	ASP
1	А	498	LYS
1	А	504	ARG
1	В	10	GLU
1	В	78	GLU
1	В	81	ARG
1	В	91	MET
1	В	108	TYR
1	В	109	VAL
1	В	114	ILE
1	В	241	LYS
1	В	284	ARG
1	В	318	ASN
1	В	330	LEU
1	В	421	ARG
1	В	435	ASP
1	В	452	GLN
1	В	476	GLN
1	В	481	ASP



Mol	Chain	Res	Type
1	В	495	ASP
1	В	515	MET
1	С	47	LEU
1	С	82	ARG
1	С	108	TYR
1	С	109	VAL
1	С	114	ILE
1	С	177	GLU
1	С	234	GLU
1	С	236	LEU
1	С	241	LYS
1	С	284	ARG
1	С	401	ASP
1	С	415	VAL
1	С	435	ASP
1	С	481	ASP
1	D	13	ASN
1	D	47	LEU
1	D	67	ARG
1	D	82	ARG
1	D	91	MET
1	D	108	TYR
1	D	128	ASP
1	D	141	ARG
1	D	181	LYS
1	D	203	ILE
1	D	205	VAL
1	D	208	ARG
1	D	239	ASP
1	D	284	ARG
1	D	289	LEU
1	D	318	ASN
1	D	330	LEU
1	D	352	PRO
1	D	387	ARG
1	D	402	LYS
1	D	417	ARG
1	D	421	ARG
1	D	435	ASP
1	D	452	GLN
1	D	460	GLN
1	D	481	ASP

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Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (23) such sidechains are listed below:

Mol	Chain	\mathbf{Res}	Type
1	А	13	ASN
1	А	54	GLN
1	А	130	HIS
1	А	283	GLN
1	А	318	ASN
1	А	335	GLN
1	А	376	GLN
1	А	445	ASN
1	А	505	HIS
1	В	13	ASN
1	В	215	GLN
1	В	271	HIS
1	В	318	ASN
1	В	324	GLN
1	С	13	ASN
1	С	318	ASN
1	С	324	GLN
1	С	445	ASN
1	С	460	GLN
1	D	7	GLN
1	D	31	HIS
1	D	318	ASN
1	D	376	GLN

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)

There are no ligands in this entry.

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	<RSRZ $>$	#RSRZ>2	$OWAB(Å^2)$	Q<0.9
1	А	494/517~(95%)	-0.39	7 (1%) 75 80	6, 16, 39, 83	0
1	В	491/517~(94%)	-0.17	19 (3%) 39 46	9, 19, 58, 119	0
1	С	489/517~(94%)	-0.27	9 (1%) 68 74	9, 19, 43, 81	0
1	D	467/517~(90%)	0.08	24 (5%) 28 35	11, 28, 64, 108	0
All	All	1941/2068~(93%)	-0.19	59 (3%) 50 57	6, 20, 54, 119	0

All (59) RSRZ outliers are listed below:

Mol	Chain	\mathbf{Res}	Type	RSRZ
1	В	497	ALA	9.6
1	D	1	MET	8.8
1	D	460	GLN	7.2
1	В	498	LYS	5.6
1	D	416	GLY	5.4
1	В	500	LEU	5.3
1	В	495	ASP	4.7
1	D	62	GLU	4.3
1	В	499	ALA	4.1
1	С	498	LYS	4.0
1	А	157	PRO	3.9
1	В	415	VAL	3.8
1	D	210	GLY	3.7
1	В	516	ALA	3.6
1	D	217	ILE	3.4
1	А	481	ASP	3.4
1	D	449	THR	3.3
1	В	481	ASP	3.3
1	В	446	PHE	3.0
1	С	390	LEU	3.0
1	В	416	GLY	3.0



Mol	Chain	Res	Type	RSRZ
1	С	500	LEU	3.0
1	С	1	MET	2.9
1	D	452	GLN	2.9
1	D	462	ALA	2.9
1	С	495	ASP	2.9
1	А	390	LEU	2.8
1	D	128	ASP	2.7
1	С	467	SER	2.7
1	А	62	GLU	2.7
1	D	451	LEU	2.7
1	D	390	LEU	2.6
1	В	157	PRO	2.6
1	А	1	MET	2.6
1	D	446	PHE	2.5
1	В	126	GLY	2.5
1	D	219	ALA	2.5
1	D	415	VAL	2.4
1	D	461	ARG	2.4
1	В	417	ARG	2.4
1	В	441	PHE	2.4
1	D	181	LYS	2.3
1	D	481	ASP	2.3
1	С	481	ASP	2.3
1	D	55	ASP	2.3
1	В	1	MET	2.3
1	В	496	TYR	2.3
1	В	515	MET	2.3
1	D	417	ARG	2.2
1	В	390	LEU	2.2
1	D	467	SER	2.2
1	D	63	GLY	2.2
1	С	414	PRO	2.2
1	А	168	GLU	2.1
1	А	495	ASP	2.1
1	В	460	GLN	2.1
1	D	456	MET	2.1
1	D	441	PHE	2.0
1	С	460	GLN	2.0

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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)

There are no ligands in this entry.

6.5 Other polymers (i)

There are no such residues in this entry.

