



# Full wwPDB X-ray Structure Validation Report ⓘ

Sep 16, 2017 – 06:52 PM EDT

PDB ID : 5IKL  
Title : Crystal structure of *P. aeruginosa* geranyl-CoA carboxylase (GCC), beta subunit  
Authors : Huang, C.S.; Jurado, A.R.; Tong, L.  
Deposited on : unknown  
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](mailto: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.

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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
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20029824
Percentile statistics	:	20161228.v01 (using entries in the PDB archive December 28th 2016)
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)	:	rb-20029824

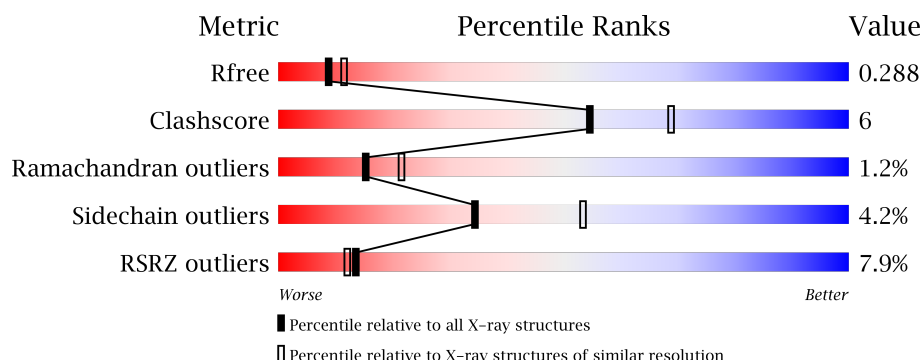
# 1 Overall quality at a glance

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))
$R_{free}$	100719	3166 (2.40-2.40)
Clashscore	112137	3674 (2.40-2.40)
Ramachandran outliers	110173	3616 (2.40-2.40)
Sidechain outliers	110143	3617 (2.40-2.40)
RSRZ outliers	101464	3195 (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. 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	B	537	 6% 81% 13% • •
1	D	537	 7% 79% 16% • 5%
1	F	537	 9% 70% 15% • 14%

## 2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 11146 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 Geranyl-CoA carboxylase, beta-subunit.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	B	514	Total	C	N	O	S	0	0	0
			3849	2424	683	725	17			
1	D	512	Total	C	N	O	S	0	0	0
			3836	2417	681	721	17			
1	F	460	Total	C	N	O	S	0	0	0
			3437	2171	605	645	16			

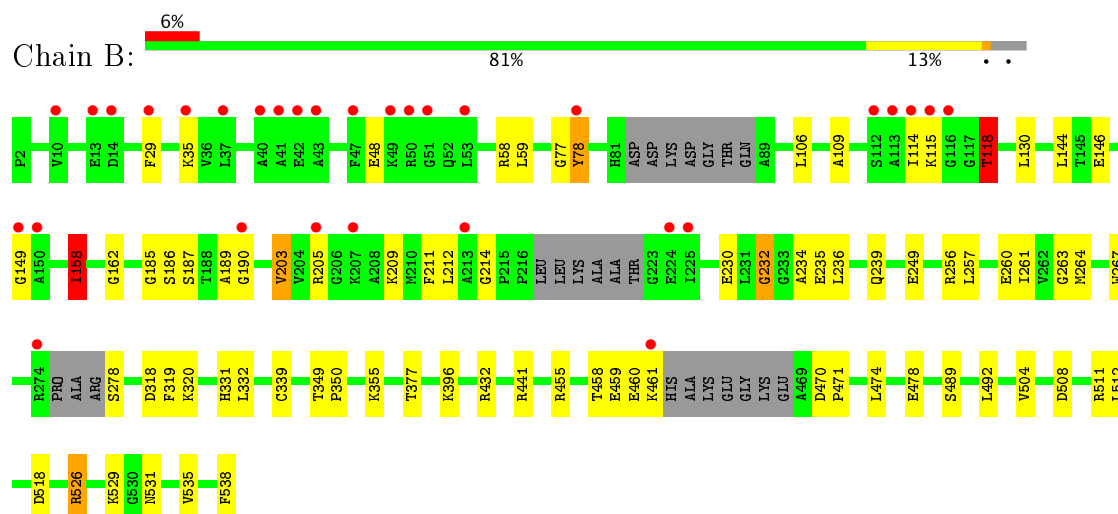
- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	B	7	Total	O	0	0
			7	7		
2	D	5	Total	O	0	0
			5	5		
2	F	12	Total	O	0	0
			12	12		

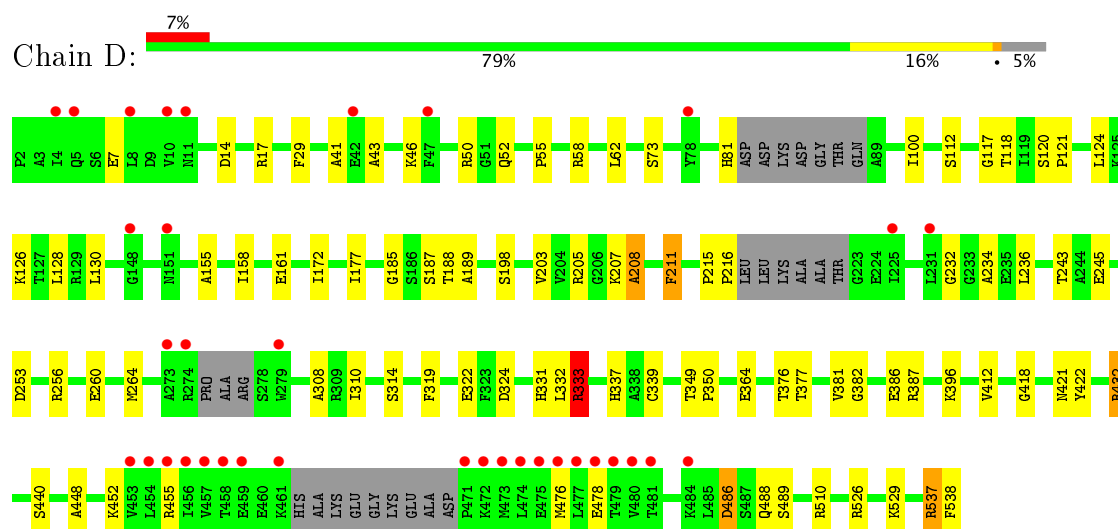
### 3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of 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: Geranyl-CoA carboxylase, beta-subunit



- Molecule 1: Geranyl-CoA carboxylase, beta-subunit



- Molecule 1: Geranyl-CoA carboxylase, beta-subunit





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 65 2 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	105.72Å 105.72Å 550.76Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	47.20 – 2.40 47.20 – 2.40	Depositor EDS
% Data completeness (in resolution range)	99.6 (47.20-2.40) 99.7 (47.20-2.40)	Depositor EDS
$R_{merge}$	0.08	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	3.03 (at 2.39Å)	Xtriage
Refinement program	REFMAC 5.8.0049	Depositor
R, $R_{free}$	0.215 , 0.282 0.228 , 0.288	Depositor DCC
$R_{free}$ test set	3660 reflections (5.32%)	DCC
Wilson B-factor (Å <sup>2</sup> )	48.2	Xtriage
Anisotropy	0.610	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.36 , 55.0	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.47$ , $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.93	EDS
Total number of atoms	11146	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	66.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.18% 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](#)

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 5$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
1	B	0.64	0/3915	0.79	4/5291 (0.1%)
1	D	0.66	0/3902	0.81	4/5272 (0.1%)
1	F	0.60	0/3497	0.76	1/4731 (0.0%)
All	All	0.63	0/11314	0.79	9/15294 (0.1%)

There are no bond length outliers.

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	432	ARG	NE-CZ-NH2	-7.57	116.52	120.30
1	B	432	ARG	CG-CD-NE	-7.52	96.01	111.80
1	D	526	ARG	NE-CZ-NH1	-6.32	117.14	120.30
1	B	432	ARG	NE-CZ-NH2	-5.65	117.48	120.30
1	B	526	ARG	NE-CZ-NH2	-5.27	117.66	120.30
1	D	333	ARG	NE-CZ-NH2	-5.21	117.69	120.30
1	D	537	ARG	NE-CZ-NH1	5.17	122.88	120.30
1	F	106	LEU	CA-CB-CG	-5.12	103.53	115.30
1	B	526	ARG	NE-CZ-NH1	5.07	122.83	120.30

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	B	3849	0	3869	39	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	D	3836	0	3861	50	0
1	F	3437	0	3460	60	0
2	B	7	0	0	0	0
2	D	5	0	0	0	0
2	F	12	0	0	1	0
All	All	11146	0	11190	134	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 (134) 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:F:78:TYR:O	1:F:81:HIS:NE2	2.19	0.76
1:B:263:GLY:O	1:F:333:ARG:NH2	2.25	0.69
1:F:78:TYR:O	1:F:81:HIS:CD2	2.48	0.67
1:B:508:ASP:OD1	1:B:511:ARG:NH1	2.27	0.67
1:F:194:GLN:HG3	1:F:195:PRO:HD3	1.76	0.66
1:B:320:LYS:HG3	1:D:245:GLU:HA	1.77	0.65
1:F:54:LEU:HD12	1:F:57:GLU:OE2	1.98	0.64
1:F:488:GLN:O	1:F:490:THR:N	2.31	0.63
1:F:332:LEU:HD13	1:F:334:ILE:HG13	1.81	0.62
1:D:253:ASP:OD1	1:D:256:ARG:NH1	2.32	0.62
1:F:146:GLU:O	1:F:186:SER:O	2.18	0.61
1:B:256:ARG:O	1:B:260:GLU:HG2	2.01	0.61
1:D:331:HIS:HB2	1:F:264:MET:HG2	1.84	0.60
1:B:106:LEU:HD21	1:B:130:LEU:HB3	1.83	0.60
1:D:52:GLN:HG2	1:D:207:LYS:HE3	1.83	0.60
1:D:198:SER:O	1:D:537:ARG:NH2	2.35	0.60
1:D:207:LYS:O	1:D:208:ALA:HB2	2.02	0.59
1:B:396:LYS:HD2	1:D:538:PHE:CE1	2.39	0.57
1:F:155:ALA:O	1:F:159:PHE:HB3	2.05	0.57
1:F:488:GLN:O	1:F:490:THR:OG1	2.20	0.56
1:F:203:VAL:HG11	1:F:234:ALA:HA	1.88	0.56
1:B:455:ARG:NH1	1:B:478:GLU:OE1	2.39	0.56
1:D:452:LYS:O	1:D:455:ARG:HB3	2.07	0.55
1:F:280:ARG:O	1:F:281:GLU:HB2	2.06	0.55
1:F:121:PRO:HA	1:F:158:ILE:HD11	1.88	0.54
1:B:115:LYS:O	1:B:118:THR:OG1	2.24	0.54
1:B:332:LEU:C	1:D:264:MET:HE1	2.28	0.54
1:D:232:GLY:HA2	1:D:236:LEU:HD23	1.88	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:538:PHE:CE1	1:F:396:LYS:HD2	2.42	0.53
1:F:374:HIS:HB2	1:F:412:VAL:HA	1.91	0.53
1:B:203:VAL:HG13	1:B:234:ALA:HB1	1.91	0.53
1:F:332:LEU:C	1:F:332:LEU:HD12	2.29	0.53
1:D:112:SER:HA	1:D:117:GLY:N	2.24	0.52
1:F:339:CYS:HA	1:F:368:THR:CG2	2.39	0.52
1:F:77:GLY:HA2	1:F:80:LEU:HD12	1.92	0.52
1:F:167:ALA:O	1:F:171:ARG:HG3	2.10	0.52
1:F:126:LYS:HA	1:F:498:LEU:HD21	1.92	0.52
1:F:290:LEU:HD13	1:F:290:LEU:O	2.10	0.52
1:D:185:GLY:O	1:D:208:ALA:HA	2.11	0.52
1:D:203:VAL:HG13	1:D:234:ALA:HB1	1.92	0.52
1:D:188:THR:HG21	1:D:211:PHE:CE1	2.46	0.51
1:F:341:LEU:HD11	1:F:373:LEU:CD1	2.41	0.51
1:B:205:ARG:NH2	1:B:249:GLU:OE1	2.44	0.50
1:B:441:ARG:HA	1:B:489:SER:O	2.13	0.49
1:F:448:ALA:HB3	1:F:449:GLN:HE21	1.77	0.49
1:F:189:ALA:HA	1:F:212:LEU:O	2.13	0.49
1:F:303:VAL:HA	1:F:306:ILE:HD12	1.95	0.49
1:D:486:ASP:HA	1:D:489:SER:HB3	1.94	0.49
1:D:333:ARG:HD2	1:F:264:MET:HE3	1.94	0.49
1:B:257:LEU:O	1:B:261:ILE:HG13	2.13	0.48
1:B:492:LEU:HD23	1:B:492:LEU:C	2.32	0.48
1:F:307:VAL:HG22	1:F:341:LEU:HD13	1.96	0.48
1:F:56:ARG:HG2	1:F:94:ILE:CD1	2.43	0.48
1:F:350:PRO:HG3	1:F:390:VAL:HB	1.96	0.48
1:D:172:ILE:HG23	1:D:177:ILE:HB	1.97	0.47
1:D:333:ARG:HD2	1:F:264:MET:CE	2.44	0.47
1:D:55:PRO:O	1:D:58:ARG:HB2	2.14	0.47
1:D:412:VAL:HG12	1:D:440:SER:HB2	1.94	0.47
1:F:401:VAL:HG12	1:F:429:LEU:HD12	1.96	0.47
1:F:455:ARG:HD2	1:F:474:LEU:CD1	2.44	0.47
1:B:118:THR:HA	1:B:149:GLY:O	2.15	0.47
1:B:211:PHE:CE1	1:B:214:GLY:HA2	2.50	0.47
1:F:452:LYS:O	1:F:456:ILE:HD12	2.15	0.47
1:F:159:PHE:CE2	1:F:160:VAL:HG23	2.49	0.47
1:F:297:PRO:HB2	1:F:414:GLY:CA	2.45	0.47
1:B:458:THR:C	1:B:460:GLU:H	2.18	0.46
1:F:203:VAL:HG12	1:F:208:ALA:HB3	1.98	0.46
1:D:17:ARG:HB2	1:D:17:ARG:CZ	2.45	0.46
1:D:188:THR:O	1:D:189:ALA:HB3	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:293:VAL:HG13	1:F:301:TYR:CE2	2.51	0.46
1:B:235:GLU:O	1:B:239:GLN:HG2	2.14	0.46
1:D:256:ARG:O	1:D:260:GLU:HG3	2.16	0.46
1:D:308:ALA:O	1:D:314:SER:OG	2.23	0.46
1:F:280:ARG:O	1:F:281:GLU:CB	2.64	0.46
1:B:209:LYS:HA	1:B:232:GLY:O	2.16	0.45
1:D:422:TYR:CD1	1:D:422:TYR:N	2.79	0.45
1:D:333:ARG:HA	1:D:337:HIS:O	2.16	0.45
1:B:455:ARG:HG3	1:B:474:LEU:HB3	1.99	0.45
1:D:126:LYS:O	1:D:130:LEU:HG	2.17	0.45
1:D:46:LYS:O	1:D:50:ARG:HG2	2.17	0.45
1:F:56:ARG:HG2	1:F:94:ILE:HD13	1.98	0.45
1:D:124:LEU:HD21	1:D:128:LEU:HD11	1.99	0.45
1:F:417:TYR:HA	1:F:443:ALA:O	2.17	0.45
1:B:529:LYS:CD	2:F:610:HOH:O	2.64	0.44
1:D:120:SER:HB2	1:D:121:PRO:HD2	1.98	0.44
1:D:207:LYS:O	1:D:208:ALA:CB	2.65	0.44
1:D:62:LEU:HG	1:D:100:ILE:HD12	1.98	0.44
1:F:453:VAL:O	1:F:457:VAL:HG13	2.17	0.44
1:F:441:ARG:HH21	1:F:490:THR:HA	1.83	0.44
1:B:205:ARG:NE	1:B:249:GLU:OE1	2.48	0.44
1:B:267:TRP:O	1:B:526:ARG:NH2	2.50	0.44
1:B:460:GLU:O	1:B:461:LYS:C	2.56	0.44
1:D:73:SER:HB2	1:D:126:LYS:HE3	2.00	0.44
1:F:293:VAL:HG13	1:F:301:TYR:CZ	2.52	0.44
1:B:189:ALA:HA	1:B:212:LEU:HA	2.00	0.44
1:F:98:GLY:O	1:F:104:ARG:HA	2.18	0.44
1:B:504:VAL:HG11	1:B:512:LEU:HD22	1.99	0.43
1:D:418:GLY:O	1:D:421:ASN:HB3	2.17	0.43
1:B:470:ASP:HA	1:B:471:PRO:HD2	1.92	0.43
1:B:535:VAL:HG13	1:F:361:GLN:HG2	2.00	0.43
1:D:396:LYS:HD2	1:F:538:PHE:CE1	2.54	0.43
1:F:382:GLY:O	1:F:386:GLU:HG2	2.19	0.42
1:D:62:LEU:HG	1:D:100:ILE:CD1	2.49	0.42
1:F:260:GLU:O	1:F:264:MET:HB2	2.19	0.42
1:B:59:LEU:HD21	1:B:109:ALA:HB2	2.01	0.42
1:B:264:MET:HE2	1:F:332:LEU:N	2.34	0.42
1:B:349:THR:HB	1:B:350:PRO:HD2	2.01	0.42
1:B:77:GLY:O	1:B:78:TYR:C	2.58	0.42
1:F:303:VAL:HG22	1:F:373:LEU:HD12	2.02	0.42
1:D:324:ASP:OD2	1:D:349:THR:OG1	2.27	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:203:VAL:CG1	1:F:208:ALA:HB3	2.50	0.42
1:D:349:THR:HB	1:D:350:PRO:HD2	2.01	0.42
1:F:449:GLN:O	1:F:453:VAL:HG23	2.20	0.42
1:D:310:ILE:O	1:D:510:ARG:NH1	2.49	0.42
1:B:146:GLU:HG3	1:B:185:GLY:HA3	2.02	0.41
1:D:381:VAL:HG12	1:D:382:GLY:H	1.85	0.41
1:D:41:ALA:C	1:D:43:ALA:H	2.24	0.41
1:B:58:ARG:HB3	1:B:144:LEU:HD13	2.02	0.41
1:D:188:THR:CG2	1:D:211:PHE:CE1	3.03	0.41
1:F:302:ASP:OD1	1:F:345:ASN:ND2	2.54	0.41
1:D:331:HIS:HB3	1:F:264:MET:HG3	2.03	0.41
1:D:215:PRO:HB2	1:D:216:PRO:HD3	2.03	0.41
1:D:319:PHE:CE2	1:F:245:GLU:HG2	2.56	0.41
1:F:454:LEU:HD23	1:F:477:LEU:HD22	2.02	0.41
1:B:319:PHE:O	1:B:355:LYS:HE3	2.19	0.41
1:D:155:ALA:O	1:D:158:ILE:HG22	2.21	0.41
1:D:486:ASP:OD1	1:D:486:ASP:N	2.54	0.41
1:B:158:ILE:O	1:B:162:GLY:N	2.54	0.41
1:D:333:ARG:CD	1:F:264:MET:HE3	2.50	0.41
1:F:332:LEU:CD1	1:F:334:ILE:HG13	2.47	0.40
1:B:211:PHE:CE1	1:B:214:GLY:CA	3.05	0.40
1:D:243:THR:HA	1:D:537:ARG:HD2	2.03	0.40
1:B:331:HIS:HB3	1:D:264:MET:HE2	2.04	0.40
1:F:453:VAL:O	1:F:457:VAL:HG22	2.21	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles [i](#)

### 5.3.1 Protein backbone [i](#)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	B	504/537 (94%)	468 (93%)	30 (6%)	6 (1%)	15 21

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	D	502/537 (94%)	465 (93%)	32 (6%)	5 (1%)	18	26
1	F	448/537 (83%)	410 (92%)	32 (7%)	6 (1%)	14	19
All	All	1454/1611 (90%)	1343 (92%)	94 (6%)	17 (1%)	15	21

All (17) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	78	TYR
1	B	118	THR
1	D	208	ALA
1	F	295	ALA
1	F	489	SER
1	B	158	ILE
1	D	118	THR
1	D	488	GLN
1	F	487	SER
1	B	459	GLU
1	D	478	GLU
1	F	155	ALA
1	F	281	GLU
1	F	297	PRO
1	D	448	ALA
1	B	190	GLY
1	B	232	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	B	392/409 (96%)	375 (96%)	17 (4%)	33	52
1	D	391/409 (96%)	370 (95%)	21 (5%)	26	41
1	F	353/409 (86%)	343 (97%)	10 (3%)	49	70
All	All	1136/1227 (93%)	1088 (96%)	48 (4%)	34	53

All (48) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	29	PHE
1	B	35	LYS
1	B	48	GLU
1	B	114	ILE
1	B	118	THR
1	B	158	ILE
1	B	186	SER
1	B	187	SER
1	B	203	VAL
1	B	230	GLU
1	B	236	LEU
1	B	278	SER
1	B	318	ASP
1	B	339	CYS
1	B	377	THR
1	B	518	ASP
1	B	531	ASN
1	D	7	GLU
1	D	14	ASP
1	D	29	PHE
1	D	81	HIS
1	D	161	GLU
1	D	187	SER
1	D	205	ARG
1	D	211	PHE
1	D	322	GLU
1	D	332	LEU
1	D	333	ARG
1	D	339	CYS
1	D	364	GLU
1	D	376	THR
1	D	377	THR
1	D	386	GLU
1	D	387	ARG
1	D	432	ARG
1	D	476	MET
1	D	486	ASP
1	D	529	LYS
1	F	145	THR
1	F	147	SER
1	F	159	PHE
1	F	211	PHE

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Mol	Chain	Res	Type
1	F	278	SER
1	F	289	LEU
1	F	303	VAL
1	F	339	CYS
1	F	461	LYS
1	F	490	THR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	531	ASN
1	D	153	ASN
1	D	365	GLN
1	F	194	GLN
1	F	449	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](#)

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

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	B	514/537 (95%)	0.11	31 (6%) 23 21	37, 59, 96, 121	0
1	D	512/537 (95%)	0.26	35 (6%) 18 16	36, 56, 111, 147	0
1	F	460/537 (85%)	0.46	51 (11%) 6 5	37, 61, 143, 186	0
All	All	1486/1611 (92%)	0.27	117 (7%) 13 12	36, 59, 118, 186	0

All (117) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	F	292	VAL	13.8
1	F	285	PRO	13.4
1	F	286	VAL	13.4
1	F	473	MET	12.3
1	F	291	GLY	11.7
1	F	469	ALA	9.9
1	D	474	LEU	8.6
1	F	461	LYS	8.5
1	F	472	LYS	8.4
1	D	473	MET	8.3
1	D	476	MET	7.9
1	D	457	VAL	7.7
1	F	460	GLU	6.7
1	F	289	LEU	6.6
1	D	472	LYS	6.6
1	F	296	ASP	6.6
1	F	293	VAL	6.3
1	D	454	LEU	6.2
1	D	10	VAL	5.9
1	D	456	ILE	5.8
1	F	485	LEU	5.7
1	D	479	THR	5.6
1	F	299	LYS	5.6

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Mol	Chain	Res	Type	RSRZ
1	D	11	ASN	5.4
1	D	477	LEU	5.3
1	D	471	PRO	5.2
1	D	480	VAL	5.2
1	F	449	GLN	5.0
1	F	484	LYS	4.9
1	B	116	GLY	4.9
1	D	5	GLN	4.8
1	F	457	VAL	4.8
1	B	40	ALA	4.7
1	D	475	GLU	4.7
1	D	458	THR	4.7
1	F	453	VAL	4.6
1	B	47	PHE	4.4
1	D	459	GLU	4.4
1	B	113	ALA	4.4
1	B	50	ARG	4.4
1	D	453	VAL	4.3
1	F	295	ALA	4.2
1	D	478	GLU	4.2
1	B	112	SER	4.1
1	F	456	ILE	4.0
1	F	474	LEU	4.0
1	B	42	GLU	3.8
1	F	478	GLU	3.8
1	B	53	LEU	3.8
1	D	461	LYS	3.6
1	F	287	GLU	3.5
1	F	458	THR	3.5
1	B	114	ILE	3.5
1	D	455	ARG	3.4
1	F	489	SER	3.4
1	D	148	GLY	3.4
1	F	116	GLY	3.3
1	F	225	ILE	3.3
1	B	37	LEU	3.2
1	F	300	PRO	3.2
1	F	480	VAL	3.2
1	F	450	ALA	3.1
1	B	115	LYS	3.1
1	D	274	ARG	3.1
1	F	284	TYR	3.1

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Mol	Chain	Res	Type	RSRZ
1	F	117	GLY	3.1
1	B	225	ILE	3.1
1	D	4	ILE	3.0
1	B	150	ALA	3.0
1	F	297	PRO	2.8
1	B	13	GLU	2.8
1	F	283	LEU	2.8
1	F	290	LEU	2.8
1	F	454	LEU	2.8
1	F	298	LYS	2.8
1	B	49	LYS	2.7
1	F	154	TYR	2.7
1	F	288	GLU	2.6
1	B	14	ASP	2.6
1	F	471	PRO	2.6
1	D	279	TRP	2.6
1	F	112	SER	2.5
1	B	43	ALA	2.5
1	B	207	LYS	2.5
1	B	149	GLY	2.5
1	B	78	TYR	2.5
1	F	52	GLN	2.4
1	F	470	ASP	2.4
1	D	151	ASN	2.4
1	F	476	MET	2.4
1	B	274	ARG	2.3
1	D	273	ALA	2.3
1	B	51	GLY	2.3
1	F	75	LEU	2.3
1	D	47	PHE	2.3
1	D	78	TYR	2.3
1	F	447	GLY	2.3
1	B	213	ALA	2.3
1	B	35	LYS	2.2
1	B	41	ALA	2.2
1	B	10	VAL	2.2
1	B	205	ARG	2.2
1	B	224	GLU	2.2
1	D	42	GLU	2.2
1	F	274	ARG	2.2
1	B	190	GLY	2.1
1	F	492	LEU	2.1

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Mol	Chain	Res	Type	RSRZ
1	F	280	ARG	2.1
1	F	119	ILE	2.1
1	B	461	LYS	2.1
1	D	481	THR	2.1
1	D	231	LEU	2.1
1	D	8	LEU	2.0
1	D	225	ILE	2.0
1	D	484	LYS	2.0
1	B	29	PHE	2.0
1	F	488	GLN	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.