



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 08:04 AM GMT

PDB ID : 3D6B
Title : 2.2 Å crystal structure of glutaryl-CoA dehydrogenase from Burkholderia pseudomallei
Authors : Seattle Structural Genomics Center for Infectious Disease (SSGCID)
Deposited on : 2008-05-19
Resolution : 2.21 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) : 1.9-1692
EDS : rb-20026688
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac : 5.8.0135
CCP4 : 6.5.0
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : trunk26865

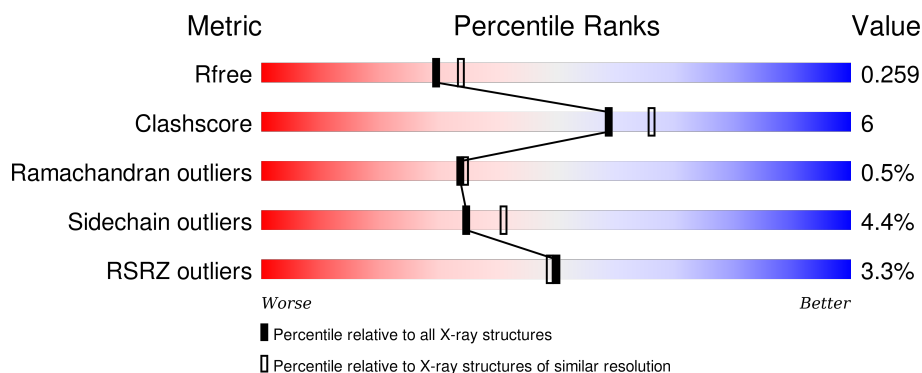
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.21 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}	91344	4405 (2.24-2.20)
Clashscore	102246	5146 (2.24-2.20)
Ramachandran outliers	100387	5065 (2.24-2.20)
Sidechain outliers	100360	5066 (2.24-2.20)
RSRZ outliers	91569	4414 (2.24-2.20)

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 $\leq 5\%$. 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	395	<div> <div>4%</div> <div>80% 13% • 5%</div> </div>
1	B	395	<div> <div>5%</div> <div>77% 12% • 8%</div> </div>
1	C	395	<div> <div>%</div> <div>83% 11% • 5%</div> </div>
1	D	395	<div> <div>2%</div> <div>84% 10% • 6%</div> </div>

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard

residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	54D	C	501	-	-	-	X

2 Entry composition [i](#)

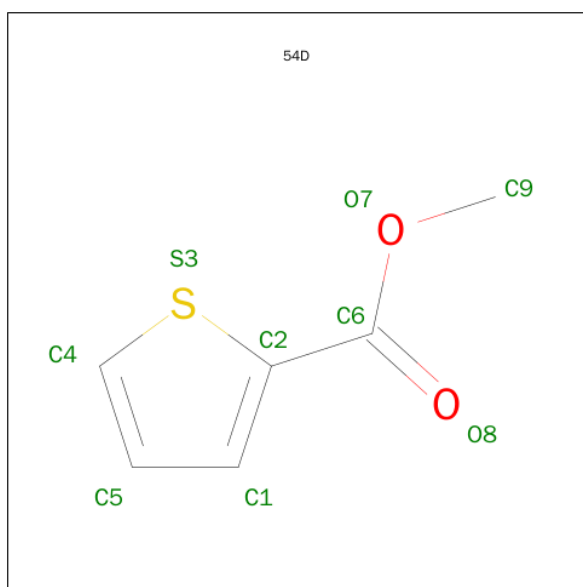
There are 3 unique types of molecules in this entry. The entry contains 11945 atoms, of which 0 are hydrogens and 0 are deuteriums.

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	374	Total	C	N	O	S	0	0	0
			2876	1822	507	531	16			
1	B	365	Total	C	N	O	S	0	0	0
			2805	1775	494	520	16			
1	C	377	Total	C	N	O	S	0	0	0
			2896	1829	514	537	16			
1	D	372	Total	C	N	O	S	0	0	0
			2859	1809	507	527	16			

- Molecule 2 is METHYL THIOPHENE-2-CARBOXYLATE (three-letter code: 54D) (formula: C₆H₆O₂S).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	C	1	Total	C	O	S	0	0
			9	6	2	1		

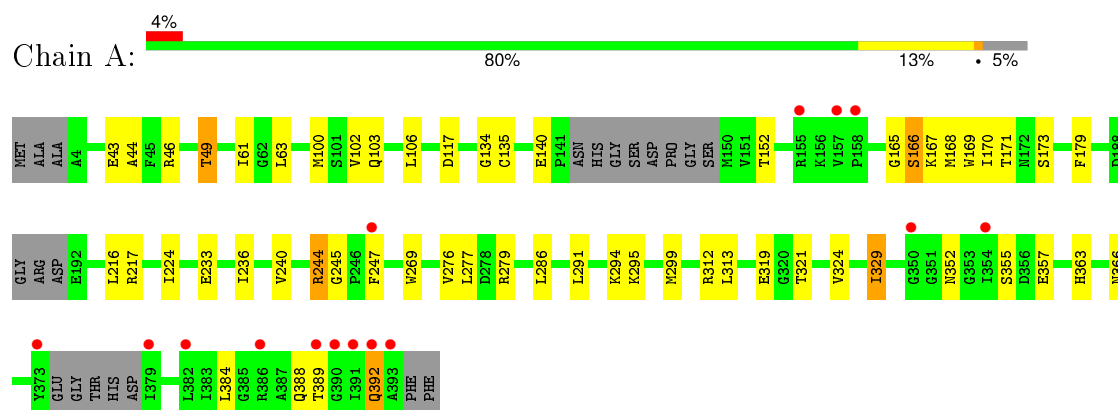
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	121	Total 121	O 121	0	0
3	B	79	Total 79	O 79	0	0
3	C	173	Total 173	O 173	0	0
3	D	127	Total 127	O 127	0	0

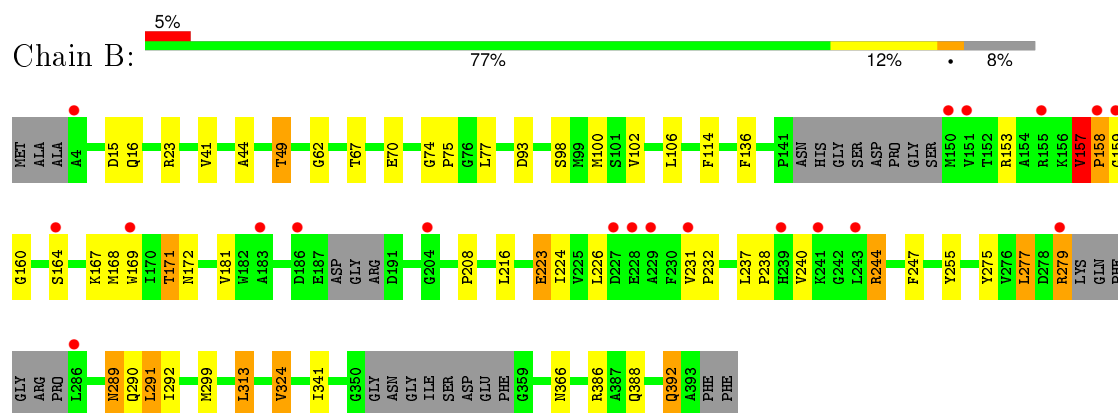
3 Residue-property plots

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.

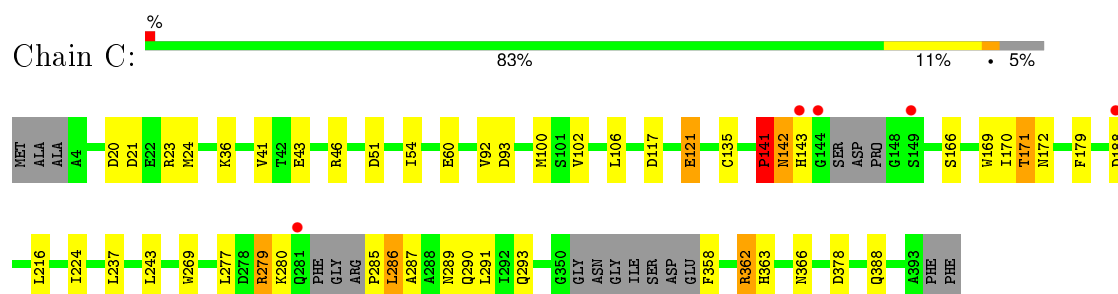
• Molecule 1: Glutaryl-CoA dehydrogenase



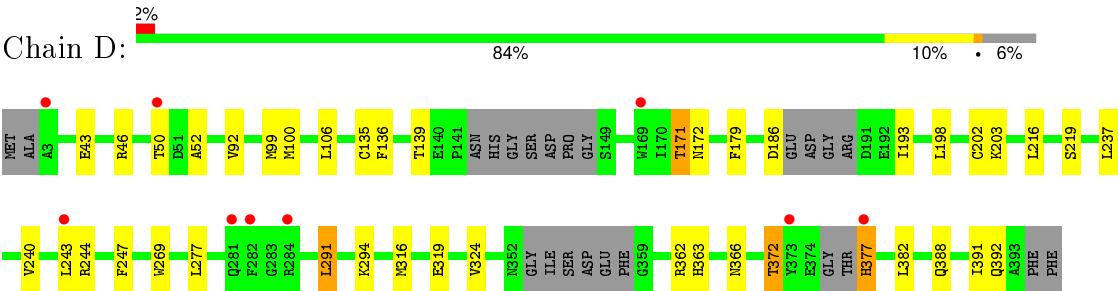
• Molecule 1: Glutaryl-CoA dehydrogenase



• 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	98.50Å 107.47Å 144.31Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	47.19 – 2.21 47.17 – 2.21	Depositor EDS
% Data completeness (in resolution range)	98.8 (47.19-2.21) 98.8 (47.17-2.21)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.17 (at 2.20Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.209 , 0.261 0.208 , 0.259	Depositor DCC
R_{free} test set	3826 reflections (5.28%)	DCC
Wilson B-factor (Å ²)	32.6	Xtriage
Anisotropy	0.121	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 37.6	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.32$	Xtriage
Outliers	0 of 76240 reflections	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	11945	wwPDB-VP
Average B, all atoms (Å ²)	36.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.60% 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, 0.375 respectively for untwinned datasets, and 0.333, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: 54D

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	0.45	0/2929	0.58	0/3955
1	B	0.45	0/2855	0.58	2/3856 (0.1%)
1	C	0.50	0/2950	0.65	1/3983 (0.0%)
1	D	0.48	0/2911	0.59	0/3930
All	All	0.47	0/11645	0.60	3/15724 (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	B	0	1

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	362	ARG	NE-CZ-NH1	-7.00	116.80	120.30
1	B	157	VAL	C-N-CD	-6.56	106.18	120.60
1	B	157	VAL	C-N-CA	5.71	145.99	122.00

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	157	VAL	Peptide

5.2 Too-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 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	2876	0	2887	39	0
1	B	2805	0	2813	50	0
1	C	2896	0	2896	34	0
1	D	2859	0	2869	30	0
2	C	9	0	6	0	0
3	A	121	0	0	4	0
3	B	79	0	0	1	0
3	C	173	0	0	3	0
3	D	127	0	0	4	0
All	All	11945	0	11471	132	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 (132) 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:44:ALA:HA	1:A:49:THR:HG23	1.30	1.11
1:B:289:ASN:HD21	1:B:291:LEU:HB2	1.32	0.94
1:B:44:ALA:HA	1:B:49:THR:HG23	1.53	0.90
1:A:247:PHE:HZ	1:A:324:VAL:HG11	1.38	0.87
1:A:43:GLU:OE2	1:A:46:ARG:NH1	2.12	0.83
1:B:247:PHE:HZ	1:B:324:VAL:HG11	1.43	0.80
1:C:117:ASP:O	1:C:121:GLU:HG2	1.85	0.77
1:A:44:ALA:HA	1:A:49:THR:CG2	2.13	0.76
1:B:244:ARG:HG3	1:B:244:ARG:HH11	1.50	0.76
1:B:289:ASN:CG	1:C:290:GLN:HE22	1.92	0.73
1:C:92:VAL:O	1:C:362:ARG:NH1	2.24	0.71
3:B:409:HOH:O	1:D:372:THR:HG21	1.92	0.70
1:A:216:LEU:H	1:A:366:ASN:HD22	1.42	0.67
1:D:203:LYS:O	3:D:587:HOH:O	2.12	0.67
1:D:216:LEU:H	1:D:366:ASN:HD22	1.43	0.67
1:D:43:GLU:OE2	1:D:46:ARG:NH1	2.27	0.66
1:B:216:LEU:H	1:B:366:ASN:HD22	1.41	0.66
1:A:168:MET:HG3	1:A:169:TRP:CD1	2.30	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:92:VAL:O	1:D:362:ARG:NH1	2.30	0.64
1:B:289:ASN:ND2	1:B:291:LEU:HB2	2.08	0.64
1:B:247:PHE:CZ	1:B:324:VAL:HG11	2.31	0.64
1:A:216:LEU:H	1:A:366:ASN:ND2	1.95	0.64
1:B:289:ASN:HD22	1:B:292:ILE:H	1.45	0.63
1:A:247:PHE:CZ	1:A:324:VAL:HG11	2.29	0.63
1:D:216:LEU:H	1:D:366:ASN:ND2	1.96	0.63
1:C:141:PRO:O	1:C:142:ASN:HB2	1.99	0.61
1:B:216:LEU:H	1:B:366:ASN:ND2	1.98	0.61
1:C:216:LEU:H	1:C:366:ASN:HD22	1.49	0.59
1:C:279:ARG:HB3	1:C:286:LEU:HD13	1.85	0.58
1:B:44:ALA:HA	1:B:49:THR:CG2	2.29	0.58
1:D:247:PHE:HZ	1:D:324:VAL:CG1	2.16	0.58
1:C:388:GLN:HE22	1:D:269:TRP:HE1	1.53	0.57
1:D:247:PHE:CZ	1:D:324:VAL:HG11	2.40	0.57
1:A:279:ARG:HG2	1:A:286:LEU:HD22	1.87	0.56
1:D:99:MET:HE2	1:D:219:SER:HA	1.87	0.56
1:B:244:ARG:NH1	1:B:244:ARG:HG3	2.19	0.56
1:A:217:ARG:NH1	3:A:447:HOH:O	2.39	0.56
1:B:289:ASN:CG	1:C:290:GLN:NE2	2.59	0.55
1:B:247:PHE:HZ	1:B:324:VAL:CG1	2.15	0.55
1:B:290:GLN:HE22	1:C:289:ASN:HA	1.71	0.55
1:A:140:GLU:HG2	1:A:166:SER:O	2.07	0.55
1:A:61:ILE:HG13	1:A:63:LEU:HG	1.89	0.55
1:B:292:ILE:HD11	1:D:377:HIS:CE1	2.42	0.55
1:D:171:THR:O	1:D:172:ASN:HB2	2.07	0.55
1:A:244:ARG:NH1	3:A:416:HOH:O	2.35	0.55
1:C:141:PRO:O	1:C:142:ASN:CB	2.54	0.55
1:A:269:TRP:HE1	1:B:388:GLN:NE2	2.05	0.55
1:B:70:GLU:HA	1:B:74:GLY:O	2.06	0.54
1:B:98:SER:O	1:B:102:VAL:HG23	2.08	0.53
1:C:51:ASP:O	1:C:54:ILE:HD12	2.09	0.52
1:A:312:ARG:HH22	1:B:16:GLN:NE2	2.07	0.52
1:A:103:GLN:OE1	1:A:134:GLY:N	2.35	0.52
1:A:279:ARG:HH12	1:C:142:ASN:ND2	2.08	0.52
1:B:15:ASP:O	1:B:23:ARG:HD2	2.09	0.52
1:A:312:ARG:HH22	1:B:16:GLN:HE21	1.59	0.51
1:C:102:VAL:HG22	1:C:106:LEU:HD12	1.93	0.51
1:A:269:TRP:HE1	1:B:388:GLN:HE22	1.59	0.51
1:B:62:GLY:O	1:B:75:PRO:HG3	2.11	0.51
1:B:114:PHE:HB2	1:B:237:LEU:HD23	1.91	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:289:ASN:ND2	1:B:292:ILE:H	2.09	0.50
1:B:157:VAL:HB	1:B:158:PRO:HB2	1.92	0.50
1:C:388:GLN:NE2	1:D:269:TRP:HE1	2.10	0.49
1:C:269:TRP:HE1	1:D:388:GLN:NE2	2.11	0.49
1:A:102:VAL:HG22	1:A:106:LEU:HD12	1.95	0.49
1:A:389:THR:HB	1:B:277:LEU:HD11	1.95	0.49
1:B:208:PRO:HG2	1:B:223:GLU:HG3	1.95	0.49
1:D:247:PHE:HZ	1:D:324:VAL:HG11	1.77	0.48
1:A:167:LYS:HB3	1:A:170:ILE:HD11	1.95	0.48
1:B:167:LYS:HB2	1:B:224:ILE:HB	1.95	0.48
1:C:287:ALA:HB3	1:D:391:ILE:HD13	1.96	0.48
1:D:52:ALA:O	3:D:615:HOH:O	2.20	0.47
1:B:168:MET:HG3	1:B:169:TRP:CD1	2.49	0.47
1:B:157:VAL:HB	1:B:158:PRO:CB	2.44	0.47
1:C:171:THR:O	1:C:172:ASN:HB2	2.15	0.47
1:D:240:VAL:HG23	1:D:244:ARG:NH1	2.29	0.47
1:B:171:THR:O	1:B:172:ASN:HB2	2.14	0.47
1:A:363:HIS:HD2	3:A:438:HOH:O	1.98	0.47
1:C:60:GLU:OE1	3:C:582:HOH:O	2.20	0.46
1:A:276:VAL:HG12	1:A:286:LEU:HD23	1.97	0.46
1:B:255:TYR:CD2	1:B:313:LEU:HD13	2.51	0.46
1:C:20:ASP:O	1:C:24:MET:HG3	2.14	0.46
1:B:291:LEU:CD1	1:C:291:LEU:HA	2.46	0.46
1:A:294:LYS:HE3	1:D:291:LEU:HD21	1.99	0.45
1:A:291:LEU:HG	1:A:295:LYS:HE2	1.98	0.45
1:D:247:PHE:HZ	1:D:324:VAL:HG13	1.82	0.45
1:C:135:CYS:SG	1:C:179:PHE:CD1	3.10	0.45
1:A:247:PHE:HZ	1:A:324:VAL:CG1	2.21	0.45
1:D:247:PHE:CZ	1:D:324:VAL:CG1	2.98	0.45
1:B:386:ARG:NH1	1:B:392:GLN:OE1	2.49	0.45
1:A:135:CYS:SG	1:A:179:PHE:CD1	3.10	0.45
1:C:280:LYS:HA	1:C:285:PRO:HA	1.99	0.45
1:D:363:HIS:HD2	3:D:498:HOH:O	2.00	0.44
1:B:255:TYR:HD2	1:B:313:LEU:HD13	1.82	0.44
1:A:388:GLN:HG3	3:A:475:HOH:O	2.17	0.44
1:A:329:ILE:HB	1:A:384:LEU:HD11	1.99	0.44
1:B:291:LEU:HD13	1:C:291:LEU:HA	1.99	0.44
1:D:135:CYS:SG	1:D:179:PHE:CD1	3.11	0.44
1:B:299:MET:HG2	1:B:341:ILE:HG23	1.98	0.44
1:C:43:GLU:OE2	1:C:46:ARG:HD2	2.18	0.44
1:D:106:LEU:HB3	1:D:136:PHE:HB2	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:170:ILE:HG21	1:A:224:ILE:HD11	2.00	0.43
1:A:295:LYS:O	1:A:299:MET:HG3	2.18	0.43
1:B:160:GLY:HA2	1:B:231:VAL:O	2.19	0.43
1:C:280:LYS:HE3	1:C:285:PRO:HG3	2.00	0.43
1:A:233:GLU:O	1:A:236:ILE:HG22	2.19	0.43
1:C:378:ASP:OD2	1:D:294:LYS:HE3	2.19	0.42
1:B:41:VAL:HG21	1:B:93:ASP:HB2	2.01	0.42
1:B:240:VAL:HG23	1:B:244:ARG:HE	1.84	0.42
1:B:277:LEU:HD12	1:B:277:LEU:HA	1.92	0.42
1:B:67:THR:HA	1:B:77:LEU:O	2.19	0.42
1:C:41:VAL:HG21	1:C:93:ASP:HB2	2.01	0.42
1:A:152:THR:HG23	1:A:165:GLY:HA3	2.01	0.42
1:B:181:VAL:HG11	1:B:226:LEU:HD11	2.00	0.42
1:A:392:GLN:HE21	1:A:392:GLN:HB3	1.65	0.42
1:B:289:ASN:OD1	1:C:290:GLN:NE2	2.53	0.41
1:C:23:ARG:HD2	3:C:564:HOH:O	2.19	0.41
1:C:43:GLU:OE1	1:C:46:ARG:NH1	2.54	0.41
1:B:231:VAL:HA	1:B:232:PRO:HD2	1.91	0.41
1:A:319:GLU:HG3	1:A:321:THR:HG23	2.03	0.41
1:C:363:HIS:HD2	3:C:550:HOH:O	2.04	0.41
1:D:50:THR:HA	3:D:572:HOH:O	2.20	0.41
1:A:352:ASN:HB3	1:C:169:TRP:CH2	2.55	0.41
1:A:44:ALA:CA	1:A:49:THR:HG23	2.23	0.41
1:C:170:ILE:HG21	1:C:224:ILE:HD11	2.02	0.41
1:B:275:TYR:O	1:B:279:ARG:HD3	2.20	0.41
1:C:293:GLN:OE1	1:D:382:LEU:HD22	2.21	0.41
1:B:106:LEU:HB3	1:B:136:PHE:HB2	2.02	0.40
1:D:316:MET:HA	1:D:319:GLU:HG2	2.03	0.40
1:A:240:VAL:HG21	1:A:245:GLY:HA2	2.02	0.40
1:D:193:ILE:HD12	1:D:243:LEU:HD12	2.04	0.40
1:B:237:LEU:HA	1:B:238:PRO:HD3	1.89	0.40
1:D:179:PHE:HB2	1:D:198:LEU:HB2	2.02	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	366/395 (93%)	357 (98%)	9 (2%)	0	100	100
1	B	355/395 (90%)	347 (98%)	5 (1%)	3 (1%)	24	21
1	C	369/395 (93%)	356 (96%)	9 (2%)	4 (1%)	17	14
1	D	362/395 (92%)	351 (97%)	11 (3%)	0	100	100
All	All	1452/1580 (92%)	1411 (97%)	34 (2%)	7 (0%)	34	34

All (7) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	157	VAL
1	B	158	PRO
1	C	141	PRO
1	C	142	ASN
1	B	159	GLY
1	C	143	HIS
1	C	188	ASP

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	297/312 (95%)	284 (96%)	13 (4%)	35	41
1	B	290/312 (93%)	275 (95%)	15 (5%)	29	32
1	C	299/312 (96%)	286 (96%)	13 (4%)	35	42
1	D	295/312 (95%)	284 (96%)	11 (4%)	41	50
All	All	1181/1248 (95%)	1129 (96%)	52 (4%)	35	41

All (52) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	49	THR
1	A	100	MET
1	A	117	ASP
1	A	166	SER
1	A	171	THR
1	A	173	SER
1	A	244	ARG
1	A	277	LEU
1	A	313	LEU
1	A	329	ILE
1	A	355	SER
1	A	357	GLU
1	A	392	GLN
1	B	49	THR
1	B	100	MET
1	B	153	ARG
1	B	157	VAL
1	B	164	SER
1	B	171	THR
1	B	223	GLU
1	B	244	ARG
1	B	277	LEU
1	B	279	ARG
1	B	289	ASN
1	B	291	LEU
1	B	313	LEU
1	B	324	VAL
1	B	392	GLN
1	C	21	ASP
1	C	36	LYS
1	C	100	MET
1	C	121	GLU
1	C	141	PRO
1	C	166	SER
1	C	171	THR
1	C	237	LEU
1	C	243	LEU
1	C	277	LEU
1	C	279	ARG
1	C	286	LEU
1	C	358	PHE
1	D	100	MET
1	D	139	THR

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Mol	Chain	Res	Type
1	D	171	THR
1	D	186	ASP
1	D	202	CYS
1	D	237	LEU
1	D	277	LEU
1	D	291	LEU
1	D	372	THR
1	D	377	HIS
1	D	392	GLN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (26) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	17	GLN
1	A	290	GLN
1	A	293	GLN
1	A	308	GLN
1	A	363	HIS
1	A	366	ASN
1	A	388	GLN
1	A	392	GLN
1	B	16	GLN
1	B	289	ASN
1	B	290	GLN
1	B	293	GLN
1	B	363	HIS
1	B	366	ASN
1	B	371	ASN
1	B	388	GLN
1	C	235	ASN
1	C	290	GLN
1	C	363	HIS
1	C	366	ASN
1	C	388	GLN
1	D	281	GLN
1	D	293	GLN
1	D	363	HIS
1	D	366	ASN
1	D	388	GLN

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 ⓘ

1 ligand is 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).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
2	54D	C	501	-	8,9,9	2.05	1 (12%)	6,11,11	3.18	3 (50%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the chemical component dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	54D	C	501	-	-	1/4/6/6	0/1/1/1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	501	54D	O7-C6	5.54	1.46	1.33

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
2	C	501	54D	C5-C4-S3	-5.11	107.57	113.23
2	C	501	54D	C9-O7-C6	2.06	120.08	115.84
2	C	501	54D	O7-C6-C2	5.14	121.23	112.42

There are no chirality outliers.

All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	C	501	54D	C9-O7-C6-C2

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 ⓘ

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, 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	374/395 (94%)	0.04	15 (4%) 42 41	21, 37, 66, 76	0
1	B	365/395 (92%)	0.21	20 (5%) 29 27	22, 41, 69, 80	0
1	C	377/395 (95%)	-0.20	5 (1%) 79 78	17, 29, 48, 63	0
1	D	372/395 (94%)	-0.13	9 (2%) 62 61	17, 31, 50, 57	0
All	All	1488/1580 (94%)	-0.02	49 (3%) 50 49	17, 35, 62, 80	0

All (49) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	373	TYR	5.3
1	A	379	ILE	4.9
1	A	389	THR	4.8
1	C	143	HIS	4.4
1	B	159	GLY	4.3
1	A	155	ARG	4.2
1	A	386	ARG	4.0
1	B	229	ALA	3.9
1	B	169	TRP	3.7
1	D	377	HIS	3.6
1	A	393	ALA	3.5
1	D	50	THR	3.5
1	B	4	ALA	3.4
1	B	239	HIS	3.4
1	A	392	GLN	3.2
1	A	390	GLY	3.1
1	B	231	VAL	3.0
1	C	149	SER	3.0
1	D	282	PHE	2.9
1	A	350	GLY	2.8
1	D	169	TRP	2.8

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Mol	Chain	Res	Type	RSRZ
1	B	186	ASP	2.7
1	B	243	LEU	2.6
1	A	391	ILE	2.6
1	B	155	ARG	2.6
1	B	227	ASP	2.5
1	B	183	ALA	2.5
1	B	151	VAL	2.5
1	A	247	PHE	2.5
1	B	286	LEU	2.5
1	D	3	ALA	2.5
1	B	228	GLU	2.4
1	B	279	ARG	2.4
1	B	164	SER	2.4
1	B	241	LYS	2.4
1	B	150	MET	2.4
1	C	281	GLN	2.4
1	B	204	GLY	2.3
1	C	144	GLY	2.3
1	D	284	ARG	2.3
1	A	354	ILE	2.3
1	C	188	ASP	2.2
1	B	158	PRO	2.2
1	D	373	TYR	2.2
1	A	158	PRO	2.1
1	D	243	LEU	2.0
1	A	382	LEU	2.0
1	D	281	GLN	2.0
1	A	157	VAL	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 carbohydrates 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. LLDF column lists the quality of electron

density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95th 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	LLDF	B-factors(\AA^2)	Q<0.9
2	54D	C	501	9/9	0.84	0.17	3.07	56,58,58,58	0

6.5 Other polymers [i](#)

There are no such residues in this entry.