



# Full wwPDB X-ray Structure Validation Report ⓘ

May 16, 2020 – 07:42 am BST

PDB ID : 3EON  
Title : 2.55Å crystal structure of native glutaryl-coa dehydrogenase from Burkholderia pseudomallei in complex with a small molecule  
Authors : Seattle Structural Genomics Center for Infectious Disease (SSGCID)  
Deposited on : 2008-09-28  
Resolution : 2.55 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](mailto: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.

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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 : 1.8.5 (274361), CSD as541be (2020)  
Xtriage (Phenix) : 1.13  
EDS : 2.11  
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) : 2.11

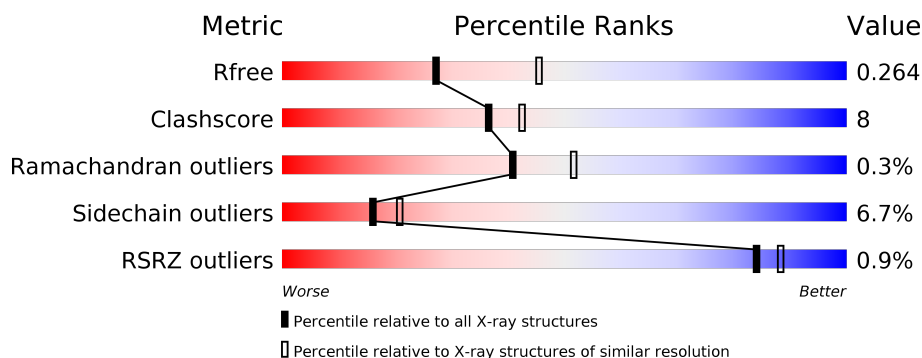
# 1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.55 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))
$R_{free}$	130704	1284 (2.56-2.52)
Clashscore	141614	1332 (2.56-2.52)
Ramachandran outliers	138981	1315 (2.56-2.52)
Sidechain outliers	138945	1315 (2.56-2.52)
RSRZ outliers	127900	1272 (2.56-2.52)

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 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	<div> <div>%</div> <div> <div></div> <div>81%</div> <div>14%</div> <div>• •</div> </div> </div>
1	B	396	<div> <div>%</div> <div> <div></div> <div>79%</div> <div>14%</div> <div>• 5%</div> </div> </div>
1	C	396	<div> <div>%</div> <div> <div></div> <div>76%</div> <div>19%</div> <div>• •</div> </div> </div>
1	D	396	<div> <div>%</div> <div> <div></div> <div>73%</div> <div>21%</div> <div>• •</div> </div> </div>

## 2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 11897 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.

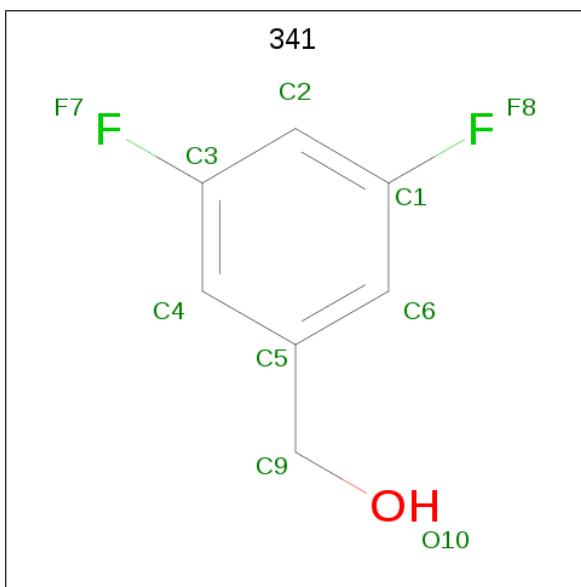
- Molecule 1 is a protein called Glutaryl-CoA dehydrogenase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	383	Total	C	N	O	S	0	0	0
			2943	1861	520	546	16			
1	B	375	Total	C	N	O	S	0	0	0
			2885	1826	510	533	16			
1	C	382	Total	C	N	O	S	0	0	0
			2933	1851	520	546	16			
1	D	380	Total	C	N	O	S	0	0	0
			2920	1851	513	540	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 (3,5-difluorophenyl)methanol (three-letter code: 341) (formula: C<sub>7</sub>H<sub>6</sub>F<sub>2</sub>O).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	C	1	Total	C	F	O	0	0
			10	7	2	1		

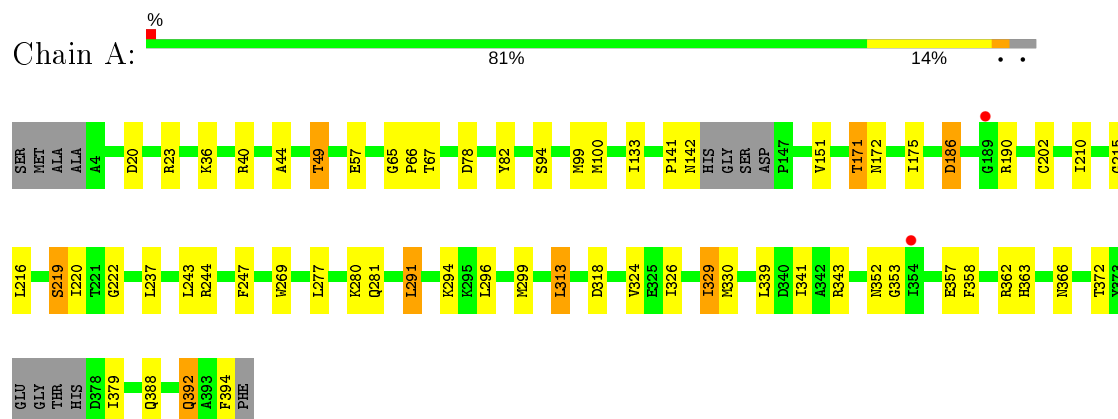
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	62	Total	O	0	0
			62	62		
3	B	54	Total	O	0	0
			54	54		
3	C	52	Total	O	0	0
			52	52		
3	D	38	Total	O	0	0
			38	38		

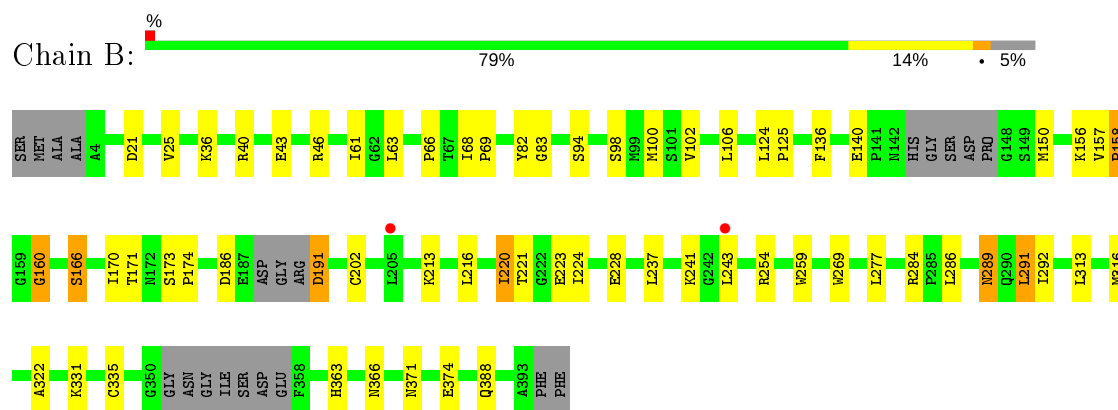
### 3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of 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.

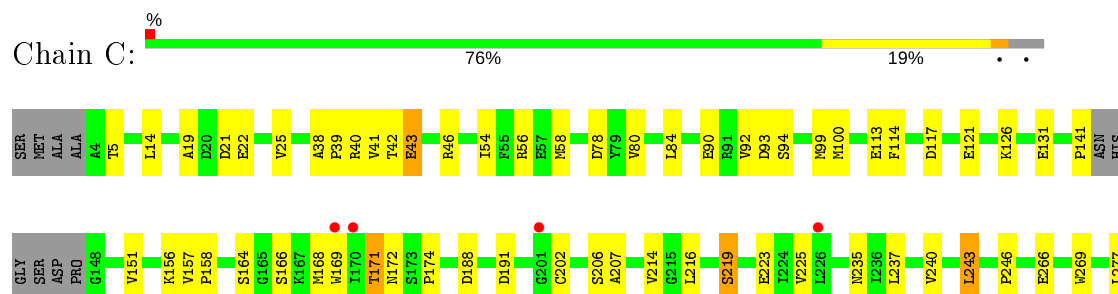
#### • Molecule 1: Glutaryl-CoA dehydrogenase



#### • Molecule 1: Glutaryl-CoA dehydrogenase

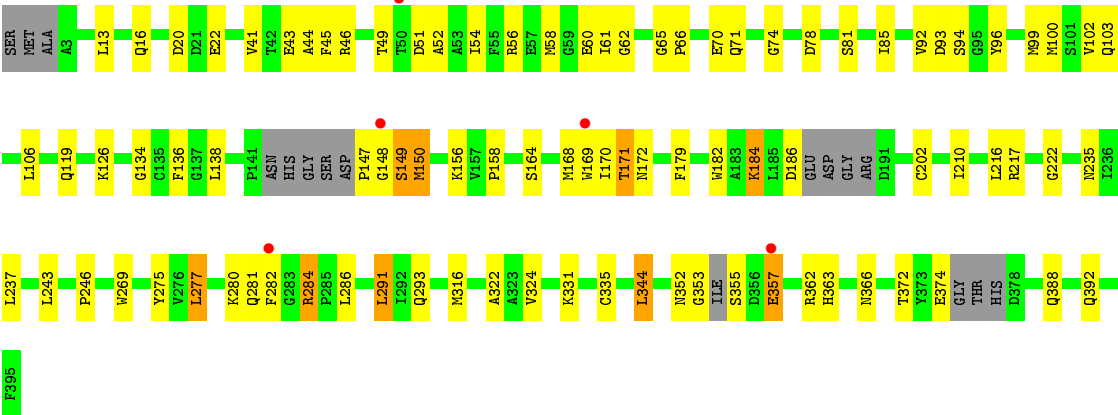


#### • Molecule 1: Glutaryl-CoA dehydrogenase





● 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, $\alpha$ , $\beta$ , $\gamma$	97.41Å 106.17Å 144.19Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	46.63 – 2.55 46.61 – 2.55	Depositor EDS
% Data completeness (in resolution range)	100.0 (46.63-2.55) 100.0 (46.61-2.55)	Depositor EDS
$R_{merge}$	0.12	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	3.57 (at 2.54Å)	Xtriage
Refinement program	REFMAC	Depositor
R, $R_{free}$	0.187 , 0.266 0.185 , 0.264	Depositor DCC
$R_{free}$ test set	2476 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	41.4	Xtriage
Anisotropy	0.059	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.31 , 31.1	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	11897	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	42.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.65% of the height of the origin peak. No significant pseudotranslation is detected.*

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

<sup>2</sup>Theoretical 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](#)

Bond lengths and bond angles in the following residue types are not validated in this section:  
341

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	0.64	0/2999	0.71	0/4050
1	B	0.67	0/2939	0.71	0/3969
1	C	0.66	0/2988	0.72	0/4035
1	D	0.66	0/2975	0.71	1/4015 (0.0%)
All	All	0.66	0/11901	0.71	1/16069 (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	D	344	LEU	CA-CB-CG	5.66	128.32	115.30

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	2943	0	2943	51	0
1	B	2885	0	2890	43	0
1	C	2933	0	2927	55	0
1	D	2920	0	2918	57	0
2	C	10	0	6	0	0
3	A	62	0	0	4	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	B	54	0	0	3	0
3	C	52	0	0	4	0
3	D	38	0	0	3	0
All	All	11897	0	11684	185	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 8.

All (185) 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:B:289:ASN:HB2	3:B:413:HOH:O	1.50	1.10
1:C:54:ILE:HG22	1:C:58:MET:HE3	1.38	1.01
1:A:353:GLY:HA3	1:C:214:VAL:HG23	1.41	0.98
1:A:44:ALA:HA	1:A:49:THR:HG23	1.46	0.96
1:A:247:PHE:HZ	1:A:324:VAL:HG11	1.25	0.95
1:B:289:ASN:ND2	1:B:292:ILE:H	1.67	0.93
1:A:247:PHE:CZ	1:A:324:VAL:HG11	2.05	0.92
1:A:215:GLY:H	1:C:352:ASN:HD21	1.22	0.88
1:C:54:ILE:HG22	1:C:58:MET:CE	2.04	0.86
1:C:157:VAL:HB	1:C:158:PRO:HD2	1.59	0.83
1:B:289:ASN:HD22	1:B:292:ILE:H	1.21	0.83
1:A:294:LYS:HE3	1:D:291:LEU:HD21	1.61	0.82
1:C:126:LYS:HG2	3:C:513:HOH:O	1.79	0.82
1:B:157:VAL:O	1:B:160:GLY:HA2	1.85	0.76
1:C:43:GLU:CD	1:C:43:GLU:H	1.87	0.76
1:B:289:ASN:HD21	1:B:291:LEU:HB2	1.51	0.74
1:A:353:GLY:HA3	1:C:214:VAL:CG2	2.17	0.72
1:B:173:SER:OG	1:B:174:PRO:HD3	1.90	0.71
1:B:291:LEU:HD12	1:C:291:LEU:HD23	1.71	0.71
1:D:54:ILE:HG22	1:D:58:MET:HE3	1.72	0.71
1:C:156:LYS:HG3	3:C:533:HOH:O	1.92	0.69
1:A:216:LEU:H	1:A:366:ASN:HD22	1.41	0.69
1:D:216:LEU:H	1:D:366:ASN:HD22	1.41	0.69
1:A:353:GLY:CA	1:C:214:VAL:HG23	2.18	0.68
1:A:388:GLN:NE2	1:B:269:TRP:HE1	1.91	0.68
1:A:353:GLY:HA2	1:A:358:PHE:CG	2.29	0.68
1:C:269:TRP:HE1	1:D:388:GLN:NE2	1.92	0.68
1:D:216:LEU:H	1:D:366:ASN:ND2	1.92	0.68
1:C:56:ARG:NH2	1:C:131:GLU:HG3	2.10	0.67
1:D:56:ARG:HH12	1:D:60:GLU:HG2	1.59	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:99:MET:CE	1:C:219:SER:HA	2.25	0.66
1:C:269:TRP:HE1	1:D:388:GLN:HE22	1.42	0.66
1:A:329:ILE:HD11	1:A:330:MET:CE	2.26	0.66
1:D:138:LEU:HD13	1:D:246:PRO:HB3	1.77	0.65
1:D:171:THR:O	1:D:172:ASN:HB2	1.97	0.65
1:A:216:LEU:H	1:A:366:ASN:ND2	1.94	0.63
1:D:92:VAL:O	1:D:362:ARG:NH1	2.32	0.63
1:A:66:PRO:HG2	1:A:82:TYR:CD2	2.35	0.62
1:C:141:PRO:HD3	1:C:168:MET:HB2	1.81	0.62
1:A:388:GLN:HE22	1:B:269:TRP:HE1	1.49	0.61
1:A:363:HIS:HD2	3:A:396:HOH:O	1.84	0.61
1:B:289:ASN:ND2	1:B:292:ILE:N	2.45	0.60
1:A:329:ILE:HD11	1:A:330:MET:HE1	1.84	0.60
1:B:186:ASP:HB3	1:B:191:ASP:N	2.16	0.60
1:C:54:ILE:CG2	1:C:58:MET:CE	2.79	0.60
1:A:294:LYS:HE3	1:D:291:LEU:CD2	2.30	0.60
1:C:361:ALA:O	1:C:365:VAL:HG22	2.02	0.60
1:C:206:SER:HB2	1:C:225:VAL:HB	1.84	0.59
1:C:216:LEU:H	1:C:366:ASN:ND2	2.00	0.59
1:C:216:LEU:H	1:C:366:ASN:HD22	1.50	0.59
1:C:90:GLU:OE2	1:C:94:SER:OG	2.07	0.59
1:C:99:MET:HE3	1:C:219:SER:HA	1.85	0.58
1:D:331:LYS:HE2	1:D:335:CYS:SG	2.42	0.58
1:D:56:ARG:NH1	1:D:60:GLU:HG2	2.17	0.58
1:A:392:GLN:HG2	1:A:394:PHE:HD2	1.68	0.58
1:C:363:HIS:HD2	3:C:502:HOH:O	1.87	0.58
1:C:157:VAL:HB	1:C:158:PRO:CD	2.30	0.58
1:A:247:PHE:HZ	1:A:324:VAL:CG1	2.09	0.58
1:D:54:ILE:HG22	1:D:58:MET:CE	2.33	0.57
1:D:281:GLN:HB2	1:D:286:LEU:HD11	1.86	0.57
1:B:216:LEU:H	1:B:366:ASN:ND2	2.03	0.57
1:A:372:THR:HG21	1:C:350:GLY:HA2	1.85	0.57
1:B:286:LEU:O	1:B:289:ASN:HB3	2.04	0.56
1:A:49:THR:HG21	3:A:431:HOH:O	2.06	0.55
1:B:363:HIS:HD2	3:B:397:HOH:O	1.88	0.55
1:B:216:LEU:H	1:B:366:ASN:HD22	1.54	0.55
1:A:362:ARG:NH1	3:A:432:HOH:O	2.39	0.55
1:C:243:LEU:O	1:C:246:PRO:HD2	2.07	0.55
1:D:316:MET:HB3	1:D:322:ALA:HB2	1.89	0.54
1:B:335:CYS:HB3	1:B:371:ASN:OD1	2.06	0.54
1:B:316:MET:HB3	1:B:322:ALA:HB2	1.88	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:43:GLU:OE2	1:D:46:ARG:NH1	2.40	0.54
1:A:291:LEU:HD13	1:D:291:LEU:HD11	1.90	0.54
1:A:372:THR:HG22	1:A:372:THR:O	2.08	0.54
1:A:329:ILE:CD1	1:A:330:MET:CE	2.86	0.54
1:D:147:PRO:HD3	1:D:243:LEU:HD11	1.90	0.54
1:B:66:PRO:HG3	1:B:82:TYR:CD2	2.42	0.54
1:A:329:ILE:CD1	1:A:330:MET:HE2	2.38	0.53
1:C:40:ARG:O	1:C:43:GLU:HG2	2.08	0.53
1:D:70:GLU:HA	1:D:74:GLY:O	2.08	0.53
1:C:322:ALA:N	3:C:525:HOH:O	2.39	0.53
1:D:171:THR:HG22	3:D:415:HOH:O	2.08	0.53
1:C:168:MET:SD	1:C:223:GLU:HG2	2.49	0.53
1:C:171:THR:O	1:C:172:ASN:HB2	2.09	0.53
1:B:21:ASP:O	1:B:25:VAL:HG23	2.09	0.52
1:C:38:ALA:HB3	1:C:39:PRO:HD3	1.91	0.52
1:C:43:GLU:N	1:C:43:GLU:CD	2.61	0.52
1:B:289:ASN:HD22	1:B:289:ASN:C	2.13	0.52
1:C:114:PHE:CD1	1:C:240:VAL:HB	2.44	0.52
1:D:41:VAL:HG21	1:D:93:ASP:HB2	1.92	0.52
1:D:70:GLU:O	1:D:71:GLN:C	2.48	0.51
1:C:388:GLN:NE2	1:D:269:TRP:HE1	2.08	0.51
1:D:280:LYS:HA	1:D:284:ARG:O	2.11	0.51
1:D:210:ILE:HG13	1:D:222:GLY:HA2	1.93	0.50
1:B:213:LYS:HD2	1:D:352:ASN:ND2	2.26	0.50
1:A:339:LEU:O	1:A:343:ARG:HG3	2.10	0.50
1:C:117:ASP:O	1:C:121:GLU:HG2	2.12	0.50
1:C:92:VAL:O	1:C:362:ARG:NH1	2.45	0.50
1:B:186:ASP:OD1	1:B:186:ASP:N	2.44	0.49
1:A:244:ARG:NH1	3:A:454:HOH:O	2.46	0.49
1:A:186:ASP:OD1	1:A:186:ASP:C	2.51	0.49
1:B:98:SER:O	1:B:102:VAL:HG23	2.12	0.48
1:D:353:GLY:O	1:D:355:SER:N	2.45	0.48
1:A:99:MET:CE	1:A:219:SER:HA	2.43	0.48
1:B:94:SER:HB2	1:B:366:ASN:HB3	1.95	0.48
1:D:102:VAL:HG22	1:D:106:LEU:HD12	1.95	0.48
1:A:313:LEU:HG	1:A:326:ILE:HG22	1.95	0.48
1:D:148:GLY:N	1:D:149:SER:HA	2.28	0.48
1:D:275:TYR:HD1	1:D:357:GLU:HG2	1.79	0.48
1:B:363:HIS:CD2	3:B:397:HOH:O	2.65	0.47
1:B:140:GLU:OE2	1:B:150:MET:HB2	2.14	0.47
1:A:171:THR:O	1:A:172:ASN:HB2	2.15	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:14:LEU:HD12	1:C:311:LEU:HD22	1.96	0.47
1:C:54:ILE:CG2	1:C:58:MET:HE2	2.44	0.47
1:D:149:SER:HB3	1:D:184:LYS:NZ	2.30	0.47
1:D:119:GLN:HE21	1:D:235:ASN:HA	1.79	0.47
1:A:329:ILE:HD13	1:A:330:MET:HE2	1.97	0.46
1:B:289:ASN:C	1:B:289:ASN:ND2	2.68	0.46
1:A:40:ARG:NH2	1:A:57:GLU:OE2	2.48	0.46
1:D:150:MET:HE1	1:D:182:TRP:HB2	1.98	0.46
1:C:295:LYS:O	1:C:299:MET:HG3	2.16	0.46
1:D:13:LEU:HB3	1:D:16:GLN:HG3	1.98	0.46
1:A:44:ALA:HA	1:A:49:THR:CG2	2.31	0.46
1:A:299:MET:HG2	1:A:341:ILE:HG23	1.98	0.46
1:A:94:SER:HB2	1:A:366:ASN:HB3	1.98	0.46
1:D:363:HIS:HD2	3:D:396:HOH:O	1.98	0.45
1:B:61:ILE:HG13	1:B:63:LEU:HG	1.98	0.45
1:D:147:PRO:HG2	1:D:149:SER:HA	1.98	0.45
1:D:45:PHE:CD1	1:D:217:ARG:HB2	2.52	0.45
1:B:140:GLU:HG2	1:B:166:SER:O	2.17	0.45
1:B:106:LEU:HB3	1:B:136:PHE:HB2	1.99	0.45
1:D:281:GLN:HG2	1:D:282:PHE:HD1	1.81	0.44
1:B:157:VAL:HB	1:B:158:PRO:HD2	1.98	0.44
1:C:80:VAL:O	1:C:84:LEU:HG	2.16	0.44
1:D:106:LEU:HB3	1:D:136:PHE:CD2	2.52	0.44
1:A:353:GLY:CA	1:C:214:VAL:CG2	2.87	0.44
1:D:148:GLY:H	1:D:149:SER:HA	1.81	0.44
1:B:331:LYS:HE2	1:B:335:CYS:SG	2.58	0.44
1:C:21:ASP:O	1:C:25:VAL:HG23	2.17	0.44
1:A:20:ASP:OD1	1:A:23:ARG:NH1	2.50	0.44
1:A:352:ASN:HB3	1:C:169:TRP:CZ3	2.53	0.44
1:A:379:ILE:HD11	1:C:281:GLN:HE22	1.83	0.44
1:A:269:TRP:HE1	1:B:388:GLN:NE2	2.16	0.44
1:C:388:GLN:HE22	1:D:269:TRP:HE1	1.66	0.44
1:D:51:ASP:OD1	1:D:52:ALA:N	2.51	0.43
1:D:62:GLY:HA2	3:D:423:HOH:O	2.17	0.43
1:D:179:PHE:CD2	1:D:179:PHE:N	2.86	0.43
1:A:99:MET:HE2	1:A:219:SER:HA	2.00	0.43
1:A:141:PRO:O	1:A:142:ASN:HB2	2.19	0.43
1:A:78:ASP:HB2	1:A:318:ASP:OD2	2.19	0.43
1:D:136:PHE:O	1:D:170:ILE:HD12	2.18	0.43
1:A:78:ASP:HB2	1:A:318:ASP:CG	2.38	0.42
1:B:124:LEU:HB2	1:B:125:PRO:HD3	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:174:PRO:HA	1:C:207:ALA:HB1	2.02	0.42
1:A:65:GLY:N	1:A:66:PRO:CD	2.83	0.42
1:B:289:ASN:HD21	1:B:291:LEU:CB	2.27	0.42
1:A:133:ILE:HD13	1:A:175:ILE:HD12	2.01	0.42
1:D:96:TYR:HA	1:D:99:MET:HE3	2.02	0.42
1:C:266:GLU:OE1	1:C:307:LEU:HD11	2.19	0.42
1:D:103:GLN:OE1	1:D:134:GLY:N	2.45	0.42
1:D:281:GLN:HB2	1:D:286:LEU:CD1	2.50	0.41
1:C:279:ARG:HA	1:C:279:ARG:HD3	1.77	0.41
1:A:296:LEU:HB3	1:B:388:GLN:HE22	1.85	0.41
1:C:42:THR:O	1:C:46:ARG:HB2	2.20	0.41
1:D:168:MET:HG3	1:D:169:TRP:CD1	2.56	0.41
1:B:220:ILE:HG13	1:B:221:THR:N	2.34	0.41
1:D:22:GLU:OE1	1:D:78:ASP:OD2	2.38	0.41
1:B:254:ARG:NE	1:B:374:GLU:OE1	2.49	0.41
1:B:36:LYS:O	1:B:40:ARG:HG3	2.21	0.41
1:C:94:SER:HB2	1:C:366:ASN:HB3	2.03	0.41
1:B:43:GLU:OE1	1:B:46:ARG:NH1	2.54	0.41
1:D:44:ALA:HA	1:D:49:THR:HB	2.02	0.41
1:D:81:SER:O	1:D:85:ILE:HG13	2.20	0.41
1:A:210:ILE:HG13	1:A:222:GLY:HA2	2.02	0.41
1:D:65:GLY:N	1:D:66:PRO:HD3	2.36	0.41
1:C:19:ALA:O	1:C:22:GLU:HB2	2.21	0.41
1:D:277:LEU:HD12	1:D:277:LEU:HA	1.90	0.41
1:D:94:SER:HB2	1:D:366:ASN:HB3	2.02	0.40
1:C:99:MET:HE2	1:C:219:SER:HA	2.02	0.40
1:C:41:VAL:HG21	1:C:93:ASP:HB2	2.03	0.40
1:B:170:ILE:HG21	1:B:224:ILE:HD11	2.03	0.40
1:D:45:PHE:CE1	1:D:217:ARG:HB2	2.57	0.40
1:B:68:ILE:HA	1:B:69:PRO:HD3	1.98	0.40
1:B:83:GLY:HA3	1:B:259:TRP:CD1	2.56	0.40
1:C:78:ASP:HB2	1:C:318:ASP:OD1	2.22	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	377/396 (95%)	361 (96%)	15 (4%)	1 (0%)	41	51
1	B	367/396 (93%)	353 (96%)	11 (3%)	3 (1%)	19	27
1	C	376/396 (95%)	360 (96%)	16 (4%)	0	100	100
1	D	370/396 (93%)	355 (96%)	14 (4%)	1 (0%)	41	51
All	All	1490/1584 (94%)	1429 (96%)	56 (4%)	5 (0%)	41	51

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	190	ARG
1	B	158	PRO
1	D	158	PRO
1	B	160	GLY
1	B	284	ARG

### 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	304/313 (97%)	284 (93%)	20 (7%)	16	22
1	B	298/313 (95%)	282 (95%)	16 (5%)	22	29
1	C	302/313 (96%)	280 (93%)	22 (7%)	14	18
1	D	301/313 (96%)	278 (92%)	23 (8%)	13	17
All	All	1205/1252 (96%)	1124 (93%)	81 (7%)	16	21

All (81) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	36	LYS

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Mol	Chain	Res	Type
1	A	49	THR
1	A	67	THR
1	A	100	MET
1	A	151	VAL
1	A	171	THR
1	A	186	ASP
1	A	202	CYS
1	A	219	SER
1	A	220	ILE
1	A	237	LEU
1	A	243	LEU
1	A	277	LEU
1	A	280	LYS
1	A	281	GLN
1	A	291	LEU
1	A	313	LEU
1	A	329	ILE
1	A	357	GLU
1	A	392	GLN
1	B	100	MET
1	B	156	LYS
1	B	166	SER
1	B	171	THR
1	B	191	ASP
1	B	202	CYS
1	B	220	ILE
1	B	223	GLU
1	B	228	GLU
1	B	237	LEU
1	B	241	LYS
1	B	243	LEU
1	B	277	LEU
1	B	289	ASN
1	B	291	LEU
1	B	313	LEU
1	C	5	THR
1	C	43	GLU
1	C	100	MET
1	C	113	GLU
1	C	151	VAL
1	C	164	SER
1	C	166	SER

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Mol	Chain	Res	Type
1	C	171	THR
1	C	188	ASP
1	C	191	ASP
1	C	202	CYS
1	C	219	SER
1	C	235	ASN
1	C	237	LEU
1	C	243	LEU
1	C	277	LEU
1	C	279	ARG
1	C	324	VAL
1	C	331	LYS
1	C	352	ASN
1	C	365	VAL
1	C	392	GLN
1	D	20	ASP
1	D	61	ILE
1	D	100	MET
1	D	126	LYS
1	D	149	SER
1	D	150	MET
1	D	156	LYS
1	D	164	SER
1	D	171	THR
1	D	184	LYS
1	D	186	ASP
1	D	202	CYS
1	D	237	LEU
1	D	277	LEU
1	D	284	ARG
1	D	291	LEU
1	D	293	GLN
1	D	324	VAL
1	D	344	LEU
1	D	357	GLU
1	D	372	THR
1	D	374	GLU
1	D	392	GLN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (22) such sidechains are listed below:



Mol	Chain	Res	Type
1	A	290	GLN
1	A	293	GLN
1	A	363	HIS
1	A	366	ASN
1	A	388	GLN
1	B	289	ASN
1	B	293	GLN
1	B	363	HIS
1	B	366	ASN
1	B	388	GLN
1	C	235	ASN
1	C	274	GLN
1	C	281	GLN
1	C	290	GLN
1	C	352	ASN
1	C	363	HIS
1	C	366	ASN
1	C	388	GLN
1	D	293	GLN
1	D	363	HIS
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 carbohydrates in this entry.

### 5.6 Ligand geometry [i](#)

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	341	C	501	-	10,10,10	0.94	0	13,13,13	1.57	4 (30%)

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	341	C	501	-	-	0/2/2/2	0/1/1/1

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	501	341	C2-C3-C4	-2.78	120.00	123.52
2	C	501	341	C1-C2-C3	2.49	120.00	116.13
2	C	501	341	C2-C1-C6	-2.44	120.44	123.52
2	C	501	341	F7-C3-C4	2.11	121.26	118.25

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 [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, 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	383/396 (96%)	-0.28	2 (0%) 91 94	25, 41, 64, 74	0
1	B	375/396 (94%)	-0.36	2 (0%) 91 94	23, 40, 56, 72	0
1	C	382/396 (96%)	-0.29	4 (1%) 82 86	24, 42, 63, 72	0
1	D	380/396 (95%)	-0.25	5 (1%) 77 82	24, 43, 61, 70	0
All	All	1520/1584 (95%)	-0.29	13 (0%) 84 88	23, 42, 62, 74	0

All (13) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	354	ILE	4.0
1	C	201	GLY	3.7
1	D	282	PHE	3.7
1	C	169	TRP	3.2
1	C	226	LEU	3.2
1	C	170	ILE	3.2
1	D	357	GLU	2.6
1	B	205	LEU	2.2
1	B	243	LEU	2.2
1	D	148	GLY	2.1
1	A	189	GLY	2.1
1	D	169	TRP	2.1
1	D	50	THR	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 [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. The B-factors column lists the minimum, median, 95<sup>th</sup> 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	B-factors( $\text{\AA}^2$ )	Q<0.9
2	341	C	501	10/10	0.87	0.19	71,74,74,74	0

### 6.5 Other polymers [i](#)

There are no such residues in this entry.