



# Full wwPDB X-ray Structure Validation Report

Feb 27, 2014 – 11:51 PM GMT

PDB ID : 3EOM  
Title : 2.4 Å crystal structure of native glutaryl-coa dehydrogenase from Burkholderia pseudomallei  
Authors : Seattle Structural Genomics Center for Infectious Disease (SSGCID)  
Deposited on : 2008-09-28  
Resolution : 2.40 Å(reported)

This is a full wwPDB validation report for a publicly released PDB entry.  
We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)  
A user guide is available at <http://wwpdb.org/ValidationPDFNotes.html>

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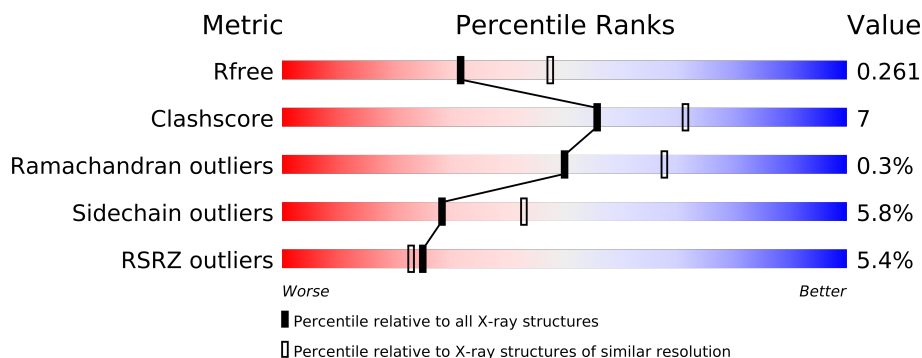
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467  
Mogul : 1.15 2013  
Xtriage (Phenix) : dev-1323  
EDS : stable22639  
Percentile statistics : 21963  
Refmac : 5.8.0049  
CCP4 : 6.3.0 (Settle)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)  
Validation Pipeline (wwPDB-VP) : stable22683

# 1 Overall quality at a glance

The reported resolution of this entry is 2.40 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))
$R_{free}$	66092	2207 (2.40-2.40)
Clashscore	79885	2789 (2.40-2.40)
Ramachandran outliers	78287	2736 (2.40-2.40)
Sidechain outliers	78261	2737 (2.40-2.40)
RSRZ outliers	66119	2210 (2.40-2.40)

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  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Mol	Chain	Length	Quality of chain
1	A	396	
1	B	396	
1	C	396	
1	D	396	

## 2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 11908 atoms, of which 0 are hydrogen and 0 are deuterium.

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 Glutaryl-CoA dehydrogenase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	387	Total	C	N	O	S	0	0	0
			2976	1881	525	554	16			
1	B	378	Total	C	N	O	S	0	0	0
			2909	1839	515	539	16			
1	C	381	Total	C	N	O	S	0	0	0
			2924	1846	517	545	16			
1	D	381	Total	C	N	O	S	0	0	0
			2932	1854	519	543	16			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	0	SER	-	EXPRESSION TAG	UNP Q3JP94
B	0	SER	-	EXPRESSION TAG	UNP Q3JP94
C	0	SER	-	EXPRESSION TAG	UNP Q3JP94
D	0	SER	-	EXPRESSION TAG	UNP Q3JP94

- Molecule 2 is water.

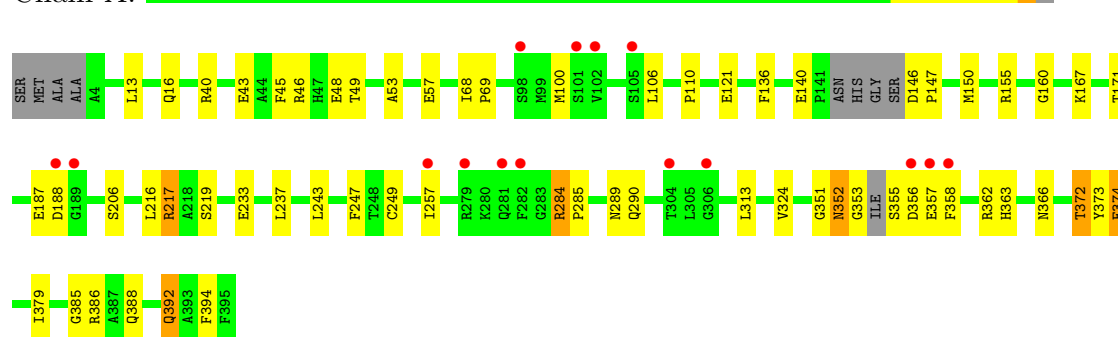
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	50	Total	O	0	0
			50	50		
2	B	34	Total	O	0	0
			34	34		
2	C	36	Total	O	0	0
			36	36		
2	D	47	Total	O	0	0
			47	47		

### 3 Residue-property plots

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.

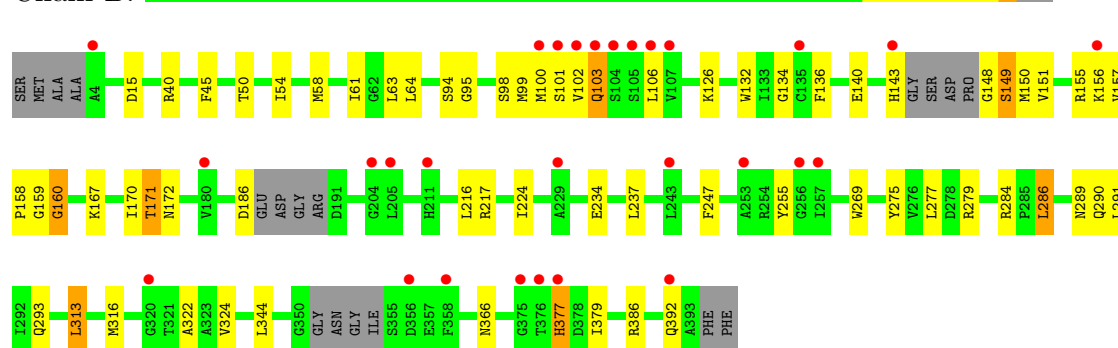
- Molecule 1: Glutaryl-CoA dehydrogenase

Chain A:



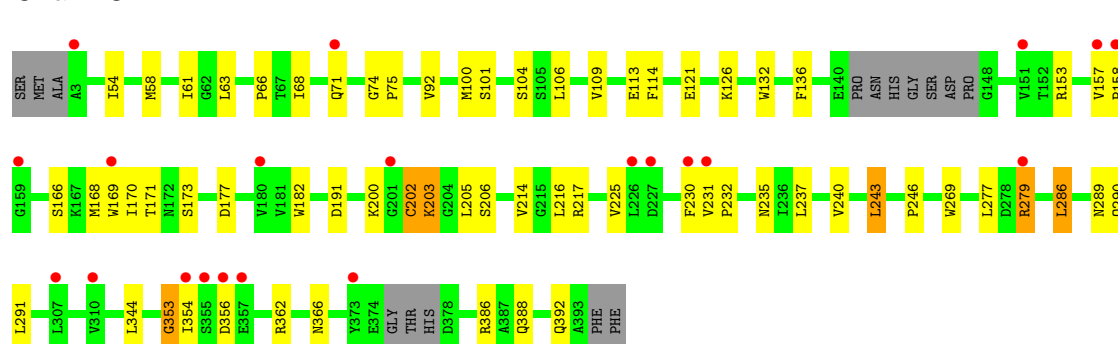
- Molecule 1: Glutaryl-CoA dehydrogenase

Chain B:



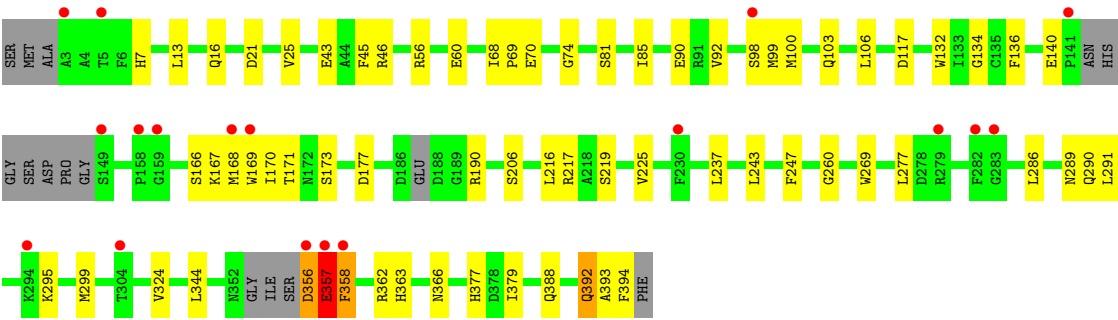
- Molecule 1: Glutaryl-CoA dehydrogenase

Chain C:



● Molecule 1: Glutaryl-CoA dehydrogenase

Chain D: 



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	98.11Å 106.77Å 145.43Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	30.00 – 2.40 29.21 – 2.40	Depositor EDS
% Data completeness (in resolution range)	99.3 (30.00-2.40) 99.3 (29.21-2.40)	Depositor EDS
$R_{merge}$	0.08	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.59 (at 2.39Å)	Xtriage
Refinement program	REFMAC 5.2	Depositor
R, $R_{free}$	0.211 , 0.264 0.210 , 0.261	Depositor DCC
$R_{free}$ test set	3035 reflections (5.32%)	DCC
Wilson B-factor (Å <sup>2</sup> )	53.2	Xtriage
Anisotropy	0.023	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.30 , 34.1	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtriage
Outliers	0 of 60090 reflections	Xtriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	11908	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	60.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.09% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

## 5 Model quality

### 5.1 Standard geometry

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	0.54	0/3034	0.63	0/4098
1	B	0.55	0/2964	0.62	0/4003
1	C	0.51	0/2977	0.66	1/4019 (0.0%)
1	D	0.54	0/2987	0.62	0/4033
All	All	0.53	0/11962	0.63	1/16153 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	353	GLY	N-CA-C	12.67	144.77	113.10

There are no chirality outliers.

There are no planarity outliers.

### 5.2 Close contacts

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 hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2976	0	2961	47	0
1	B	2909	0	2906	40	0
1	C	2924	0	2924	42	0
1	D	2932	0	2928	40	0
2	A	50	0	0	2	0
2	B	34	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	C	36	0	0	0	0
2	D	47	0	0	2	0
All	All	11908	0	11719	155	0

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 7.

All (155) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:355:SER:N	1:A:358:PHE:HD2	1.63	0.97
1:A:355:SER:N	1:A:358:PHE:CD2	2.38	0.92
1:A:146:ASP:HB3	1:A:147:PRO:HD3	1.55	0.86
1:A:290:GLN:HE22	1:D:289:ASN:HD21	1.26	0.83
1:B:377:HIS:CE1	1:B:379:ILE:HG22	2.15	0.82
1:A:355:SER:O	1:A:358:PHE:N	2.16	0.79
1:B:275:TYR:O	1:B:279:ARG:HG2	1.85	0.76
1:D:356:ASP:C	1:D:358:PHE:H	1.90	0.75
1:A:290:GLN:NE2	1:D:289:ASN:HD21	1.84	0.74
1:A:247:PHE:HZ	1:A:324:VAL:HG11	1.53	0.74
1:B:377:HIS:HE1	1:B:379:ILE:HG22	1.52	0.73
1:B:159:GLY:N	1:B:160:GLY:HA2	2.03	0.71
1:B:157:VAL:HB	1:B:158:PRO:HD2	1.70	0.71
1:B:140:GLU:OE2	1:B:150:MET:HB2	1.91	0.70
1:B:50:THR:HG21	1:B:99:MET:CE	2.22	0.70
1:B:103:GLN:HE22	1:B:134:GLY:H	1.39	0.70
1:D:43:GLU:OE2	1:D:46:ARG:NH1	2.25	0.69
1:D:216:LEU:H	1:D:366:ASN:HD22	1.38	0.68
1:B:279:ARG:HB2	1:B:286:LEU:HD22	1.75	0.67
1:A:290:GLN:HE22	1:D:289:ASN:ND2	1.92	0.67
1:A:353:GLY:C	1:A:355:SER:N	2.49	0.66
1:D:21:ASP:O	1:D:25:VAL:HG23	1.96	0.66
1:C:279:ARG:HB3	1:C:286:LEU:HD22	1.77	0.66
1:C:243:LEU:O	1:C:246:PRO:HD2	1.96	0.65
1:D:356:ASP:OD2	1:D:357:GLU:N	2.30	0.65
1:A:355:SER:O	1:A:357:GLU:N	2.30	0.64
1:A:247:PHE:HZ	1:A:324:VAL:CG1	2.09	0.64
1:A:355:SER:O	1:A:356:ASP:C	2.35	0.64
1:B:50:THR:HG21	1:B:99:MET:HE3	1.81	0.62
1:D:92:VAL:O	1:D:362:ARG:NH1	2.33	0.62
1:C:203:LYS:HE2	1:C:230:PHE:HB3	1.82	0.61
1:C:54:ILE:HG22	1:C:58:MET:CE	2.31	0.61
1:D:377:HIS:HD2	2:D:400:HOH:O	1.84	0.60

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:388:GLN:HE22	1:B:269:TRP:HE1	1.48	0.60
1:A:388:GLN:NE2	1:B:269:TRP:HE1	2.01	0.59
1:B:247:PHE:HZ	1:B:324:VAL:HG11	1.67	0.59
1:C:206:SER:HB2	1:C:225:VAL:HB	1.85	0.58
1:A:43:GLU:OE2	1:A:46:ARG:NH1	2.35	0.58
1:C:54:ILE:CG2	1:C:58:MET:HE2	2.33	0.58
1:D:216:LEU:H	1:D:366:ASN:ND2	2.02	0.58
1:A:13:LEU:HB3	1:A:16:GLN:HG3	1.86	0.58
1:D:99:MET:HE2	1:D:219:SER:HA	1.86	0.58
1:B:159:GLY:H	1:B:160:GLY:HA2	1.69	0.57
1:C:269:TRP:HE1	1:D:388:GLN:HE22	1.49	0.57
1:D:356:ASP:C	1:D:358:PHE:N	2.56	0.57
1:B:98:SER:O	1:B:102:VAL:HG23	2.05	0.56
1:D:7:HIS:CD2	1:D:13:LEU:HD21	2.41	0.56
1:A:362:ARG:NH1	2:A:420:HOH:O	2.34	0.56
1:D:393:ALA:O	1:D:394:PHE:HB2	2.06	0.56
1:C:353:GLY:C	1:C:354:ILE:HD12	2.27	0.55
1:C:54:ILE:HG22	1:C:58:MET:HE2	1.89	0.55
1:A:216:LEU:H	1:A:366:ASN:HD22	1.54	0.54
1:D:168:MET:HG3	1:D:169:TRP:CD1	2.43	0.54
1:A:216:LEU:H	1:A:366:ASN:ND2	2.05	0.54
1:B:40:ARG:HH21	1:B:54:ILE:HG12	1.72	0.54
1:C:388:GLN:HE22	1:D:269:TRP:HE1	1.55	0.54
1:A:187:GLU:O	1:A:188:ASP:C	2.45	0.54
1:A:257:ILE:CD1	1:A:374:GLU:HG3	2.38	0.53
1:B:45:PHE:O	1:B:217:ARG:NH2	2.41	0.53
1:C:354:ILE:O	1:C:354:ILE:CG2	2.57	0.53
1:D:206:SER:HB3	1:D:225:VAL:HB	1.90	0.53
1:A:363:HIS:HD2	2:A:399:HOH:O	1.92	0.52
1:D:81:SER:O	1:D:85:ILE:HG13	2.09	0.52
1:A:247:PHE:CZ	1:A:324:VAL:HG11	2.37	0.52
1:A:45:PHE:O	1:A:217:ARG:NH2	2.42	0.52
1:A:385:GLY:HA3	1:B:293:GLN:HB3	1.91	0.52
1:B:247:PHE:CZ	1:B:324:VAL:HG11	2.45	0.52
1:D:45:PHE:O	1:D:217:ARG:NH2	2.43	0.51
1:B:316:MET:HB3	1:B:322:ALA:HB2	1.92	0.51
1:C:386:ARG:HH11	1:C:392:GLN:HE21	1.59	0.51
1:A:140:GLU:OE1	1:A:150:MET:HG3	2.10	0.51
1:A:40:ARG:NH2	1:A:57:GLU:OE2	2.44	0.51
1:B:216:LEU:H	1:B:366:ASN:HD22	1.59	0.51
1:A:386:ARG:HG3	1:A:392:GLN:HA	1.92	0.51
1:D:103:GLN:OE1	1:D:134:GLY:N	2.29	0.51

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:D:140:GLU:HG2	1:D:166:SER:O	2.12	0.50
1:C:170:ILE:HG22	1:C:173:SER:HB3	1.93	0.50
1:B:149:SER:O	1:B:149:SER:OG	2.30	0.50
1:D:106:LEU:O	1:D:136:PHE:HD2	1.95	0.50
1:D:356:ASP:O	1:D:358:PHE:N	2.45	0.49
1:B:95:GLY:O	1:B:99:MET:HG3	2.12	0.49
1:C:354:ILE:HD12	1:C:354:ILE:N	2.28	0.49
1:D:392:GLN:OE1	1:D:394:PHE:HA	2.13	0.48
1:A:353:GLY:HA2	1:C:214:VAL:HG23	1.95	0.48
1:B:106:LEU:HB3	1:B:136:PHE:CG	2.49	0.48
1:C:114:PHE:CD1	1:C:240:VAL:HB	2.48	0.48
1:B:50:THR:HG21	1:B:99:MET:HE1	1.95	0.48
1:C:61:ILE:HG13	1:C:63:LEU:HG	1.94	0.48
1:B:64:LEU:HD22	1:B:103:GLN:HG2	1.96	0.48
1:A:140:GLU:HG2	1:A:167:LYS:HD3	1.96	0.48
1:C:168:MET:HG3	1:C:169:TRP:CD1	2.49	0.48
1:C:66:PRO:HA	1:C:75:PRO:HG2	1.95	0.48
1:C:177:ASP:HA	1:C:200:LYS:HB2	1.96	0.47
1:B:126:LYS:HD2	1:B:132:TRP:CE2	2.50	0.47
1:A:372:THR:HG22	1:A:373:TYR:CD1	2.50	0.47
1:A:160:GLY:HA2	1:A:233:GLU:HG2	1.97	0.47
1:D:356:ASP:C	1:D:356:ASP:OD2	2.53	0.47
1:C:153:ARG:NH1	1:C:191:ASP:OD1	2.47	0.47
1:C:216:LEU:H	1:C:366:ASN:HD22	1.61	0.47
1:C:104:SER:O	1:C:109:VAL:HG23	2.14	0.46
1:B:61:ILE:HG13	1:B:63:LEU:HG	1.96	0.46
1:D:295:LYS:O	1:D:299:MET:HG3	2.16	0.46
1:C:54:ILE:HG22	1:C:58:MET:HE3	1.96	0.46
1:B:216:LEU:H	1:B:366:ASN:ND2	2.14	0.46
1:A:146:ASP:HB3	1:A:147:PRO:CD	2.38	0.45
1:B:157:VAL:HB	1:B:158:PRO:CD	2.44	0.45
1:C:170:ILE:CG2	1:C:173:SER:HB3	2.46	0.45
1:C:136:PHE:CE2	1:C:182:TRP:NE1	2.81	0.45
1:B:171:THR:O	1:B:172:ASN:HB2	2.17	0.45
1:A:106:LEU:HB3	1:A:136:PHE:CD2	2.52	0.45
1:A:284:ARG:HG3	1:A:285:PRO:HD2	1.99	0.45
1:A:355:SER:C	1:A:357:GLU:N	2.69	0.45
1:C:354:ILE:O	1:C:354:ILE:HG22	2.17	0.44
1:B:54:ILE:O	1:B:58:MET:HG3	2.16	0.44
1:D:363:HIS:HD2	2:D:397:HOH:O	1.99	0.44
1:C:386:ARG:NH1	1:C:392:GLN:HE21	2.14	0.44
1:D:70:GLU:HA	1:D:74:GLY:O	2.18	0.44

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:C:232:PRO:HB2	1:C:235:ASN:HD22	1.83	0.44
1:D:13:LEU:HB3	1:D:16:GLN:HG3	2.00	0.43
1:A:351:GLY:O	1:A:352:ASN:HB2	2.18	0.43
1:D:392:GLN:HB3	1:D:392:GLN:HE21	1.67	0.43
1:A:392:GLN:HG2	1:A:394:PHE:HD2	1.84	0.43
1:C:92:VAL:O	1:C:362:ARG:NH1	2.50	0.43
1:C:68:ILE:O	1:C:74:GLY:HA3	2.18	0.43
1:C:106:LEU:HB3	1:C:136:PHE:CG	2.53	0.42
1:C:203:LYS:CE	1:C:230:PHE:HB3	2.48	0.42
1:A:110:PRO:HB3	1:A:249:CYS:SG	2.59	0.42
1:B:148:GLY:O	1:B:150:MET:N	2.53	0.42
1:A:386:ARG:NE	1:A:392:GLN:HB2	2.34	0.42
1:C:388:GLN:NE2	1:D:269:TRP:HE1	2.16	0.42
1:D:56:ARG:O	1:D:60:GLU:HG2	2.20	0.42
1:B:143:HIS:CE1	1:B:151:VAL:HG13	2.55	0.42
1:A:289:ASN:HD21	1:D:290:GLN:HE22	1.68	0.42
1:C:202:CYS:O	1:C:205:LEU:HB3	2.20	0.42
1:B:170:ILE:HG21	1:B:224:ILE:HD11	2.01	0.42
1:A:48:GLU:HB2	1:A:217:ARG:NH2	2.35	0.41
1:D:167:LYS:HB3	1:D:170:ILE:HD11	2.02	0.41
1:B:290:GLN:HE22	1:C:289:ASN:HB3	1.85	0.41
1:A:68:ILE:HA	1:A:69:PRO:HD3	1.94	0.41
1:B:140:GLU:HG2	1:B:167:LYS:HD3	2.02	0.41
1:C:216:LEU:H	1:C:366:ASN:ND2	2.19	0.41
1:A:106:LEU:HB3	1:A:136:PHE:CG	2.55	0.41
1:C:231:VAL:HG12	1:C:235:ASN:HB2	2.03	0.41
1:D:132:TRP:HA	1:D:177:ASP:OD1	2.21	0.41
1:C:157:VAL:HB	1:C:158:PRO:HD2	2.03	0.41
1:B:289:ASN:HB3	1:C:290:GLN:HE22	1.84	0.41
1:B:255:TYR:HD2	1:B:313:LEU:HD13	1.85	0.41
1:B:94:SER:HB2	1:B:366:ASN:HB3	2.03	0.41
1:C:126:LYS:HD2	1:C:132:TRP:CE2	2.55	0.41
1:A:352:ASN:HB3	1:C:169:TRP:CH2	2.57	0.40
1:A:372:THR:HG22	1:A:373:TYR:HD1	1.85	0.40
1:D:247:PHE:CZ	1:D:324:VAL:HG11	2.56	0.40
1:A:53:ALA:O	1:A:57:GLU:HG3	2.21	0.40
1:D:90:GLU:OE1	1:D:260:GLY:HA3	2.21	0.40
1:D:68:ILE:HA	1:D:69:PRO:HD3	1.95	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles

### 5.3.1 Protein backbone ⓘ

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	381/396 (96%)	363 (95%)	17 (4%)	1 (0%)	50	68
1	B	370/396 (93%)	357 (96%)	11 (3%)	2 (0%)	38	53
1	C	375/396 (95%)	362 (96%)	13 (4%)	0	100	100
1	D	373/396 (94%)	357 (96%)	15 (4%)	1 (0%)	50	68
All	All	1499/1584 (95%)	1439 (96%)	56 (4%)	4 (0%)	50	68

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	149	SER
1	A	352	ASN
1	D	357	GLU
1	B	160	GLY

### 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	307/313 (98%)	291 (95%)	16 (5%)	32	49
1	B	301/313 (96%)	282 (94%)	19 (6%)	25	38
1	C	301/313 (96%)	283 (94%)	18 (6%)	27	41
1	D	302/313 (96%)	285 (94%)	17 (6%)	30	45
All	All	1211/1252 (97%)	1141 (94%)	70 (6%)	28	43

All (70) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	49	THR
1	A	100	MET
1	A	121	GLU
1	A	155	ARG
1	A	171	THR
1	A	206	SER
1	A	217	ARG
1	A	219	SER
1	A	237	LEU
1	A	243	LEU
1	A	284	ARG
1	A	313	LEU
1	A	372	THR
1	A	374	GLU
1	A	379	ILE
1	A	392	GLN
1	B	15	ASP
1	B	100	MET
1	B	101	SER
1	B	103	GLN
1	B	155	ARG
1	B	156	LYS
1	B	171	THR
1	B	186	ASP
1	B	234	GLU
1	B	237	LEU
1	B	277	LEU
1	B	284	ARG
1	B	286	LEU
1	B	291	LEU
1	B	313	LEU
1	B	344	LEU
1	B	377	HIS
1	B	386	ARG
1	B	392	GLN
1	C	71	GLN
1	C	100	MET
1	C	101	SER
1	C	113	GLU
1	C	121	GLU
1	C	166	SER
1	C	171	THR
1	C	202	CYS

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Mol	Chain	Res	Type
1	C	203	LYS
1	C	217	ARG
1	C	237	LEU
1	C	243	LEU
1	C	277	LEU
1	C	279	ARG
1	C	286	LEU
1	C	291	LEU
1	C	344	LEU
1	C	356	ASP
1	D	98	SER
1	D	100	MET
1	D	117	ASP
1	D	171	THR
1	D	173	SER
1	D	190	ARG
1	D	237	LEU
1	D	243	LEU
1	D	277	LEU
1	D	286	LEU
1	D	291	LEU
1	D	344	LEU
1	D	356	ASP
1	D	357	GLU
1	D	358	PHE
1	D	379	ILE
1	D	392	GLN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (24) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	281	GLN
1	A	290	GLN
1	A	293	GLN
1	A	366	ASN
1	A	388	GLN
1	B	16	GLN
1	B	47	HIS
1	B	103	GLN
1	B	143	HIS
1	B	290	GLN
1	B	293	GLN

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Mol	Chain	Res	Type
1	B	366	ASN
1	B	377	HIS
1	B	388	GLN
1	C	235	ASN
1	C	290	GLN
1	C	366	ASN
1	C	388	GLN
1	C	392	GLN
1	D	7	HIS
1	D	281	GLN
1	D	293	GLN
1	D	366	ASN
1	D	388	GLN

### 5.3.3 RNA ⓘ

There are no RNA chains 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 ⓘ

There are no ligands in this entry.

### 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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	387/396 (97%)	0.26	15 (3%) 37 35	41, 56, 78, 90	0
1	B	378/396 (95%)	0.37	28 (7%) 14 13	39, 61, 77, 90	0
1	C	381/396 (96%)	0.34	21 (5%) 24 22	40, 66, 87, 92	0
1	D	381/396 (96%)	0.28	18 (4%) 30 28	38, 60, 79, 90	0
All	All	1527/1584 (96%)	0.31	82 (5%) 25 23	38, 60, 81, 92	0

All (82) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	3	ALA	6.6
1	B	102	VAL	4.3
1	B	205	LEU	4.3
1	C	356	ASP	4.2
1	C	151	VAL	3.8
1	B	101	SER	3.7
1	D	141	PRO	3.6
1	B	375	GLY	3.6
1	B	253	ALA	3.6
1	C	230	PHE	3.6
1	D	282	PHE	3.5
1	B	358	PHE	3.4
1	C	158	PRO	3.4
1	B	376	THR	3.4
1	B	180	VAL	3.3
1	D	358	PHE	3.3
1	A	358	PHE	3.3
1	B	377	HIS	3.3
1	B	4	ALA	3.3
1	D	149	SER	3.2
1	B	107	VAL	3.1

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Mol	Chain	Res	Type	RSRZ
1	C	373	TYR	3.1
1	B	156	LYS	3.1
1	A	282	PHE	3.1
1	D	230	PHE	3.1
1	A	357	GLU	3.1
1	C	201	GLY	3.0
1	B	106	LEU	3.0
1	B	356	ASP	3.0
1	C	355	SER	3.0
1	D	158	PRO	2.9
1	C	159	GLY	2.9
1	C	310	VAL	2.7
1	A	102	VAL	2.7
1	C	226	LEU	2.7
1	C	169	TRP	2.7
1	B	143	HIS	2.7
1	D	357	GLU	2.7
1	B	392	GLN	2.7
1	C	71	GLN	2.7
1	C	357	GLU	2.6
1	A	189	GLY	2.6
1	D	279	ARG	2.6
1	B	257	ILE	2.6
1	B	229	ALA	2.5
1	A	281	GLN	2.5
1	B	104	SER	2.5
1	B	320	GLY	2.5
1	B	103	GLN	2.5
1	B	204	GLY	2.5
1	A	356	ASP	2.4
1	B	211	HIS	2.4
1	C	231	VAL	2.4
1	C	3	ALA	2.4
1	A	257	ILE	2.4
1	C	227	ASP	2.4
1	B	100	MET	2.4
1	A	188	ASP	2.4
1	D	356	ASP	2.4
1	D	169	TRP	2.4
1	A	101	SER	2.3
1	A	105	SER	2.3
1	B	105	SER	2.3

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Mol	Chain	Res	Type	RSRZ
1	A	279	ARG	2.3
1	C	157	VAL	2.3
1	D	159	GLY	2.3
1	D	283	GLY	2.3
1	B	135	CYS	2.3
1	C	307	LEU	2.2
1	D	304	THR	2.2
1	A	98	SER	2.2
1	A	306	GLY	2.1
1	C	354	ILE	2.1
1	D	5	THR	2.1
1	D	168	MET	2.1
1	C	279	ARG	2.1
1	C	180	VAL	2.1
1	B	243	LEU	2.0
1	D	98	SER	2.0
1	A	304	THR	2.0
1	B	256	GLY	2.0
1	D	294	LYS	2.0

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

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

## 6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

## 6.4 Ligands ⓘ

There are no ligands in this entry.

## 6.5 Other polymers ⓘ

There are no such residues in this entry.