



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 11:11 AM UTC

PDB ID : 3EOM / pdb_00003eom
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 X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity	:	4-5-2 with Phenix2.0
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

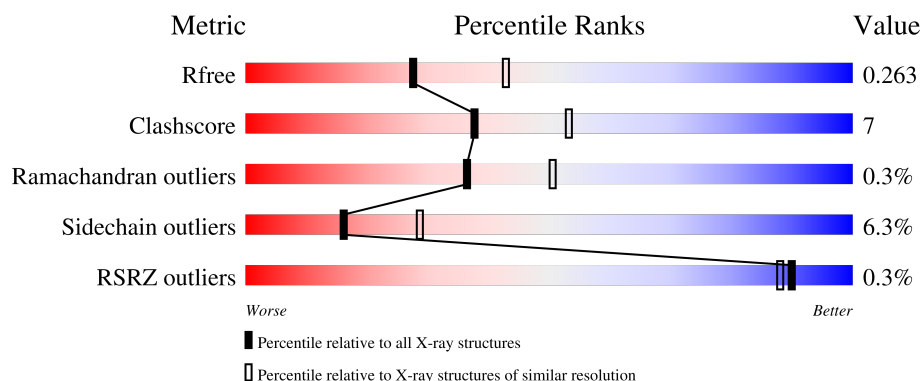
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.40 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}	180053	4912 (2.40-2.40)
Clashscore	190562	5391 (2.40-2.40)
Ramachandran outliers	187476	5320 (2.40-2.40)
Sidechain outliers	187428	5321 (2.40-2.40)
RSRZ outliers	180081	4916 (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 of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	396	 80% 16% . .
1	B	396	 78% 16% . 5%
1	C	396	 79% 16% . .
1	D	396	 77% 18% . .

2 Entry composition

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

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called 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

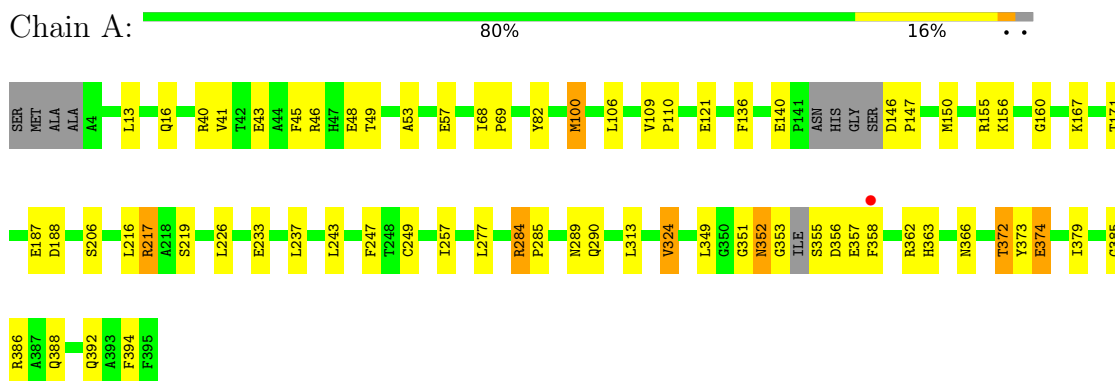
- Molecule 2 is water.

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		

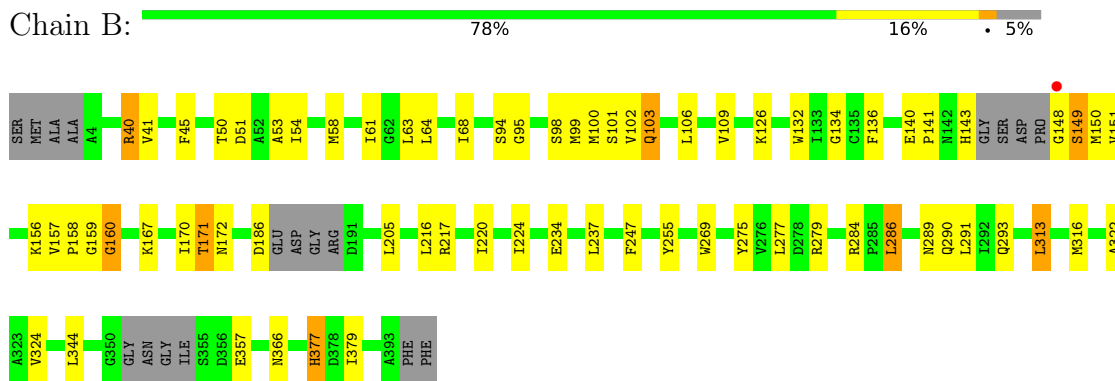
3 Residue-property plots [i](#)

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.

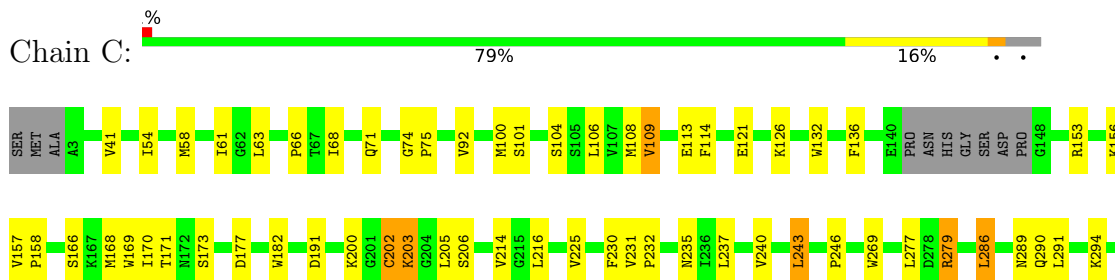
- Molecule 1: Glutaryl-CoA dehydrogenase

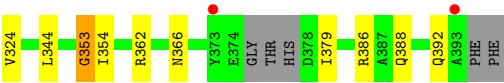


- Molecule 1: Glutaryl-CoA dehydrogenase

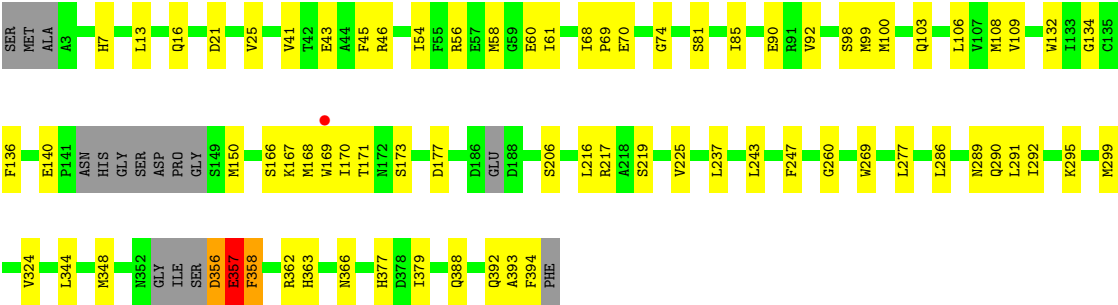
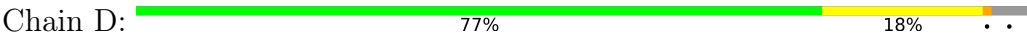


- Molecule 1: Glutaryl-CoA dehydrogenase





● Molecule 1: Glutaryl-CoA dehydrogenase



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	98.11Å 106.77Å 145.43Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	30.00 – 2.40 30.00 – 2.40	Depositor EDS
% Data completeness (in resolution range)	99.3 (30.00-2.40) 99.2 (30.00-2.40)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.59 (at 2.39Å)	Xtriage
Refinement program	REFMAC	Depositor
R, R_{free}	0.211 , 0.264 0.208 , 0.263	Depositor DCC
R_{free} test set	3035 reflections (5.02%)	wwPDB-VP
Wilson B-factor (Å ²)	53.2	Xtriage
Anisotropy	0.023	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.29 , 23.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	11908	wwPDB-VP
Average B, all atoms (Å ²)	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.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality [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).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.69	1/3034 (0.0%)	0.93	1/4098 (0.0%)
1	B	0.68	1/2964 (0.0%)	0.94	3/4003 (0.1%)
1	C	0.66	1/2977 (0.0%)	1.00	2/4019 (0.0%)
1	D	0.69	1/2987 (0.0%)	0.94	1/4033 (0.0%)
All	All	0.68	4/11962 (0.0%)	0.95	7/16153 (0.0%)

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	109	VAL	CA-CB	6.60	1.57	1.54
1	A	109	VAL	CA-CB	6.26	1.57	1.54
1	D	109	VAL	CA-CB	5.92	1.57	1.54
1	B	109	VAL	CA-CB	5.02	1.57	1.54

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	353	GLY	N-CA-C	22.37	144.77	115.47
1	D	41	VAL	N-CA-C	7.12	117.89	110.62
1	C	41	VAL	N-CA-C	7.09	117.85	110.62
1	B	41	VAL	N-CA-C	5.85	116.59	110.62
1	A	41	VAL	N-CA-C	5.17	115.90	110.62
1	B	68	ILE	CA-C-N	5.00	125.00	119.89
1	B	68	ILE	C-N-CA	5.00	125.00	119.89

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen

atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2976	0	2961	50	0
1	B	2909	0	2906	42	0
1	C	2924	0	2924	43	0
1	D	2932	0	2928	43	0
2	A	50	0	0	2	0
2	B	34	0	0	0	0
2	C	36	0	0	0	0
2	D	47	0	0	2	0
All	All	11908	0	11719	164	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 7.

All (164) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A: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:B:50:THR:HG21	1:B:99:MET:HE1	1.60	0.81
1:B:54:ILE:HG22	1:B:58:MET:HE2	1.64	0.80
1:A:355:SER:O	1:A:358:PHE:N	2.16	0.79
1:D:356:ASP:C	1:D:358:PHE:H	1.90	0.78
1:B:275:TYR:O	1:B:279:ARG:HG2	1.85	0.76
1:D:54:ILE:HG22	1:D:58:MET:HE2	1.69	0.74
1:A:247:PHE:HZ	1:A:324:VAL:HG11	1.53	0.74
1:A:290:GLN:NE2	1:D:289:ASN:HD21	1.84	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:A:353:GLY:C	1:A:355:SER:N	2.49	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:A:355:SER:O	1:A:356:ASP:C	2.35	0.68
1:D:216:LEU:H	1:D:366:ASN:HD22	1.38	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:C:279:ARG:HB3	1:C:286:LEU:HD22	1.77	0.66
1:D:21:ASP:O	1:D:25:VAL:HG23	1.96	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:247:PHE:HZ	1:A:324:VAL:CG1	2.09	0.64
1:A:355:SER:O	1:A:357:GLU:N	2.30	0.64
1:C:54:ILE:HG22	1:C:58:MET:HE3	1.79	0.63
1:C:68:ILE:HG13	1:C:108:MET:HE2	1.80	0.63
1:B:50:THR:CG2	1:B:99:MET:HE1	2.28	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
1:A:388:GLN:HE22	1:B:269:TRP:HE1	1.48	0.60
1:C:353:GLY:C	1:C:354:ILE:HD12	2.27	0.59
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:D:99:MET:HE2	1:D:219:SER:HA	1.85	0.59
1:A:43:GLU:OE2	1:A:46:ARG:NH1	2.35	0.58
1:A:187:GLU:O	1:A:188:ASP:C	2.45	0.58
1:C:206:SER:HB2	1:C:225:VAL:HB	1.85	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: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: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: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: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:CG2	1:C:354:ILE:O	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:81:SER:O	1:D:85:ILE:HG13	2.09	0.52
1:A:45:PHE:O	1:A:217:ARG:NH2	2.42	0.52
1:A:247:PHE:CZ	1:A:324:VAL:HG11	2.37	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:356:ASP:C	1:D:356:ASP:OD2	2.53	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:A:140:GLU:OE1	1:A:150:MET:HG3	2.10	0.51
1:C:386:ARG:HH11	1:C:392:GLN:HE21	1.59	0.51
1:A:40:ARG:NH2	1:A:57:GLU:OE2	2.44	0.51
1:A:386:ARG:HG3	1:A:392:GLN:HA	1.92	0.51
1:B:216:LEU:H	1:B:366:ASN:HD22	1.59	0.51
1:D:103:GLN:OE1	1:D:134:GLY:N	2.29	0.51
1:D:356:ASP:C	1:D:358:PHE:N	2.56	0.50
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:A:355:SER:C	1:A:357:GLU:N	2.69	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:C:61:ILE:HG13	1:C:63:LEU:HG	1.94	0.48
1:A:140:GLU:HG2	1:A:167:LYS:HD3	1.96	0.48
1:B:64:LEU:HD22	1:B:103:GLN:HG2	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:D:356:ASP:O	1:D:358:PHE:N	2.45	0.47
1:A:372:THR:HG22	1:A:373:TYR:CD1	2.50	0.47
1:B:126:LYS:HD2	1:B:132:TRP:CE2	2.50	0.47
1:A:160:GLY:HA2	1:A:233:GLU:HG2	1.97	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:C:54:ILE:CG2	1:C:58:MET:HE2	2.46	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:295:LYS:O	1:D:299:MET:HG3	2.16	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:A:40:ARG:HH22	1:A:57:GLU:CD	2.23	0.45
1:B:157:VAL:HB	1:B:158:PRO:CD	2.44	0.45
1:D:292:ILE:HD12	1:D:348:MET:HE3	1.99	0.45
1:B:171:THR:O	1:B:172:ASN:HB2	2.17	0.45
1:C:136:PHE:CE2	1:C:182:TRP:NE1	2.81	0.45
1:C:170:ILE:CG2	1:C:173:SER:HB3	2.46	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: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:C:232:PRO:HB2	1:C:235:ASN:HD22	1.83	0.44
1:D:70:GLU:HA	1:D:74:GLY:O	2.18	0.44
1:B:51:ASP:C	1:B:53:ALA:H	2.26	0.43
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:HE21	1:D:392:GLN:HB3	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:D:68:ILE:HG13	1:D:108:MET:HE2	2.00	0.42
1:A:82:TYR:HE2	1:A:100:MET:HE1	1.83	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:A:289:ASN:HD21	1:D:290:GLN:HE22	1.68	0.42
1:B:143:HIS:CE1	1:B:151:VAL:HG13	2.55	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:A:82:TYR:CE2	1:A:100:MET:HE1	2.55	0.42
1:B:170:ILE:HG21	1:B:224:ILE:HD11	2.01	0.42
1:C:202:CYS:O	1:C:205:LEU:HB3	2.20	0.42
1:A:48:GLU:HB2	1:A:217:ARG:NH2	2.35	0.41
1:C:54:ILE:CG2	1:C:58:MET:CE	2.97	0.41
1:B:290:GLN:HE22	1:C:289:ASN:HB3	1.85	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:167:LYS:HB3	1:D:170:ILE:HD11	2.02	0.41
1:A:68:ILE:HA	1:A:69:PRO:HD3	1.94	0.41
1:A:106:LEU:HB3	1:A:136:PHE:CG	2.55	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:C:231:VAL:HG12	1:C:235:ASN:HB2	2.03	0.41
1:B:255:TYR:HD2	1:B:313:LEU:HD13	1.85	0.41
1:B:289:ASN:HB3	1:C:290:GLN:HE22	1.84	0.41
1:C:157:VAL:HB	1:C:158:PRO:HD2	2.03	0.41
1:D:132:TRP:HA	1:D:177:ASP:OD1	2.21	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%)	36	50
1	B	370/396 (93%)	357 (96%)	11 (3%)	2 (0%)	24	37
1	C	375/396 (95%)	362 (96%)	13 (4%)	0	100	100
1	D	373/396 (94%)	357 (96%)	15 (4%)	1 (0%)	36	50
All	All	1499/1584 (95%)	1439 (96%)	56 (4%)	4 (0%)	36	50

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%)	287 (94%)	20 (6%)	15	27
1	B	301/313 (96%)	281 (93%)	20 (7%)	15	26
1	C	301/313 (96%)	281 (93%)	20 (7%)	15	26
1	D	302/313 (96%)	286 (95%)	16 (5%)	20	36
All	All	1211/1252 (97%)	1135 (94%)	76 (6%)	16	29

All (76) 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	156	LYS
1	A	171	THR
1	A	206	SER
1	A	217	ARG
1	A	219	SER
1	A	226	LEU
1	A	237	LEU
1	A	243	LEU
1	A	277	LEU
1	A	284	ARG
1	A	313	LEU
1	A	324	VAL
1	A	349	LEU
1	A	372	THR

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Mol	Chain	Res	Type
1	A	374	GLU
1	A	379	ILE
1	B	40	ARG
1	B	100	MET
1	B	101	SER
1	B	103	GLN
1	B	141	PRO
1	B	156	LYS
1	B	171	THR
1	B	186	ASP
1	B	205	LEU
1	B	220	ILE
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	357	GLU
1	B	377	HIS
1	C	71	GLN
1	C	100	MET
1	C	101	SER
1	C	113	GLU
1	C	121	GLU
1	C	156	LYS
1	C	166	SER
1	C	171	THR
1	C	202	CYS
1	C	203	LYS
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	294	LYS
1	C	324	VAL
1	C	344	LEU
1	C	379	ILE

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Mol	Chain	Res	Type
1	D	61	ILE
1	D	98	SER
1	D	100	MET
1	D	150	MET
1	D	171	THR
1	D	173	SER
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

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (31) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	47	HIS
1	A	235	ASN
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	251	ASN
1	B	290	GLN
1	B	366	ASN
1	B	377	HIS
1	B	388	GLN
1	C	17	GLN
1	C	235	ASN
1	C	290	GLN
1	C	308	GLN
1	C	366	ASN
1	C	388	GLN

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Mol	Chain	Res	Type
1	C	392	GLN
1	D	7	HIS
1	D	34	GLN
1	D	47	HIS
1	D	71	GLN
1	D	281	GLN
1	D	293	GLN
1	D	366	ASN
1	D	388	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 oligosaccharides 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, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	387/396 (97%)	-0.09	1 (0%) 90 88	41, 56, 78, 90	0
1	B	378/396 (95%)	-0.02	1 (0%) 90 88	39, 61, 77, 90	0
1	C	381/396 (96%)	0.11	2 (0%) 87 85	40, 66, 87, 92	0
1	D	381/396 (96%)	0.02	1 (0%) 90 88	38, 60, 79, 90	0
All	All	1527/1584 (96%)	0.01	5 (0%) 90 88	38, 60, 81, 92	0

All (5) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	169	TRP	2.4
1	B	148	GLY	2.4
1	C	373	TYR	2.1
1	A	358	PHE	2.1
1	C	393	ALA	2.0

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.