



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 4, 2026 – 10:52 PM UTC

PDB ID : 5IKL / pdb_00005ikl
Title : Crystal structure of P. aeruginosa geranyl-CoA carboxylase (GCC), beta sub-unit
Authors : Huang, C.S.; Jurado, A.R.; Tong, L.
Deposited on : 2016-03-03
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

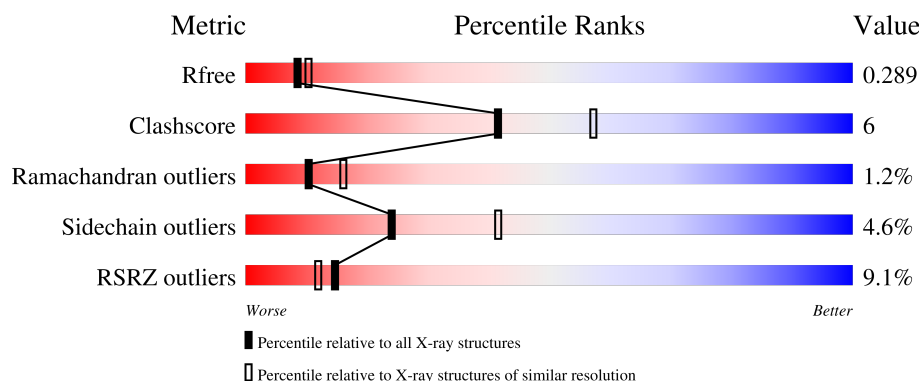
1 Overall quality at a glance

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	B	537	6% 80% 15% • •
1	D	537	9% 77% 17% • 5%
1	F	537	10% 68% 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			

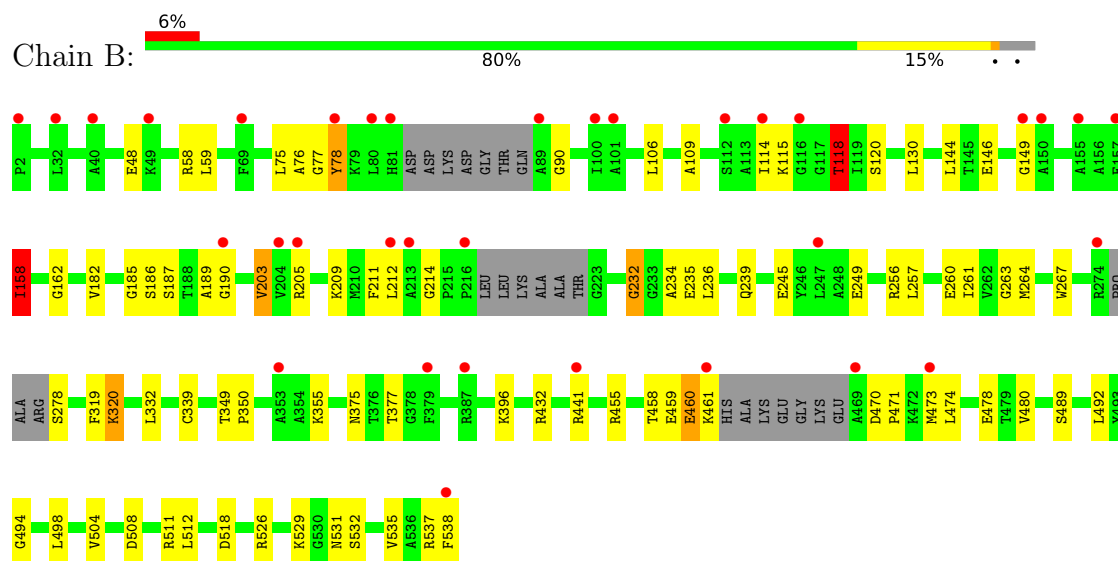
- Molecule 2 is water.

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		

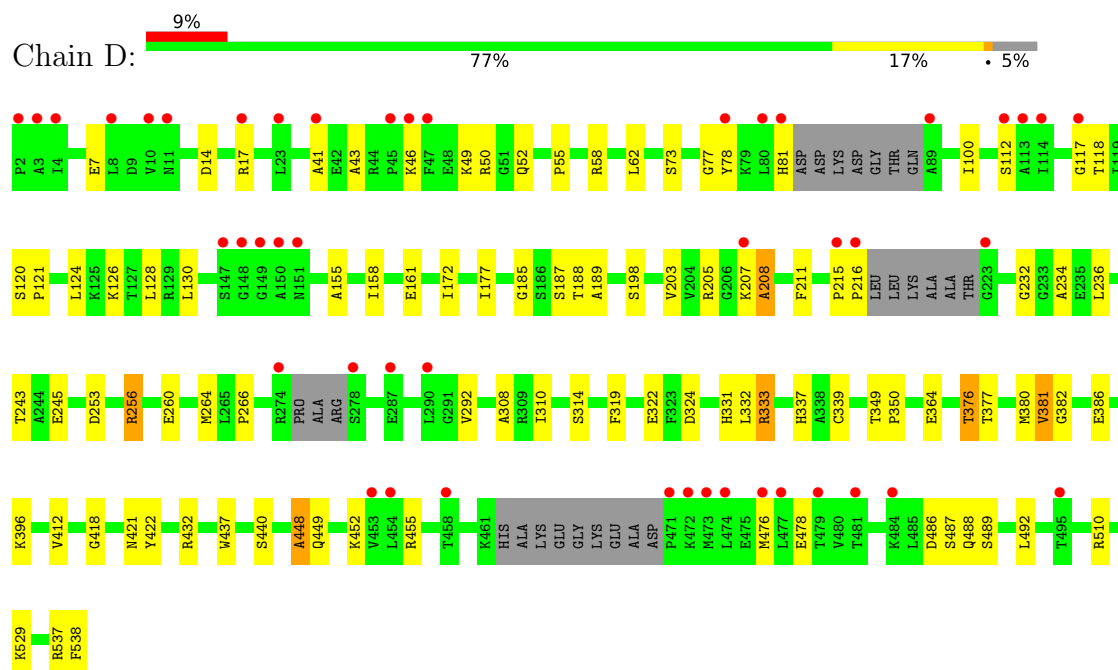
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA, 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: Geranyl-CoA carboxylase, beta-subunit

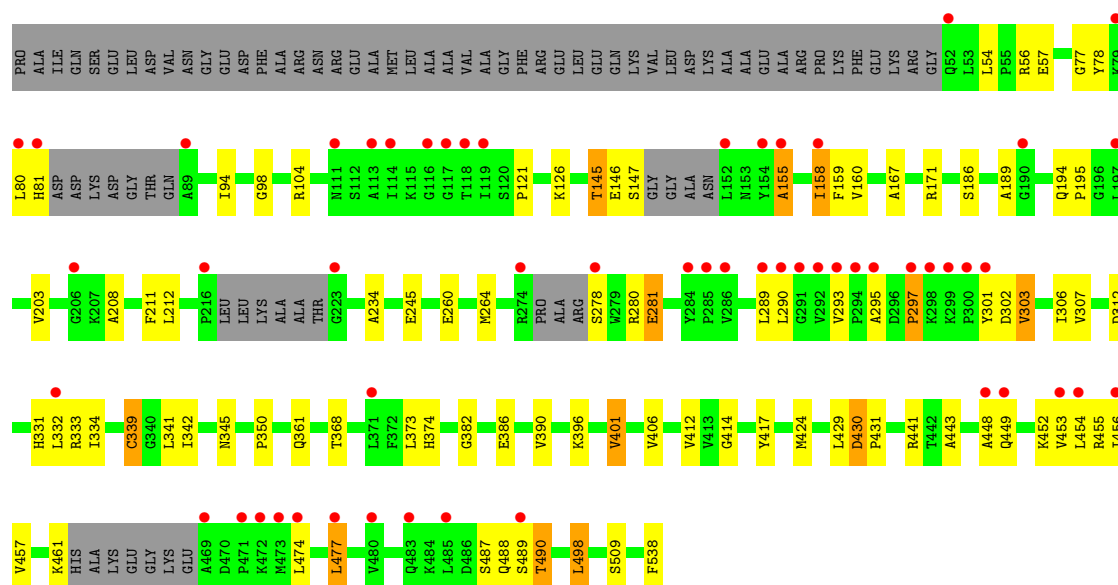


- Molecule 1: Geranyl-CoA carboxylase, beta-subunit



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

Chain F: 10% 68% 15% 14%



4 Data and refinement statistics

Property	Value	Source
Space group	P 65 2 2	Depositor
Cell constants a, b, c, α , β , γ	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) 99.6 (47.20-2.40)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.03 (at 2.39Å)	Xtriage
Refinement program	REFMAC 5.8.0049	Depositor
R, R_{free}	0.215 , 0.282 0.228 , 0.289	Depositor DCC
R_{free} test set	3660 reflections (5.03%)	wwPDB-VP
Wilson B-factor (Å ²)	48.2	Xtriage
Anisotropy	0.610	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 39.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	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 ²)	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.*

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

5.1 Standard geometry

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# $ Z > 5$	RMSZ	# $ Z > 5$
1	B	0.91	1/3915 (0.0%)	1.04	6/5291 (0.1%)
1	D	0.92	1/3902 (0.0%)	1.05	3/5272 (0.1%)
1	F	0.88	1/3497 (0.0%)	1.00	7/4731 (0.1%)
All	All	0.90	3/11314 (0.0%)	1.03	16/15294 (0.1%)

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	F	430	ASP	C-O	-7.20	1.20	1.23
1	D	266	PRO	CA-CB	-6.34	1.49	1.53
1	B	375	ASN	CA-C	-5.41	1.47	1.53

All (16) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	532	SER	N-CA-C	7.47	119.06	111.07
1	D	437	TRP	CA-C-N	7.43	127.45	119.28
1	D	437	TRP	C-N-CA	7.43	127.45	119.28
1	F	406	VAL	CA-C-N	-7.38	112.17	119.78
1	F	406	VAL	C-N-CA	-7.38	112.17	119.78
1	B	432	ARG	CG-CD-NE	-7.27	96.01	112.00
1	F	509	SER	N-CA-C	6.40	119.08	111.33
1	D	376	THR	CB-CA-C	-6.26	98.92	109.50
1	F	401	VAL	N-CA-C	-5.80	104.86	110.72
1	B	182	VAL	CB-CA-C	-5.79	103.89	111.25
1	B	90	GLY	N-CA-C	-5.63	106.89	115.00
1	B	480	VAL	N-CA-C	-5.62	105.25	110.53
1	F	430	ASP	CA-C-N	-5.26	113.27	119.84
1	F	430	ASP	C-N-CA	-5.26	113.27	119.84
1	B	494	GLY	N-CA-C	-5.07	106.36	112.49
1	F	145	THR	CB-CA-C	-5.04	100.98	109.50

There are no chirality outliers.

There are no planarity outliers.

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	B	3849	0	3869	40	0
1	D	3836	0	3861	54	0
1	F	3437	0	3460	62	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	143	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 (143) 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:B:264:MET:HE2	1:F:331:HIS:HB3	1.79	0.63
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:332:LEU:C	1:F:332:LEU:HD12	2.29	0.57
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:B:332:LEU:C	1:D:264:MET:HE1	2.30	0.56
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:D:232:GLY:HA2	1:D:236:LEU:HD23	1.88	0.54
1:B:538:PHE:CE1	1:F:396:LYS:HD2	2.42	0.53
1:B:492:LEU:C	1:B:492:LEU:HD23	2.32	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:D:112:SER:HA	1:D:117:GLY:N	2.24	0.52
1:F:77:GLY:HA2	1:F:80:LEU:HD12	1.92	0.52
1:F:339:CYS:HA	1:F:368:THR:CG2	2.39	0.52
1:F:126:LYS:HA	1:F:498:LEU:HD21	1.92	0.52
1:F:167:ALA:O	1:F:171:ARG:HG3	2.10	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:B:458:THR:C	1:B:460:GLU:H	2.18	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:B:257:LEU:O	1:B:261:ILE:HG13	2.13	0.48
1:B:460:GLU:O	1:B:461:LYS:C	2.56	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:55:PRO:O	1:D:58:ARG:HB2	2.14	0.47
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:77:GLY:O	1:B:78:TYR:C	2.58	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:41:ALA:C	1:D:43:ALA:H	2.24	0.46
1:D:188:THR:O	1:D:189:ALA:HB3	2.16	0.46
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:46:LYS:O	1:D:50:ARG:HG2	2.17	0.45
1:D:126:LYS:O	1:D:130:LEU:HG	2.17	0.45
1:D:380:MET:HE3	1:D:380:MET:HA	1.99	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:62:LEU:HG	1:D:100:ILE:HD12	1.98	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:124:LEU:HD23	1:D:124:LEU:C	2.41	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:245:GLU:CD	1:B:537:ARG:HH21	2.26	0.44
1:B:267:TRP:O	1:B:526:ARG:NH2	2.50	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:448:ALA:O	1:D:449:GLN:C	2.60	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:F:312:ASP:CG	1:F:333:ARG:O	2.61	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:D:333:ARG:HD2	1:F:264:MET:HE3	2.00	0.43
1:D:487:SER:C	1:D:489:SER:H	2.26	0.43
1:D:77:GLY:O	1:D:78:TYR:C	2.60	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:349:THR:HB	1:B:350:PRO:HD2	2.01	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
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: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:D:245:GLU:CD	1:D:537:ARG:HH11	2.29	0.41
1:F:302:ASP:OD1	1:F:345:ASN:ND2	2.54	0.41
1:B:75:LEU:O	1:B:76:ALA:C	2.60	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:158:ILE:O	1:B:162:GLY:N	2.54	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: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:F:430:ASP:O	1:F:431:PRO:C	2.61	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:342:ILE:HG22	1:F:424:MET:HE1	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%)	10	16
1	D	502/537 (94%)	465 (93%)	32 (6%)	5 (1%)	12	20
1	F	448/537 (83%)	410 (92%)	32 (7%)	6 (1%)	9	14
All	All	1454/1611 (90%)	1343 (92%)	94 (6%)	17 (1%)	10	16

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

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Mol	Chain	Res	Type
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%)	374 (95%)	18 (5%)	24	41
1	D	391/409 (96%)	369 (94%)	22 (6%)	19	33
1	F	353/409 (86%)	341 (97%)	12 (3%)	32	54
All	All	1136/1227 (93%)	1084 (95%)	52 (5%)	24	41

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

Mol	Chain	Res	Type
1	B	48	GLU
1	B	114	ILE
1	B	118	THR
1	B	120	SER
1	B	158	ILE
1	B	186	SER
1	B	187	SER
1	B	203	VAL
1	B	236	LEU
1	B	278	SER
1	B	320	LYS
1	B	339	CYS
1	B	377	THR
1	B	460	GLU
1	B	473	MET
1	B	498	LEU
1	B	518	ASP
1	B	531	ASN
1	D	7	GLU
1	D	14	ASP

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Mol	Chain	Res	Type
1	D	49	LYS
1	D	81	HIS
1	D	161	GLU
1	D	187	SER
1	D	205	ARG
1	D	256	ARG
1	D	292	VAL
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	381	VAL
1	D	386	GLU
1	D	432	ARG
1	D	476	MET
1	D	492	LEU
1	D	529	LYS
1	F	145	THR
1	F	147	SER
1	F	158	ILE
1	F	211	PHE
1	F	278	SER
1	F	289	LEU
1	F	303	VAL
1	F	339	CYS
1	F	461	LYS
1	F	477	LEU
1	F	490	THR
1	F	498	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (13) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	11	ASN
1	B	326	GLN
1	B	449	GLN
1	D	52	GLN
1	D	137	ASN
1	D	153	ASN

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Mol	Chain	Res	Type
1	D	326	GLN
1	D	365	GLN
1	D	388	GLN
1	F	194	GLN
1	F	375	ASN
1	F	439	ASN
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 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

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	B	514/537 (95%)	0.47	34 (6%)	24 20	37, 59, 96, 121	0
1	D	512/537 (95%)	0.49	46 (8%)	15 12	36, 56, 111, 147	0
1	F	460/537 (85%)	0.72	55 (11%)	9 6	37, 61, 143, 186	0
All	All	1486/1611 (92%)	0.56	135 (9%)	15 12	36, 59, 118, 186	0

All (135) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	F	291	GLY	6.6
1	F	289	LEU	6.6
1	F	286	VAL	6.4
1	D	8	LEU	5.4
1	F	292	VAL	5.4
1	F	285	PRO	5.2
1	F	114	ILE	4.9
1	F	472	LYS	4.8
1	F	474	LEU	4.7
1	B	247	LEU	4.6
1	D	471	PRO	4.6
1	F	469	ALA	4.5
1	F	473	MET	4.4
1	B	2	PRO	4.4
1	D	223	GLY	4.3
1	F	300	PRO	4.3
1	D	216	PRO	4.2
1	D	47	PHE	4.2
1	D	78	TYR	4.2
1	F	471	PRO	4.0
1	F	119	ILE	4.0
1	D	114	ILE	4.0
1	F	301	TYR	4.0

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Mol	Chain	Res	Type	RSRZ
1	B	89	ALA	3.9
1	F	299	LYS	3.9
1	F	297	PRO	3.7
1	D	10	VAL	3.7
1	F	223	GLY	3.7
1	D	80	LEU	3.7
1	D	2	PRO	3.7
1	F	113	ALA	3.6
1	F	290	LEU	3.6
1	D	278	SER	3.5
1	F	485	LEU	3.5
1	D	17	ARG	3.5
1	D	89	ALA	3.5
1	F	274	ARG	3.5
1	F	295	ALA	3.5
1	B	212	LEU	3.4
1	F	116	GLY	3.4
1	F	284	TYR	3.4
1	F	454	LEU	3.3
1	F	81	HIS	3.3
1	F	293	VAL	3.3
1	D	477	LEU	3.3
1	D	150	ALA	3.2
1	B	538	PHE	3.2
1	D	81	HIS	3.2
1	B	213	ALA	3.2
1	B	205	ARG	3.2
1	B	81	HIS	3.1
1	F	152	LEU	3.1
1	F	206	GLY	3.1
1	F	449	GLN	3.1
1	B	469	ALA	3.1
1	B	216	PRO	3.1
1	B	155	ALA	3.0
1	F	117	GLY	3.0
1	F	216	PRO	3.0
1	F	294	PRO	3.0
1	D	23	LEU	3.0
1	F	155	ALA	2.9
1	F	453	VAL	2.9
1	B	274	ARG	2.9
1	D	113	ALA	2.9

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Mol	Chain	Res	Type	RSRZ
1	D	11	ASN	2.9
1	D	274	ARG	2.9
1	B	69	PHE	2.9
1	B	112	SER	2.9
1	D	112	SER	2.8
1	F	477	LEU	2.8
1	F	480	VAL	2.7
1	F	89	ALA	2.7
1	D	472	LYS	2.7
1	D	476	MET	2.7
1	D	4	ILE	2.7
1	D	148	GLY	2.7
1	F	118	THR	2.6
1	F	448	ALA	2.6
1	B	157	GLU	2.6
1	B	190	GLY	2.6
1	B	80	LEU	2.6
1	D	479	THR	2.6
1	F	154	TYR	2.5
1	B	116	GLY	2.5
1	B	150	ALA	2.5
1	D	3	ALA	2.5
1	B	473	MET	2.5
1	D	215	PRO	2.4
1	F	158	ILE	2.4
1	F	197	LEU	2.4
1	B	100	ILE	2.4
1	B	461	LYS	2.4
1	D	45	PRO	2.4
1	F	79	LYS	2.4
1	B	387	ARG	2.4
1	D	473	MET	2.4
1	D	46	LYS	2.4
1	D	290	LEU	2.3
1	F	52	GLN	2.3
1	D	41	ALA	2.3
1	D	117	GLY	2.3
1	B	78	TYR	2.3
1	B	32	LEU	2.2
1	B	49	LYS	2.2
1	F	489	SER	2.2
1	D	151	ASN	2.2

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Mol	Chain	Res	Type	RSRZ
1	F	483	GLN	2.2
1	D	149	GLY	2.2
1	D	147	SER	2.2
1	F	278	SER	2.2
1	F	80	LEU	2.2
1	D	458	THR	2.2
1	D	481	THR	2.2
1	B	149	GLY	2.2
1	D	474	LEU	2.2
1	B	379	PHE	2.2
1	F	298	LYS	2.2
1	B	101	ALA	2.1
1	F	111	ASN	2.1
1	D	495	THR	2.1
1	D	207	LYS	2.1
1	D	454	LEU	2.1
1	B	204	VAL	2.1
1	B	40	ALA	2.1
1	F	332	LEU	2.1
1	F	371	LEU	2.1
1	F	456	ILE	2.1
1	B	353	ALA	2.1
1	F	190	GLY	2.1
1	D	453	VAL	2.0
1	D	287	GLU	2.0
1	B	114	ILE	2.0
1	D	484	LYS	2.0
1	B	441	ARG	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.