Full wwPDB X-ray Structure Validation Report ⓘ

Jan 31, 2016 – 08:52 PM GMT

PDB ID	:	1MHZ
Title	:	METHANE MONOOXYGENASE HYDROXYLASE
Authors	:	Elango, N.; Radhakrishnan, R.; Froland, W.A.; Waller, B.J.; Earhart, C.A.; Lipscomb, J.D.; Ohlendorf, D.H.
Deposited on	:	1996-10-21
Resolution	:	2.70 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.
We welcome your comments at validation@mail.wwpdb.org
A user guide is available at
http://wwpdb.org/validation/2016/XrayValidationReportHelp
with specific help available everywhere you see the ⓘ symbol.

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

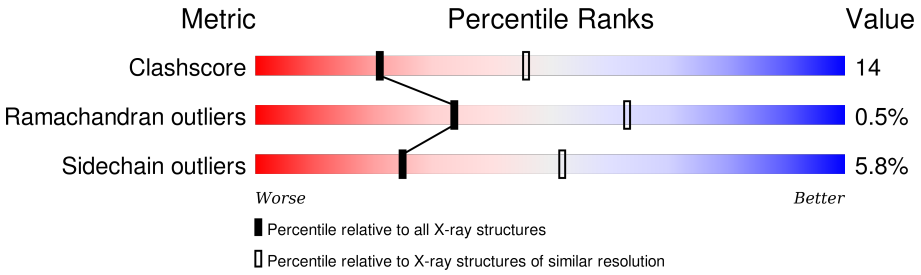
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	trunk26865

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.70 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))
Clashscore	102246	2422 (2.70-2.70)
Ramachandran outliers	100387	2382 (2.70-2.70)
Sidechain outliers	100360	2382 (2.70-2.70)

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 on the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=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.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	B	395	69% 26%
2	D	521	64% 31%
3	G	169	64% 33%

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 10542 atoms, of which 1939 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 METHANE MONOOXYGENASE HYDROXYLASE.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
			Total	C	H	N	O	S			
1	B	383	3808	1989	700	537	577	5	0	0	0

There are 27 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	255	TYR	MET	CONFLICT	UNP P27354
B	256	ASP	ILE	CONFLICT	UNP P27354
B	348	VAL	-	INSERTION	UNP P27354
B	349	ALA	SER	CONFLICT	UNP P27354
B	350	GLY	ARG	CONFLICT	UNP P27354
B	352	THR	ASP	CONFLICT	UNP P27354
B	353	ASP	ARG	CONFLICT	UNP P27354
B	?	-	ARG	DELETION	UNP P27354
B	?	-	ARG	DELETION	UNP P27354
B	?	-	ARG	DELETION	UNP P27354
B	?	-	LEU	DELETION	UNP P27354
B	?	-	ARG	DELETION	UNP P27354
B	?	-	GLY	DELETION	UNP P27354
B	356	GLY	ALA	CONFLICT	UNP P27354
B	357	VAL	ALA	CONFLICT	UNP P27354
B	359	GLU	SER	CONFLICT	UNP P27354
B	361	LEU	ILE	CONFLICT	UNP P27354
B	362	GLN	GLY	CONFLICT	UNP P27354
B	364	VAL	-	INSERTION	UNP P27354
B	365	PHE	-	INSERTION	UNP P27354
B	366	GLY	-	INSERTION	UNP P27354
B	367	ASP	-	INSERTION	UNP P27354
B	368	TRP	-	INSERTION	UNP P27354
B	369	LYS	SER	CONFLICT	UNP P27354
B	371	ASP	-	INSERTION	UNP P27354
B	372	TYR	THR	CONFLICT	UNP P27354
B	373	ALA	PRO	ENGINEERED INSERTION	UNP P27354

- Molecule 2 is a protein called METHANE MONOOXYGENASE HYDROXYLASE.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
2	D	510	Total	C	H	N	O	S	0	0	0
			5058	2649	920	720	757	12			

There are 14 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
D	?	-	ASP	DELETION	UNP P27353
D	?	-	ALA	DELETION	UNP P27353
D	?	-	LEU	DELETION	UNP P27353
D	?	-	LYS	DELETION	UNP P27353
D	?	-	VAL	DELETION	UNP P27353
D	37	TRP	ARG	CONFLICT	UNP P27353
D	195	GLY	ARG	CONFLICT	UNP P27353
D	209	GLU	ASP	CONFLICT	UNP P27353
D	210	ALA	THR	CONFLICT	UNP P27353
D	225	SER	ILE	CONFLICT	UNP P27353
D	226	ALA	GLY	CONFLICT	UNP P27353
D	329	PRO	-	INSERTION	UNP P27353
D	331	SER	VAL	CONFLICT	UNP P27353
D	357	GLY	ALA	CONFLICT	UNP P27353

- Molecule 3 is a protein called METHANE MONOOXYGENASE HYDROXYLASE.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
3	G	167	Total	C	H	N	O	S	0	0	0
			1662	868	311	230	252	1			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
G	88	ALA	ARG	CONFLICT	UNP P27355
G	109	GLU	ASP	CONFLICT	UNP P27355
G	110	ALA	GLY	CONFLICT	UNP P27355
G	160	ARG	PRO	CONFLICT	UNP P27355

- Molecule 4 is FE (III) ION (three-letter code: FE) (formula: Fe).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	D	2	Total	Fe	0	0
			2	2		

- Molecule 5 is water.

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	H	O		
5	D	4	12	8	4	0	0

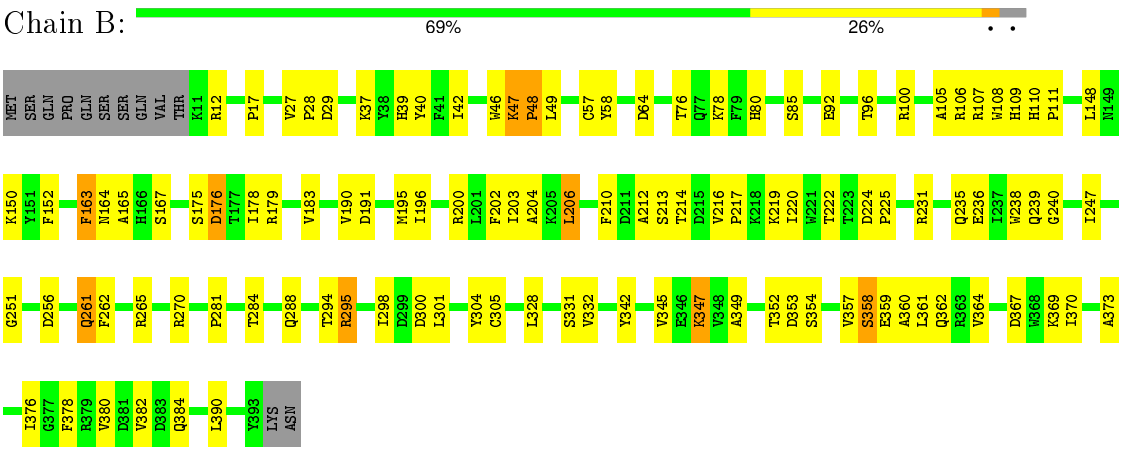
3 Residue-property plots (i)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density (RSRZ > 2). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

Note EDS was not executed.

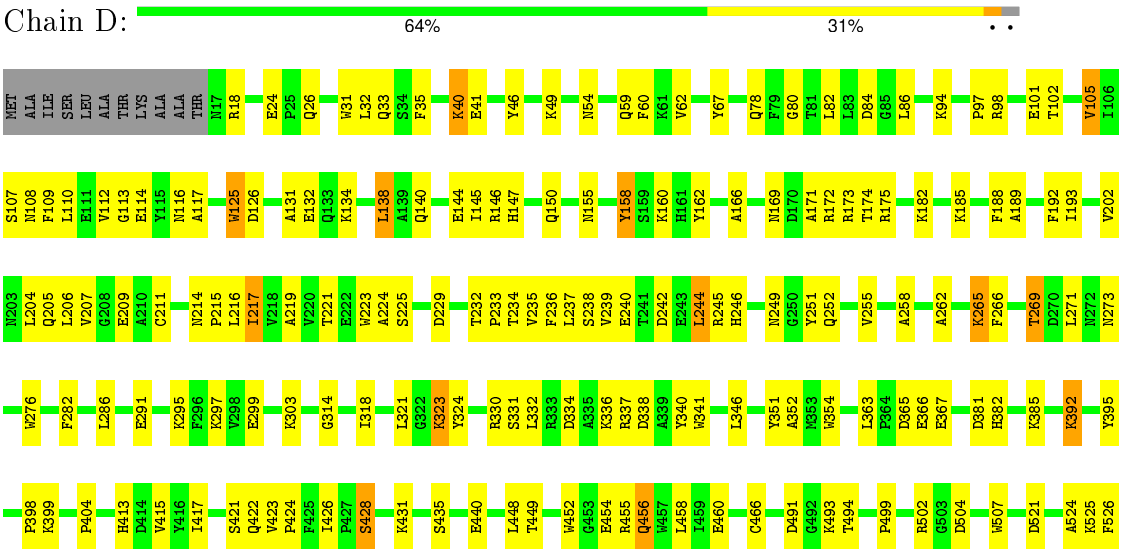
- Molecule 1: METHANE MONOOXYGENASE HYDROXYLASE

Chain B:



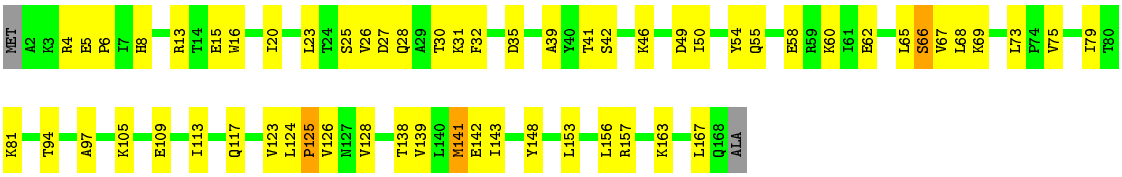
- Molecule 2: METHANE MONOOXYGENASE HYDROXYLASE

Chain D:



- Molecule 3: METHANE MONOOXYGENASE HYDROXYLASE

Chain G:


MET A2 K3 R4 E5 P6 I7 H8 R13 T14 E15 W16 I20 L23 T24 S25 V26 D27 Q28 A29 T30 K31 F32 D35 A39 Y40 T41 S42 K46 D49 I50 Y54 Q55 E58 R59 K60 I61 E62 L65 S66 V67 L68 K69 L73 P74 V75 I79 T80
K81 T94 A97 K105 E109 I113 Q117 V123 L124 P125 V126 N127 V128 T138 V139 L140 M141 E142 I143 Y148 L153 L156 R157 K163 L167 Q168 ALA

4 Data and refinement statistics (i)

Xtriage (Phenix) and EDS were not executed - this section will therefore be incomplete.

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α, β, γ	293.38Å 64.01Å 143.65Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	5.00 – 2.70	Depositor
% Data completeness (in resolution range)	89.3 (5.00-2.70)	Depositor
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	X-PLOR 3.1	Depositor
R, R_{free}	0.152 , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	10542	wwPDB-VP
Average B, all atoms (Å^2)	15.0	wwPDB-VP

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: FE

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	B	0.63	0/3201	0.75	0/4356
2	D	0.63	0/4267	0.78	2/5797 (0.0%)
3	G	0.63	0/1377	0.76	0/1863
All	All	0.63	0/8845	0.76	2/12016 (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
2	D	0	2

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	D	138	LEU	CA-CB-CG	5.75	128.52	115.30
2	D	346	LEU	CA-CB-CG	5.08	126.97	115.30

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	D	46	TYR	Sidechain
2	D	67	TYR	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	B	3108	700	2942	80	0
2	D	4138	920	3934	139	0
3	G	1351	311	1387	42	0
4	D	2	0	0	0	0
5	D	4	8	0	0	0
All	All	8603	1939	8263	241	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 14.

All (241) 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)
2:D:352:ALA:HA	2:D:404:PRO:HB2	1.58	0.85
2:D:109:PHE:O	2:D:112:VAL:HG12	1.81	0.80
2:D:244:LEU:HD13	2:D:245:ARG:H	1.46	0.80
2:D:244:LEU:HD13	2:D:245:ARG:N	1.98	0.79
2:D:334:ASP:HA	2:D:337:ARG:HE	1.49	0.78
2:D:224:ALA:HB1	2:D:229:ASP:HB3	1.68	0.74
2:D:107:SER:HB3	2:D:155:ASN:HD21	1.53	0.74
3:G:125:PRO:HB2	3:G:128:VAL:HG23	1.70	0.74
2:D:202:VAL:HA	2:D:206:LEU:HD13	1.70	0.74
2:D:421:SER:O	2:D:422:GLN:HB2	1.86	0.73
2:D:221:THR:HG22	2:D:233:PRO:HA	1.73	0.71
1:B:295:ARG:HG2	1:B:295:ARG:HH11	1.54	0.71
2:D:398:PRO:HG3	2:D:507:TRP:CD1	2.26	0.70
2:D:334:ASP:HA	2:D:337:ARG:NE	2.08	0.68
1:B:76:THR:HG22	2:D:466:CYS:SG	2.34	0.67
1:B:196:ILE:O	1:B:200:ARG:HG3	1.94	0.67
3:G:124:LEU:HD12	3:G:125:PRO:HD2	1.77	0.67
1:B:295:ARG:NH1	1:B:295:ARG:HG2	2.07	0.67
3:G:157:ARG:HH21	3:G:167:LEU:HD11	1.61	0.65
1:B:294:THR:O	1:B:298:ILE:HG12	1.98	0.64
1:B:92:GLU:OE1	3:G:126:VAL:HG23	1.97	0.64
2:D:525:LYS:HE2	2:D:526:PHE:CZ	2.33	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:60:PHE:CE2	2:D:245:ARG:HA	2.35	0.62
3:G:139:VAL:O	3:G:143:ILE:HG13	1.99	0.62
1:B:64:ASP:OD2	3:G:8:HIS:HD2	1.83	0.62
1:B:262:PHE:HD2	1:B:364:VAL:HG21	1.64	0.62
2:D:60:PHE:CZ	2:D:244:LEU:HD22	2.34	0.61
2:D:381:ASP:O	2:D:385:LYS:HD2	1.99	0.61
2:D:266:PHE:O	2:D:269:THR:HG22	2.01	0.61
1:B:47:LYS:HB3	1:B:48:PRO:HD3	1.83	0.60
3:G:113:ILE:O	3:G:117:GLN:HG3	2.00	0.60
1:B:110:HIS:HB3	1:B:111:PRO:HD3	1.82	0.60
2:D:202:VAL:HG11	2:D:271:LEU:HA	1.84	0.59
1:B:42:ILE:HD13	1:B:57:CYS:HB2	1.83	0.59
2:D:491:ASP:HB2	2:D:493:LYS:NZ	2.18	0.59
1:B:108:TRP:O	1:B:111:PRO:HD2	2.01	0.59
2:D:233:PRO:O	2:D:237:LEU:HG	2.03	0.58
3:G:25:SER:HB3	3:G:28:GLN:HB2	1.83	0.58
1:B:106:ARG:HG3	1:B:106:ARG:HH11	1.68	0.58
1:B:376:ILE:HD11	1:B:378:PHE:HB2	1.86	0.58
2:D:158:TYR:HD1	2:D:162:TYR:HB2	1.68	0.58
2:D:221:THR:CG2	2:D:233:PRO:HA	2.34	0.58
2:D:365:ASP:OD1	2:D:367:GLU:HG2	2.04	0.58
2:D:82:LEU:HD23	2:D:86:LEU:HD12	1.86	0.58
2:D:330:ARG:HG3	2:D:452:TRP:HH2	1.69	0.57
1:B:328:LEU:O	1:B:332:VAL:HG23	2.05	0.57
2:D:244:LEU:HD13	2:D:245:ARG:HG3	1.85	0.57
2:D:413:HIS:HD2	2:D:428:SER:HB2	1.69	0.57
3:G:16:TRP:O	3:G:20:ILE:HG13	2.04	0.57
3:G:26:VAL:HG11	3:G:73:LEU:HD11	1.86	0.56
2:D:251:TYR:CD1	2:D:321:LEU:HD21	2.40	0.56
2:D:354:TRP:CH2	2:D:499:PRO:HD3	2.41	0.56
2:D:171:ALA:HA	2:D:174:THR:OG1	2.07	0.55
2:D:59:GLN:NE2	2:D:252:GLN:HG2	2.21	0.55
1:B:236:GLU:O	1:B:240:GLY:HA3	2.06	0.55
2:D:192:PHE:CE1	2:D:204:LEU:HA	2.42	0.54
1:B:222:THR:HA	1:B:231:ARG:NE	2.23	0.54
1:B:281:PRO:HA	1:B:284:THR:OG1	2.08	0.54
1:B:347:LYS:CE	1:B:353:ASP:HB3	2.37	0.54
1:B:219:LYS:HB2	1:B:219:LYS:NZ	2.23	0.54
2:D:323:LYS:HG2	2:D:324:TYR:CD2	2.43	0.54
1:B:300:ASP:O	1:B:304:TYR:HB3	2.08	0.54
2:D:125:TRP:CD1	2:D:134:LYS:HB3	2.43	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:369:LYS:HA	1:B:373:ALA:HB3	1.89	0.53
1:B:191:ASP:O	1:B:195:MET:HG2	2.08	0.53
2:D:395:TYR:CE1	2:D:404:PRO:HG2	2.44	0.53
2:D:60:PHE:HE2	2:D:245:ARG:HA	1.73	0.53
3:G:125:PRO:HB2	3:G:128:VAL:CG2	2.38	0.53
1:B:261:GLN:HA	1:B:261:GLN:OE1	2.09	0.53
2:D:435:SER:O	2:D:449:THR:HA	2.08	0.53
1:B:148:LEU:O	1:B:152:PHE:HB3	2.08	0.53
2:D:147:HIS:CE1	2:D:239:VAL:HG13	2.43	0.53
2:D:232:THR:HB	2:D:233:PRO:HD3	1.92	0.52
2:D:521:ASP:OD2	2:D:524:ALA:HB2	2.09	0.52
2:D:276:TRP:CE3	2:D:331:SER:HB2	2.45	0.52
2:D:251:TYR:HD1	2:D:321:LEU:HD21	1.75	0.51
3:G:4:ARG:HH11	3:G:4:ARG:HG2	1.75	0.51
1:B:96:THR:HB	1:B:100:ARG:NH2	2.26	0.51
3:G:54:TYR:CE2	3:G:55:GLN:HG2	2.45	0.51
1:B:165:ALA:O	1:B:247:ILE:HG21	2.11	0.51
2:D:78:GLN:HE21	2:D:235:VAL:HA	1.75	0.51
2:D:49:LYS:HG2	3:G:142:GLU:HG3	1.93	0.51
3:G:79:ILE:N	3:G:79:ILE:HD12	2.25	0.51
2:D:273:ASN:ND2	2:D:456:GLN:HE21	2.09	0.51
2:D:382:HIS:CD2	2:D:431:LYS:HD2	2.46	0.51
3:G:8:HIS:HA	3:G:13:ARG:NH1	2.25	0.50
1:B:376:ILE:CD1	1:B:378:PHE:HB2	2.41	0.50
1:B:57:CYS:O	1:B:58:TYR:HB2	2.11	0.50
1:B:39:HIS:CE1	2:D:172:ARG:HB2	2.47	0.49
1:B:109:HIS:CE1	2:D:146:ARG:HB2	2.47	0.49
3:G:15:GLU:HG3	3:G:16:TRP:N	2.26	0.49
2:D:108:ASN:OD1	2:D:175:ARG:HD3	2.13	0.49
2:D:205:GLN:NE2	2:D:249:ASN:HB3	2.27	0.49
3:G:157:ARG:NH2	3:G:167:LEU:HD11	2.27	0.49
2:D:158:TYR:CD1	2:D:162:TYR:HB2	2.48	0.49
2:D:491:ASP:HB2	2:D:493:LYS:HZ2	1.77	0.49
3:G:69:LYS:HA	3:G:73:LEU:HD12	1.95	0.49
3:G:153:LEU:HB3	3:G:157:ARG:HH11	1.78	0.49
1:B:47:LYS:CB	1:B:48:PRO:HD3	2.42	0.49
1:B:150:LYS:HG2	1:B:216:VAL:HG11	1.94	0.49
2:D:244:LEU:CD1	2:D:245:ARG:HG3	2.43	0.49
2:D:216:LEU:HD13	2:D:286:LEU:HD13	1.94	0.49
2:D:395:TYR:HE1	2:D:404:PRO:HG2	1.78	0.49
1:B:150:LYS:HB3	1:B:220:ILE:HD12	1.95	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:98:ARG:NH1	2:D:295:LYS:HA	2.27	0.49
1:B:265:ARG:HB2	1:B:288:GLN:NE2	2.28	0.48
1:B:204:ALA:HB2	1:B:212:ALA:HB2	1.94	0.48
1:B:85:SER:HB3	2:D:193:ILE:HD11	1.96	0.48
1:B:203:ILE:HG21	1:B:210:PHE:CE2	2.48	0.48
2:D:219:ALA:O	2:D:223:TRP:HD1	1.96	0.48
2:D:80:GLY:O	2:D:84:ASP:HB3	2.14	0.48
2:D:32:LEU:O	2:D:35:PHE:HB2	2.13	0.48
2:D:40:LYS:HE2	2:D:41:GLU:HG3	1.96	0.48
3:G:153:LEU:HB3	3:G:157:ARG:NH1	2.29	0.48
2:D:330:ARG:HG3	2:D:452:TRP:CH2	2.49	0.48
2:D:33:GLN:HA	2:D:131:ALA:HB3	1.95	0.48
2:D:140:GLN:O	2:D:144:GLU:HG2	2.13	0.47
1:B:367:ASP:O	1:B:370:ILE:HG12	2.13	0.47
1:B:167:SER:HB2	2:D:126:ASP:HB2	1.96	0.47
3:G:105:LYS:O	3:G:109:GLU:HG2	2.14	0.47
3:G:5:GLU:HB3	3:G:6:PRO:CD	2.44	0.47
2:D:491:ASP:CG	2:D:493:LYS:HG2	2.35	0.47
2:D:102:THR:O	2:D:105:VAL:HG13	2.15	0.47
2:D:185:LYS:O	2:D:189:ALA:HB3	2.15	0.47
2:D:217:ILE:HG13	2:D:236:PHE:CD2	2.50	0.47
2:D:246:HIS:CD2	2:D:246:HIS:N	2.83	0.47
1:B:295:ARG:CG	1:B:295:ARG:HH11	2.22	0.47
2:D:82:LEU:HG	2:D:234:THR:HG21	1.96	0.47
3:G:41:THR:O	3:G:42:SER:OG	2.29	0.47
3:G:5:GLU:HB3	3:G:6:PRO:HD2	1.97	0.47
1:B:231:ARG:HG2	1:B:235:GLN:OE1	2.15	0.46
2:D:146:ARG:O	2:D:150:GLN:HG3	2.15	0.46
2:D:107:SER:HB3	2:D:155:ASN:ND2	2.26	0.46
2:D:235:VAL:O	2:D:238:SER:HB3	2.15	0.46
1:B:96:THR:HB	1:B:100:ARG:HH22	1.80	0.46
2:D:113:GLY:CA	2:D:188:PHE:HB3	2.45	0.46
1:B:213:SER:HB2	2:D:31:TRP:CZ3	2.51	0.46
1:B:64:ASP:CG	3:G:8:HIS:HD2	2.18	0.46
1:B:37:LYS:HB3	1:B:40:TYR:HB3	1.96	0.46
3:G:58:GLU:O	3:G:62:GLU:HG3	2.15	0.46
2:D:113:GLY:HA2	2:D:188:PHE:HB3	1.98	0.46
3:G:60:LYS:HE2	3:G:60:LYS:HA	1.98	0.46
1:B:163:PHE:CD1	1:B:190:VAL:HB	2.51	0.45
1:B:358:SER:OG	1:B:390:LEU:HD11	2.16	0.45
2:D:458:LEU:HD13	3:G:156:LEU:HB3	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:360:ALA:O	1:B:364:VAL:HG23	2.16	0.45
1:B:347:LYS:HA	1:B:352:THR:OG1	2.16	0.45
2:D:214:ASN:HB3	2:D:215:PRO:CD	2.47	0.45
1:B:179:ARG:O	1:B:183:VAL:HG23	2.17	0.45
2:D:502:ARG:NH1	2:D:504:ASP:OD1	2.50	0.45
1:B:239:GLN:HA	1:B:239:GLN:OE1	2.17	0.45
2:D:242:ASP:HA	2:D:245:ARG:HH12	1.82	0.44
3:G:66:SER:HA	3:G:69:LYS:HD3	2.00	0.44
2:D:392:LYS:HB3	2:D:392:LYS:NZ	2.32	0.44
2:D:160:LYS:HB3	2:D:160:LYS:NZ	2.32	0.44
2:D:24:GLU:HB3	2:D:26:GLN:OE1	2.18	0.44
1:B:76:THR:HA	2:D:466:CYS:HB2	1.98	0.44
1:B:176:ASP:O	1:B:179:ARG:HB3	2.18	0.44
2:D:303:LYS:HE2	2:D:303:LYS:HB3	1.86	0.44
2:D:351:TYR:CE2	2:D:363:LEU:HD23	2.53	0.44
1:B:347:LYS:HE3	1:B:353:ASP:HB3	1.99	0.44
1:B:301:LEU:O	1:B:305:CYS:HB2	2.17	0.44
2:D:318:ILE:HD13	2:D:318:ILE:HA	1.84	0.44
1:B:359:GLU:HA	1:B:362:GLN:HB2	2.00	0.44
2:D:314:GLY:O	2:D:318:ILE:HB	2.16	0.44
2:D:33:GLN:OE1	2:D:132:GLU:HB2	2.18	0.44
1:B:213:SER:HB2	2:D:31:TRP:CH2	2.52	0.44
1:B:214:THR:HA	1:B:217:PRO:HG2	1.99	0.44
3:G:124:LEU:HD12	3:G:125:PRO:CD	2.47	0.44
2:D:182:LYS:HB3	2:D:422:GLN:HG2	1.99	0.43
2:D:273:ASN:CG	2:D:456:GLN:HE21	2.22	0.43
2:D:413:HIS:HD2	2:D:428:SER:CB	2.31	0.43
2:D:49:LYS:HZ2	2:D:266:PHE:HB3	1.84	0.43
2:D:262:ALA:HA	2:D:265:LYS:HE3	2.01	0.43
1:B:164:ASN:HB3	1:B:238:TRP:CE2	2.53	0.43
2:D:363:LEU:HD11	2:D:395:TYR:CD2	2.52	0.43
2:D:202:VAL:HA	2:D:206:LEU:CD1	2.46	0.43
1:B:373:ALA:O	1:B:376:ILE:HG13	2.18	0.43
2:D:144:GLU:OE1	2:D:144:GLU:HA	2.19	0.43
2:D:440:GLU:HB3	3:G:163:LYS:HB3	1.99	0.43
2:D:49:LYS:HB2	2:D:49:LYS:HE3	1.75	0.43
2:D:59:GLN:HE21	2:D:252:GLN:HG2	1.83	0.43
2:D:166:ALA:HA	2:D:169:ASN:OD1	2.19	0.43
2:D:242:ASP:HA	2:D:245:ARG:NH1	2.33	0.43
1:B:76:THR:HB	2:D:422:GLN:NE2	2.33	0.43
1:B:353:ASP:O	1:B:357:VAL:HG23	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:399:LYS:HD2	2:D:399:LYS:HA	1.82	0.43
1:B:175:SER:HB3	1:B:178:ILE:HD12	2.00	0.43
1:B:109:HIS:HB2	2:D:145:ILE:HG22	2.00	0.42
2:D:417:ILE:HG23	2:D:422:GLN:O	2.19	0.42
2:D:205:GLN:HA	2:D:209:GLU:OE1	2.19	0.42
3:G:94:THR:O	3:G:97:ALA:HB3	2.18	0.42
2:D:125:TRP:HD1	2:D:134:LYS:HB3	1.82	0.42
2:D:223:TRP:CZ3	2:D:297:LYS:HA	2.55	0.42
2:D:116:ASN:CG	2:D:189:ALA:HA	2.40	0.42
3:G:65:LEU:O	3:G:68:LEU:HB2	2.19	0.42
3:G:138:THR:HA	3:G:141:MET:HE2	2.00	0.42
1:B:262:PHE:CE2	1:B:361:LEU:HD23	2.55	0.42
1:B:46:TRP:CH2	1:B:106:ARG:HG2	2.54	0.42
1:B:39:HIS:HE1	2:D:172:ARG:H	1.68	0.42
3:G:30:THR:HG23	3:G:123:VAL:HG22	2.00	0.42
2:D:255:VAL:HG22	2:D:324:TYR:CZ	2.54	0.42
2:D:209:GLU:O	2:D:214:ASN:HB2	2.19	0.42
2:D:291:GLU:O	2:D:297:LYS:HE3	2.20	0.42
2:D:40:LYS:O	2:D:40:LYS:HG2	2.20	0.42
1:B:202:PHE:O	1:B:206:LEU:HD13	2.19	0.42
1:B:342:TYR:O	1:B:345:VAL:HG22	2.20	0.42
1:B:27:VAL:HA	1:B:28:PRO:HD3	1.83	0.42
2:D:258:ALA:HB2	2:D:324:TYR:CD1	2.55	0.42
2:D:117:ALA:CB	2:D:144:GLU:HG3	2.50	0.42
1:B:214:THR:O	1:B:217:PRO:HG2	2.20	0.42
3:G:23:LEU:HD21	3:G:32:PHE:CD2	2.55	0.42
2:D:258:ALA:CB	2:D:324:TYR:HD1	2.32	0.41
2:D:273:ASN:HA	2:D:273:ASN:HD22	1.59	0.41
1:B:92:GLU:HG2	3:G:126:VAL:CG2	2.49	0.41
2:D:340:TYR:CD1	2:D:341:TRP:CE2	3.08	0.41
2:D:97:PRO:O	2:D:101:GLU:HG2	2.20	0.41
1:B:105:ALA:CB	1:B:107:ARG:HG3	2.50	0.41
3:G:153:LEU:HA	3:G:153:LEU:HD23	1.65	0.41
2:D:110:LEU:O	2:D:114:GLU:HG2	2.20	0.41
3:G:39:ALA:HA	3:G:46:LYS:HB2	2.02	0.41
2:D:258:ALA:HB2	2:D:324:TYR:HD1	1.84	0.41
2:D:415:VAL:HG22	2:D:426:ILE:HG12	2.02	0.41
2:D:244:LEU:HD13	2:D:245:ARG:CG	2.50	0.41
2:D:171:ALA:C	2:D:173:ARG:H	2.24	0.41
2:D:493:LYS:HG3	2:D:494:THR:N	2.35	0.41
1:B:294:THR:HG22	1:B:298:ILE:HG12	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:G:4:ARG:NH1	3:G:4:ARG:HG2	2.35	0.41
2:D:223:TRP:HZ2	2:D:299:GLU:O	2.04	0.41
1:B:224:ASP:HA	1:B:225:PRO:HD2	1.72	0.41
2:D:286:LEU:HA	2:D:286:LEU:HD23	1.97	0.41
2:D:98:ARG:HH11	2:D:295:LYS:HA	1.85	0.40
2:D:188:PHE:CE1	2:D:282:PHE:CE2	3.08	0.40
2:D:423:VAL:HA	2:D:424:PRO:HD3	1.87	0.40
1:B:12:ARG:HD2	1:B:12:ARG:HH11	1.72	0.40
1:B:80:HIS:CE1	2:D:460:GLU:HG2	2.56	0.40
1:B:96:THR:HG22	1:B:100:ARG:HH21	1.86	0.40
2:D:455:ARG:NH1	3:G:148:TYR:O	2.55	0.40
2:D:41:GLU:N	2:D:41:GLU:OE1	2.55	0.40
1:B:251:GLY:O	1:B:256:ASP:HB2	2.21	0.40
2:D:207:VAL:O	2:D:211:CYS:HB3	2.21	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	B	381/395 (96%)	348 (91%)	30 (8%)	3 (1%)	24 51
2	D	508/521 (98%)	469 (92%)	38 (8%)	1 (0%)	52 80
3	G	165/169 (98%)	155 (94%)	9 (6%)	1 (1%)	30 59
All	All	1054/1085 (97%)	972 (92%)	77 (7%)	5 (0%)	34 63

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	48	PRO
2	D	18	ARG
1	B	349	ALA

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Mol	Chain	Res	Type
3	G	50	ILE
1	B	382	VAL

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	B	315/327 (96%)	298 (95%)	17 (5%)	27	56
2	D	423/430 (98%)	399 (94%)	24 (6%)	25	53
3	G	144/145 (99%)	134 (93%)	10 (7%)	19	43
All	All	882/902 (98%)	831 (94%)	51 (6%)	25	52

All (51) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	17	PRO
1	B	29	ASP
1	B	47	LYS
1	B	49	LEU
1	B	78	LYS
1	B	163	PHE
1	B	176	ASP
1	B	206	LEU
1	B	261	GLN
1	B	270	ARG
1	B	295	ARG
1	B	331	SER
1	B	347	LYS
1	B	354	SER
1	B	358	SER
1	B	380	VAL
1	B	384	GLN
2	D	40	LYS
2	D	54	ASN
2	D	62	VAL

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Mol	Chain	Res	Type
2	D	94	LYS
2	D	105	VAL
2	D	125	TRP
2	D	138	LEU
2	D	158	TYR
2	D	217	ILE
2	D	225	SER
2	D	240	GLU
2	D	244	LEU
2	D	265	LYS
2	D	269	THR
2	D	323	LYS
2	D	332	LEU
2	D	336	LYS
2	D	338	ASP
2	D	366	GLU
2	D	392	LYS
2	D	428	SER
2	D	448	LEU
2	D	454	GLU
2	D	456	GLN
3	G	27	ASP
3	G	31	LYS
3	G	35	ASP
3	G	49	ASP
3	G	66	SER
3	G	67	VAL
3	G	75	VAL
3	G	81	LYS
3	G	125	PRO
3	G	141	MET

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (15) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	39	HIS
1	B	269	GLN
2	D	59	GLN
2	D	78	GLN
2	D	155	ASN
2	D	161	HIS
2	D	252	GLN

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Mol	Chain	Res	Type
2	D	273	ASN
2	D	343	HIS
2	D	344	HIS
2	D	388	ASN
2	D	413	HIS
2	D	422	GLN
2	D	456	GLN
3	G	8	HIS

5.3.3 RNA

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates

There are no carbohydrates in this entry.

5.6 Ligand geometry

Of 2 ligands modelled in this entry, 2 are monoatomic - leaving 0 for Mogul analysis.

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

EDS was not executed - this section will therefore be empty.

6.2 Non-standard residues in protein, DNA, RNA chains

EDS was not executed - this section will therefore be empty.

6.3 Carbohydrates

EDS was not executed - this section will therefore be empty.

6.4 Ligands

EDS was not executed - this section will therefore be empty.

6.5 Other polymers

EDS was not executed - this section will therefore be empty.