Full wwPDB X-ray Structure Validation Report (i)

Sep 13, 2020 – 10:40 AM BST

PDB ID	:	2VSQ
Title	:	Structure of surfactin A synthetase C (SrfA-C), a nonribosomal peptide synthetase termination module
Authors	:	Tanovic, A.; Samel, S.A.; Essen, L.-O.; Marahiel, M.A.
Deposited on	:	2008-04-29
Resolution	:	2.60 Å(reported)

The following versions of software and data (see references (i)) 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	:	2.14.4.dev1
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)	:	2.14.4.dev1

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.60 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	Percentile Ranks	Value
Rfree		0.283
Clashscore		14
Ramachandran outliers		2.8%
Sidechain outliers		10.4%
RSRZ outliers		11.9%

Worse — *Better*

▮ Percentile relative to all X-ray structures

▯ Percentile relative to X-ray structures of similar resolution
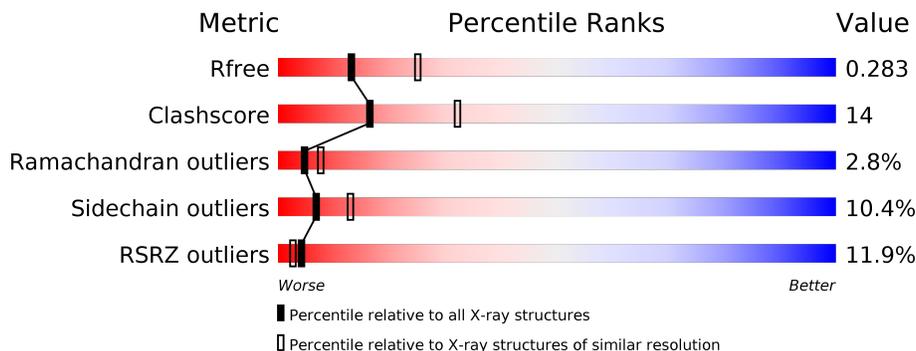
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	3163 (2.60-2.60)
Clashscore	141614	3518 (2.60-2.60)
Ramachandran outliers	138981	3455 (2.60-2.60)
Sidechain outliers	138945	3455 (2.60-2.60)
RSRZ outliers	127900	3104 (2.60-2.60)

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 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 <=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	1304	12% / 67% / 25% / 5% ·

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	LEU	A	2291	-	-	-	X

2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 10109 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 SURFACTIN SYNTHETASE SUBUNIT 3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	1273	Total 10056	C 6409	N 1685	O 1924	S 38	0	0	0

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	26	ALA	PRO	conflict	UNP Q08787
A	33	SER	THR	conflict	UNP Q08787
A	235	PRO	LEU	conflict	UNP Q08787
A	1003	ALA	SER	engineered mutation	UNP Q08787
A	1223	ILE	MET	conflict	UNP Q08787
A	1240	MET	ASN	conflict	UNP Q08787

- Molecule 2 is LEUCINE (three-letter code: LEU) (formula: $C_6H_{13}NO_2$).
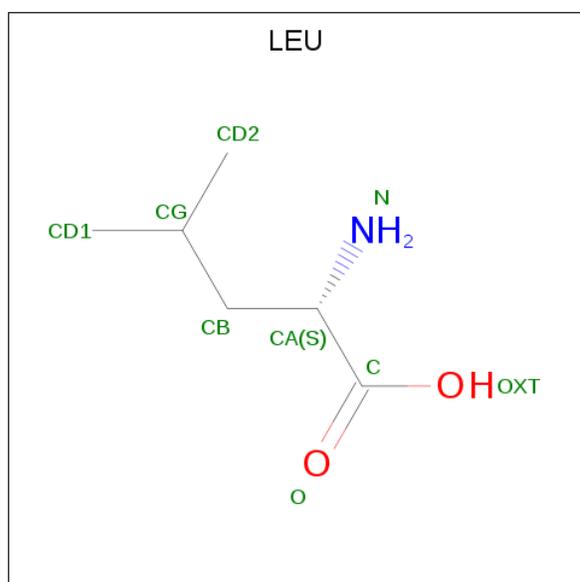
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total 9	C 6	N 1	O 2	0	0

- Molecule 3 is SULFATE ION (three-letter code: SO4) (formula: O_4S).
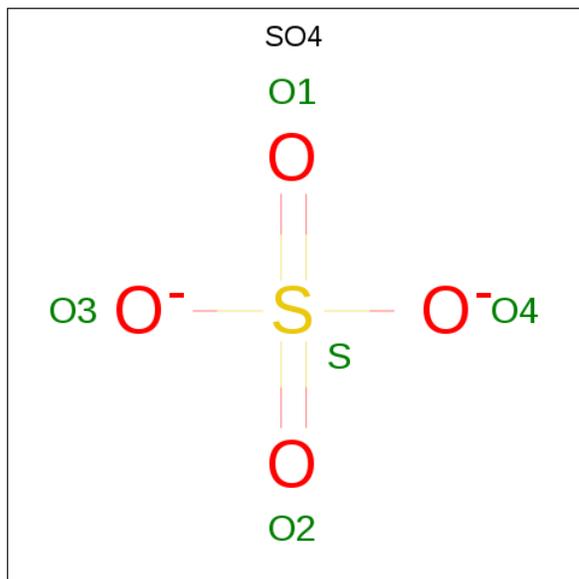
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total 5	O 4	S 1	0	0

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	39	Total 39	O 39	0	0

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: SURFACTIN SYNTHETASE SUBUNIT 3
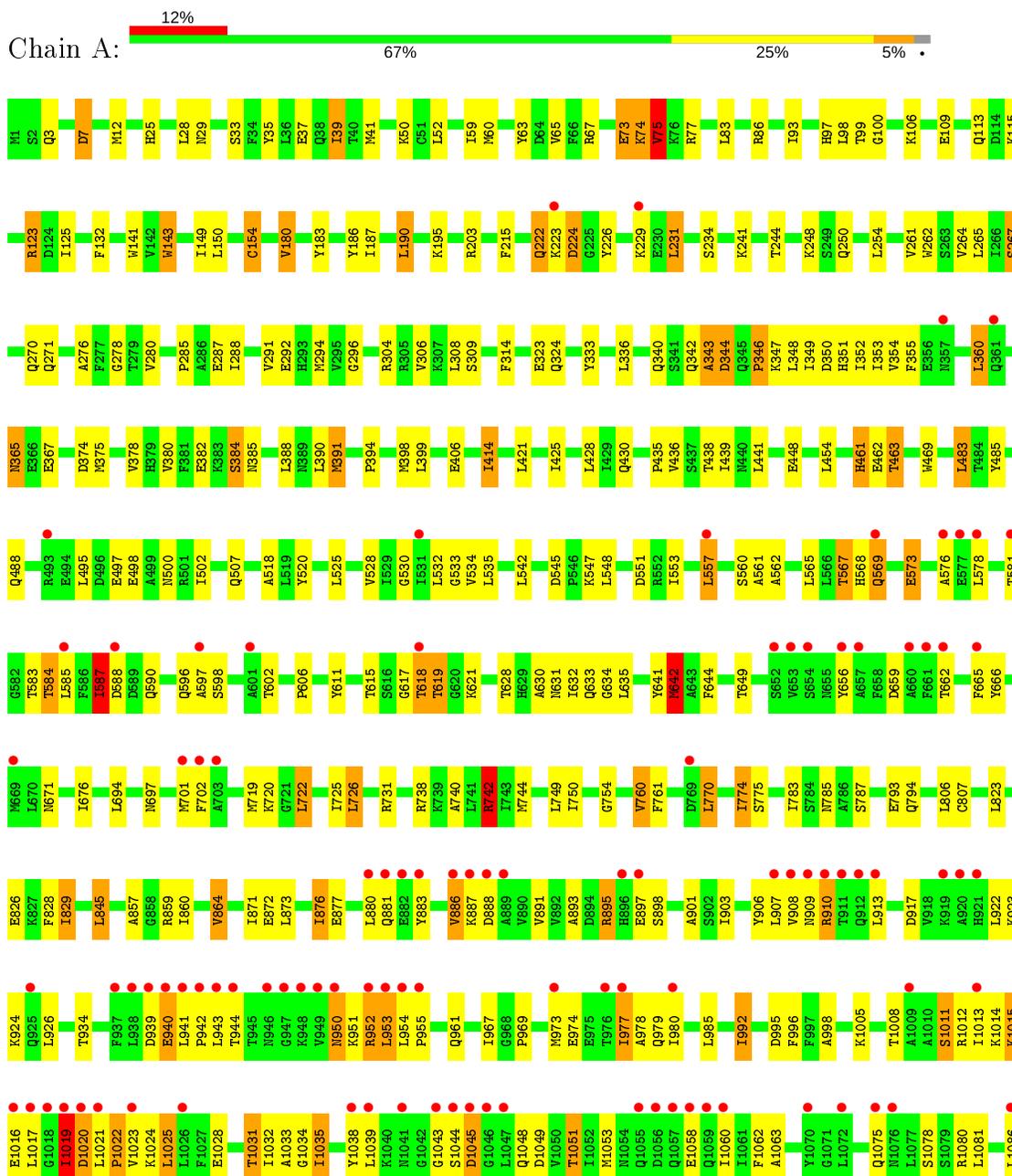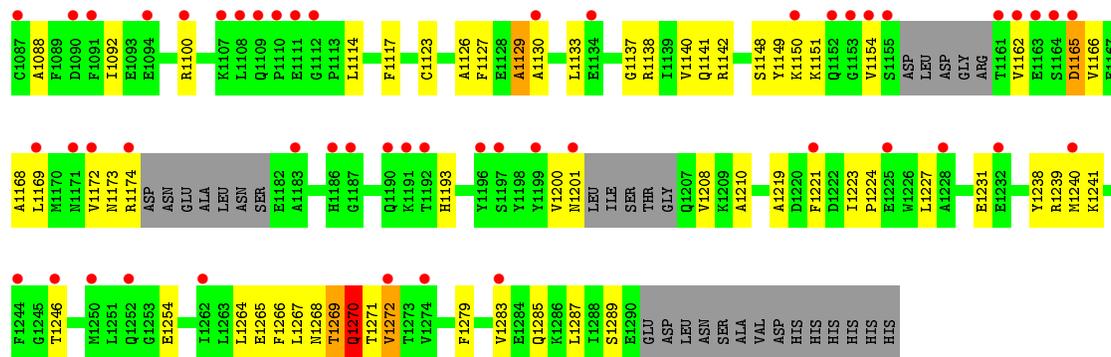
4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	83.11Å 106.56Å 92.40Å 90.00° 97.35° 90.00°	Depositor
Resolution (Å)	82.50 – 2.60 37.06 – 2.60	Depositor EDS
% Data completeness (in resolution range)	93.1 (82.50-2.60) 92.5 (37.06-2.60)	Depositor EDS
R_{merge}	0.04	Depositor
R_{sym}	(Not available)	Depositor
$<I/\sigma(I)>$ [1]	1.90 (at 2.61Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.213 , 0.272 0.219 , 0.283	Depositor DCC
R_{free} test set	1040 reflections (2.28%)	wwPDB-VP
Wilson B-factor (Å^2)	69.8	Xtriage
Anisotropy	0.013	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.31 , 76.7	EDS
L-test for twinning[2]	$<|L|> = 0.49$, $<L^2> = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	10109	wwPDB-VP
Average B, all atoms (Å^2)	70.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.19% of the height of the origin peak. No significant pseudotranslation is detected.*

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[1]Intensities estimated from amplitudes.
[2]Theoretical values of $<|L|>$, $<L^2>$ 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: SO4

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	0.53	4/10270 (0.0%)	0.64	3/13922 (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	A	0	3

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	596	GLN	CD-NE2	12.98	1.65	1.32
1	A	596	GLN	CD-OE1	8.68	1.43	1.24
1	A	143	TRP	CB-CG	-5.59	1.40	1.50
1	A	154	CYS	CB-SG	-5.17	1.73	1.81

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	596	GLN	CG-CD-OE1	-13.48	94.65	121.60
1	A	596	GLN	CG-CD-NE2	6.68	132.73	116.70
1	A	742	ARG	NE-CZ-NH1	5.48	123.04	120.30

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	462	GLU	Peptide
1	A	567	THR	Peptide
1	A	587	ILE	Peptide

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	10056	0	9872	285	0
2	A	9	0	10	0	0
3	A	5	0	0	0	0
4	A	39	0	0	0	0
All	All	10109	0	9882	285	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 14.

All (285) 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:876:ILE:HD11	1:A:891:VAL:CG2	1.60	1.31
1:A:876:ILE:CD1	1:A:891:VAL:HG21	1.61	1.29
1:A:587:ILE:O	1:A:587:ILE:HD13	1.53	1.09
1:A:60:MET:HE2	1:A:125:ILE:HD13	1.38	1.05
1:A:1021:LEU:HD22	1:A:1022:PRO:HD2	1.43	1.00
1:A:39:ILE:HD11	1:A:378:VAL:HG13	1.49	0.94
1:A:483:LEU:HD13	1:A:525:LEU:HD12	1.51	0.91
1:A:463:THR:HG23	1:A:606:PRO:HG2	1.52	0.90
1:A:725:ILE:CG2	1:A:749:LEU:HD13	2.04	0.87
1:A:943:LEU:O	1:A:944:THR:HG22	1.76	0.85
1:A:644:PHE:HB2	1:A:671:ASN:HD22	1.40	0.84
1:A:783:ILE:HD12	1:A:785:ASN:H	1.46	0.79
1:A:611:TYR:CZ	1:A:662:THR:HG21	2.17	0.79
1:A:967:ILE:O	1:A:992:ILE:HD13	1.86	0.76
1:A:883:TYR:CE1	1:A:913:LEU:HD13	2.21	0.76
1:A:618:THR:HG23	1:A:621:LYS:O	1.87	0.75
1:A:241:LYS:O	1:A:244:THR:HG22	1.87	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:264:VAL:HG22	1:A:436:VAL:HG11	1.68	0.74
1:A:611:TYR:OH	1:A:662:THR:HG21	1.88	0.73
1:A:1092:ILE:HG21	1:A:1100:ARG:HD2	1.70	0.73
1:A:973:MET:O	1:A:977:ILE:HG23	1.89	0.73
1:A:725:ILE:CG2	1:A:749:LEU:CD1	2.67	0.72
1:A:628:THR:HG22	1:A:631:ASN:H	1.55	0.72
1:A:740:ALA:HB1	1:A:744:MET:CE	2.20	0.72
1:A:952:ARG:HD3	1:A:953:LEU:HD23	1.72	0.71
1:A:1166:VAL:HG21	1:A:1193:HIS:HA	1.72	0.71
1:A:39:ILE:CD1	1:A:378:VAL:HG13	2.20	0.71
1:A:463:THR:CG2	1:A:606:PRO:HG2	2.21	0.71
1:A:1019:ILE:HD13	1:A:1019:ILE:O	1.91	0.70
1:A:365:ASN:N	1:A:365:ASN:HD22	1.89	0.70
1:A:74:LYS:O	1:A:75:VAL:HG13	1.92	0.69
1:A:583:THR:CG2	1:A:585:LEU:HD11	2.22	0.69
1:A:1264:LEU:O	1:A:1268:ASN:N	2.25	0.69
1:A:278:GLY:HA3	1:A:352:ILE:HG22	1.72	0.69
1:A:888:ASP:HB2	1:A:908:VAL:HG22	1.74	0.68
1:A:587:ILE:O	1:A:587:ILE:CD1	2.39	0.68
1:A:1031:THR:HG22	1:A:1034:GLY:H	1.58	0.68
1:A:754:GLY:HA3	1:A:761:PHE:HA	1.76	0.68
1:A:1268:ASN:O	1:A:1270:GLN:N	2.27	0.68
1:A:60:MET:HE1	1:A:125:ILE:CG2	2.24	0.67
1:A:641:TYR:O	1:A:642:MET:O	2.11	0.67
1:A:528:VAL:HG13	1:A:665:PHE:HE1	1.60	0.67
1:A:520:TYR:O	1:A:567:THR:HG23	1.95	0.66
1:A:725:ILE:HG23	1:A:749:LEU:CD1	2.25	0.66
1:A:642:MET:C	1:A:642:MET:SD	2.74	0.66
1:A:573:GLU:HG2	1:A:576:ALA:HB2	1.77	0.66
1:A:1039:LEU:HD23	1:A:1043:GLY:HA2	1.77	0.66
1:A:977:ILE:HD11	1:A:1032:ILE:HG23	1.76	0.65
1:A:725:ILE:HG23	1:A:749:LEU:HD13	1.78	0.65
1:A:463:THR:HG23	1:A:606:PRO:CG	2.26	0.65
1:A:864:VAL:HG11	1:A:893:ALA:CB	2.26	0.64
1:A:738:ARG:NH2	1:A:770:LEU:HD12	2.13	0.64
1:A:99:THR:HG22	1:A:100:GLY:N	2.11	0.63
1:A:583:THR:HG22	1:A:585:LEU:CD1	2.28	0.63
1:A:1013:ILE:O	1:A:1019:ILE:N	2.32	0.63
1:A:1023:VAL:HG23	1:A:1024:LYS:H	1.64	0.63
1:A:60:MET:CE	1:A:125:ILE:HG21	2.29	0.63
1:A:1149:TYR:HB2	1:A:1227:LEU:HD22	1.80	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:876:ILE:HD12	1:A:876:ILE:C	2.20	0.63
1:A:774:ILE:HG22	1:A:774:ILE:O	1.99	0.62
1:A:934:THR:HG22	1:A:961:GLN:HB3	1.81	0.62
1:A:215:PHE:H	1:A:270:GLN:HE22	1.45	0.62
1:A:864:VAL:HG23	1:A:871:ILE:HB	1.80	0.62
1:A:41:MET:CE	1:A:375:MET:SD	2.88	0.62
1:A:1039:LEU:HD23	1:A:1043:GLY:CA	2.30	0.62
1:A:1014:LYS:O	1:A:1015:LYS:CB	2.49	0.61
1:A:1219:ALA:HB2	1:A:1246:THR:HG22	1.83	0.61
1:A:340:GLN:NE2	1:A:346:PRO:O	2.34	0.61
1:A:992:ILE:O	1:A:1031:THR:HG23	2.00	0.61
1:A:895:ARG:HD2	1:A:901:ALA:HB2	1.82	0.61
1:A:1013:ILE:HD12	1:A:1013:ILE:C	2.21	0.60
1:A:995:ASP:HB3	1:A:998:ALA:HB3	1.84	0.60
1:A:502:ILE:HD11	1:A:587:ILE:CG1	2.31	0.60
1:A:35:TYR:OH	1:A:1024:LYS:NZ	2.34	0.60
1:A:1060:ILE:HG21	1:A:1062:PHE:CZ	2.36	0.60
1:A:60:MET:HE1	1:A:125:ILE:HG21	1.83	0.59
1:A:880:LEU:O	1:A:886:VAL:HG11	2.02	0.59
1:A:63:TYR:CE2	1:A:180:VAL:HG21	2.38	0.59
1:A:883:TYR:HE1	1:A:913:LEU:HD13	1.68	0.59
1:A:944:THR:O	1:A:944:THR:HG23	2.01	0.59
1:A:93:ILE:HD13	1:A:132:PHE:CE2	2.38	0.58
1:A:530:GLY:O	1:A:534:VAL:HG23	2.04	0.58
1:A:1092:ILE:HD13	1:A:1100:ARG:CD	2.33	0.58
1:A:1051:THR:HB	1:A:1088:ALA:HB3	1.83	0.58
1:A:41:MET:HE3	1:A:375:MET:SD	2.44	0.58
1:A:738:ARG:NH2	1:A:770:LEU:CD1	2.68	0.57
1:A:495:LEU:HD11	1:A:532:LEU:HD12	1.86	0.57
1:A:485:TYR:HB3	1:A:525:LEU:HD22	1.86	0.57
1:A:502:ILE:HG22	1:A:533:GLY:HA3	1.87	0.57
1:A:744:MET:CE	1:A:749:LEU:HD11	2.35	0.57
1:A:641:TYR:CD2	1:A:642:MET:HE3	2.40	0.57
1:A:1032:ILE:HA	1:A:1035:ILE:HG23	1.87	0.56
1:A:1172:VAL:C	1:A:1173:ASN:HD22	2.08	0.56
1:A:583:THR:HG22	1:A:585:LEU:HD11	1.84	0.56
1:A:719:MET:HA	1:A:722:LEU:HD22	1.88	0.56
1:A:485:TYR:HB3	1:A:525:LEU:CD2	2.34	0.56
1:A:567:THR:HG22	1:A:568:HIS:N	2.21	0.56
1:A:573:GLU:O	1:A:576:ALA:HB2	2.06	0.56
1:A:1021:LEU:HD13	1:A:1022:PRO:N	2.22	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1014:LYS:HA	1:A:1020:ASP:HA	1.87	0.55
1:A:63:TYR:HE2	1:A:180:VAL:HG21	1.70	0.55
1:A:576:ALA:HB3	1:A:578:LEU:HD12	1.89	0.55
1:A:65:VAL:HB	1:A:149:ILE:HB	1.89	0.55
1:A:1231:GLU:HA	1:A:1238:TYR:CD2	2.42	0.54
1:A:528:VAL:HG13	1:A:665:PHE:CE1	2.41	0.54
1:A:41:MET:HE2	1:A:375:MET:SD	2.48	0.54
1:A:254:LEU:HD12	1:A:254:LEU:H	1.73	0.54
1:A:744:MET:HE1	1:A:749:LEU:HD11	1.90	0.54
1:A:343:ALA:O	1:A:344:ASP:HB2	2.08	0.54
1:A:502:ILE:HD11	1:A:587:ILE:HG12	1.90	0.54
1:A:1224:PRO:HG2	1:A:1227:LEU:HD12	1.91	0.53
1:A:439:ILE:HG22	1:A:441:LEU:HD13	1.91	0.53
1:A:942:PRO:O	1:A:950:ASN:HB3	2.09	0.53
1:A:641:TYR:C	1:A:642:MET:HE3	2.28	0.53
1:A:941:LEU:HD12	1:A:941:LEU:N	2.24	0.53
1:A:845:LEU:HD13	1:A:860:ILE:HG13	1.91	0.53
1:A:60:MET:CE	1:A:125:ILE:CG2	2.86	0.53
1:A:744:MET:HE3	1:A:749:LEU:CD2	2.39	0.52
1:A:576:ALA:HB3	1:A:578:LEU:CD1	2.39	0.52
1:A:701:MET:O	1:A:725:ILE:HD12	2.10	0.52
1:A:1053:MET:HE2	1:A:1075:GLN:HA	1.91	0.52
1:A:262:TRP:CD1	1:A:353:ILE:HD11	2.44	0.52
1:A:676:ILE:N	1:A:676:ILE:HD12	2.25	0.52
1:A:502:ILE:HD11	1:A:587:ILE:HG13	1.91	0.52
1:A:725:ILE:HG21	1:A:749:LEU:CD1	2.38	0.51
1:A:1092:ILE:HD13	1:A:1100:ARG:HD2	1.91	0.51
1:A:1172:VAL:HG23	1:A:1173:ASN:ND2	2.25	0.51
1:A:7:ASP:C	1:A:7:ASP:OD2	2.49	0.51
1:A:744:MET:HE3	1:A:749:LEU:HD21	1.93	0.51
1:A:231:LEU:HD12	1:A:414:ILE:HG22	1.93	0.50
1:A:99:THR:CG2	1:A:100:GLY:N	2.74	0.50
1:A:642:MET:N	1:A:642:MET:HE3	2.27	0.50
1:A:725:ILE:HG21	1:A:749:LEU:HD13	1.91	0.50
1:A:439:ILE:HG22	1:A:441:LEU:CD1	2.41	0.50
1:A:568:HIS:O	1:A:569:GLN:CB	2.60	0.50
1:A:659:ASP:O	1:A:760:VAL:HG22	2.12	0.50
1:A:73:GLU:O	1:A:74:LYS:HD3	2.12	0.50
1:A:738:ARG:CZ	1:A:770:LEU:HD12	2.42	0.50
1:A:187:ILE:HD12	1:A:187:ILE:N	2.27	0.49
1:A:224:ASP:OD1	1:A:224:ASP:N	2.38	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:944:THR:O	1:A:944:THR:CG2	2.60	0.49
1:A:909:ASN:O	1:A:910:ARG:CB	2.60	0.49
1:A:1015:LYS:O	1:A:1017:LEU:N	2.46	0.49
1:A:12:MET:SD	1:A:12:MET:N	2.86	0.49
1:A:150:LEU:HD22	1:A:154:CYS:CB	2.42	0.49
1:A:285:PRO:HD2	1:A:291:VAL:HG21	1.95	0.49
1:A:845:LEU:HB3	1:A:857:ALA:HB3	1.94	0.49
1:A:1023:VAL:HG23	1:A:1024:LYS:N	2.26	0.49
1:A:1114:LEU:O	1:A:1141:GLN:N	2.45	0.49
1:A:264:VAL:HG22	1:A:436:VAL:CG1	2.39	0.49
1:A:314:PHE:CD1	1:A:428:LEU:HD22	2.47	0.49
1:A:583:THR:HG22	1:A:585:LEU:HD12	1.95	0.48
1:A:845:LEU:HD13	1:A:860:ILE:CG1	2.43	0.48
1:A:642:MET:CE	1:A:642:MET:N	2.77	0.48
1:A:1162:VAL:HG12	1:A:1193:HIS:CE1	2.48	0.48
1:A:186:TYR:CE2	1:A:190:LEU:HD22	2.49	0.48
1:A:731:ARG:HH12	1:A:872:GLU:CD	2.17	0.48
1:A:97:HIS:CE1	1:A:98:LEU:HD21	2.49	0.48
1:A:1005:LYS:HA	1:A:1008:THR:HB	1.94	0.48
1:A:1126:ALA:O	1:A:1129:ALA:HB3	2.13	0.48
1:A:1142:ARG:NH2	1:A:1267:LEU:HD23	2.29	0.48
1:A:873:LEU:HD23	1:A:877:GLU:OE1	2.14	0.48
1:A:350:ASP:HB3	1:A:351:HIS:HD1	1.79	0.48
1:A:1172:VAL:HG23	1:A:1173:ASN:HD22	1.78	0.47
1:A:288:ILE:HB	1:A:291:VAL:HB	1.95	0.47
1:A:560:SER:O	1:A:561:ALA:HB3	2.15	0.47
1:A:922:LEU:HD22	1:A:926:LEU:HD12	1.96	0.47
1:A:553:ILE:HG22	1:A:557:LEU:HD22	1.95	0.47
1:A:1021:LEU:HD22	1:A:1022:PRO:CD	2.29	0.47
1:A:1063:ALA:HA	1:A:1117:PHE:HB3	1.97	0.47
1:A:1266:PHE:O	1:A:1269:THR:HG23	2.15	0.47
1:A:545:ASP:HB3	1:A:548:LEU:HD13	1.95	0.47
1:A:881:GLN:O	1:A:886:VAL:HG21	2.14	0.47
1:A:150:LEU:HD22	1:A:154:CYS:HB3	1.97	0.47
1:A:346:PRO:O	1:A:348:LEU:N	2.48	0.47
1:A:873:LEU:HD21	1:A:891:VAL:O	2.14	0.47
1:A:565:LEU:O	1:A:584:THR:HA	2.14	0.47
1:A:606:PRO:O	1:A:628:THR:HG23	2.15	0.47
1:A:261:VAL:HG21	1:A:425:ILE:CD1	2.45	0.46
1:A:488:GLN:N	1:A:488:GLN:OE1	2.48	0.46
1:A:1123:CYS:SG	1:A:1148:SER:HB3	2.55	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1151:LYS:NZ	1:A:1201:ASN:O	2.48	0.46
1:A:995:ASP:HB3	1:A:998:ALA:CB	2.45	0.46
1:A:1078:SER:HA	1:A:1086:LEU:HD11	1.97	0.46
1:A:1238:TYR:CE2	1:A:1240:MET:HE1	2.50	0.46
1:A:60:MET:HE1	1:A:125:ILE:HG23	1.97	0.46
1:A:261:VAL:HG21	1:A:425:ILE:HD13	1.97	0.46
1:A:469:TRP:HE1	1:A:633:GLN:HE21	1.63	0.46
1:A:360:LEU:N	1:A:360:LEU:HD22	2.30	0.45
1:A:1133:LEU:O	1:A:1137:GLY:N	2.49	0.45
1:A:183:TYR:HA	1:A:294:MET:HE3	1.98	0.45
1:A:740:ALA:HB1	1:A:744:MET:HE2	1.95	0.45
1:A:1031:THR:CG2	1:A:1033:ALA:HB3	2.46	0.45
1:A:906:TYR:C	1:A:907:LEU:HD12	2.37	0.45
1:A:573:GLU:O	1:A:573:GLU:HG2	2.17	0.45
1:A:628:THR:O	1:A:631:ASN:HB2	2.16	0.45
1:A:618:THR:O	1:A:619:THR:C	2.55	0.45
1:A:806:LEU:C	1:A:806:LEU:HD23	2.37	0.45
1:A:1169:LEU:O	1:A:1172:VAL:HG22	2.17	0.45
1:A:234:SER:CB	1:A:398:MET:O	2.65	0.45
1:A:495:LEU:HD11	1:A:532:LEU:CD1	2.46	0.45
1:A:1130:ALA:HA	1:A:1133:LEU:HD12	1.98	0.45
1:A:641:TYR:O	1:A:641:TYR:CG	2.69	0.45
1:A:1221:PHE:HE2	1:A:1223:ILE:HD12	1.82	0.45
1:A:542:LEU:C	1:A:542:LEU:HD23	2.36	0.45
1:A:649:THR:HG23	1:A:676:ILE:HD11	1.98	0.45
1:A:725:ILE:HG23	1:A:749:LEU:HD12	1.96	0.45
1:A:52:LEU:HD21	1:A:141:TRP:CH2	2.52	0.44
1:A:183:TYR:HA	1:A:294:MET:CE	2.47	0.44
1:A:365:ASN:N	1:A:365:ASN:ND2	2.59	0.44
1:A:702:PHE:C	1:A:702:PHE:CD2	2.90	0.44
1:A:942:PRO:O	1:A:950:ASN:CB	2.66	0.44
1:A:39:ILE:CD1	1:A:378:VAL:CG1	2.92	0.44
1:A:744:MET:HE3	1:A:749:LEU:CD1	2.48	0.44
1:A:435:PRO:O	1:A:438:THR:HB	2.17	0.44
1:A:985:LEU:HD21	1:A:996:PHE:CZ	2.52	0.44
1:A:1127:PHE:CE1	1:A:1208:VAL:HG13	2.53	0.44
1:A:1133:LEU:HD13	1:A:1140:VAL:HG22	1.99	0.44
1:A:226:TYR:CE2	1:A:384:SER:HB2	2.52	0.44
1:A:542:LEU:C	1:A:542:LEU:CD2	2.86	0.44
1:A:642:MET:HE1	1:A:750:ILE:CD1	2.48	0.44
1:A:806:LEU:HD23	1:A:807:CYS:N	2.32	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:141:TRP:CE2	1:A:143:TRP:NE1	2.85	0.43
1:A:351:HIS:HB2	1:A:388:LEU:O	2.19	0.43
1:A:634:GLY:HA2	1:A:785:ASN:HD22	1.82	0.43
1:A:60:MET:HE2	1:A:125:ILE:HG21	1.99	0.43
1:A:1045:ASP:HA	1:A:1049:ASP:HB3	2.00	0.43
1:A:1114:LEU:HD11	1:A:1138:ARG:CZ	2.49	0.43
1:A:267:SER:OG	1:A:308:LEU:HD12	2.18	0.43
1:A:725:ILE:HD12	1:A:726:LEU:N	2.34	0.43
1:A:829:ILE:HA	1:A:829:ILE:HD13	1.78	0.43
1:A:744:MET:HE3	1:A:749:LEU:HD11	2.01	0.43
1:A:1154:VAL:HG13	1:A:1200:VAL:O	2.19	0.43
1:A:573:GLU:O	1:A:573:GLU:CG	2.67	0.43
1:A:1162:VAL:CG1	1:A:1193:HIS:CE1	3.02	0.42
1:A:507:GLN:HE22	1:A:602:THR:HG22	1.84	0.42
1:A:67:ARG:HD2	1:A:83:LEU:O	2.19	0.42
1:A:1021:LEU:HD21	1:A:1038:TYR:CD2	2.55	0.42
1:A:1080:ARG:O	1:A:1081:LEU:HD23	2.19	0.42
1:A:980:ILE:HD11	1:A:1013:ILE:CG2	2.48	0.42
1:A:518:ALA:O	1:A:565:LEU:HD12	2.19	0.42
1:A:535:LEU:HD11	1:A:666:TYR:OH	2.19	0.42
1:A:954:LEU:HB3	1:A:955:PRO:HD2	2.00	0.42
1:A:1140:VAL:HB	1:A:1210:ALA:HB2	2.01	0.42
1:A:190:LEU:HD11	1:A:333:TYR:CB	2.50	0.42
1:A:742:ARG:HH11	1:A:742:ARG:HG2	1.83	0.42
1:A:942:PRO:O	1:A:943:LEU:HD13	2.18	0.42
1:A:980:ILE:HG22	1:A:1012:ARG:CZ	2.49	0.42
1:A:414:ILE:N	1:A:414:ILE:CD1	2.82	0.42
1:A:500:ASN:HB3	1:A:598:SER:O	2.20	0.42
1:A:1165:ASP:HA	1:A:1168:ALA:HB3	2.00	0.42
1:A:1264:LEU:O	1:A:1265:GLU:C	2.57	0.42
1:A:83:LEU:HD12	1:A:86:ARG:HD2	2.01	0.42
1:A:33:SER:HB3	1:A:115:LYS:O	2.20	0.42
1:A:336:LEU:HD21	1:A:349:ILE:HD11	2.01	0.41
1:A:497:GLU:HB3	1:A:597:ALA:HB1	2.02	0.41
1:A:628:THR:HG22	1:A:630:ALA:N	2.35	0.41
1:A:360:LEU:HD22	1:A:360:LEU:H	1.85	0.41
1:A:908:VAL:HG11	1:A:941:LEU:HD12	2.02	0.41
1:A:520:TYR:HB2	1:A:565:LEU:HD11	2.03	0.41
1:A:908:VAL:HG11	1:A:940:GLU:HA	2.01	0.41
1:A:1025:LEU:HD12	1:A:1028:GLU:HB2	2.03	0.41
1:A:93:ILE:CD1	1:A:132:PHE:CE2	3.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:203:ARG:HH21	1:A:342:GLN:HE22	1.69	0.41
1:A:355:PHE:CE2	1:A:394:PRO:HD3	2.55	0.41
1:A:740:ALA:HB1	1:A:744:MET:HE1	2.00	0.41
1:A:3:GLN:HE22	1:A:123:ARG:CZ	2.34	0.41
1:A:974:GLU:O	1:A:978:ALA:N	2.50	0.41
1:A:985:LEU:HD21	1:A:996:PHE:CE1	2.55	0.41
1:A:276:ALA:HA	1:A:304:ARG:O	2.21	0.41
1:A:1114:LEU:HB2	1:A:1140:VAL:HA	2.02	0.41
1:A:149:ILE:O	1:A:296:GLY:HA2	2.20	0.41
1:A:498:GLU:O	1:A:502:ILE:HD13	2.21	0.41
1:A:793:GLU:H	1:A:793:GLU:CD	2.24	0.41
1:A:28:LEU:HD22	1:A:1011:SER:HB2	2.02	0.40
1:A:1271:THR:O	1:A:1272:VAL:C	2.59	0.40
1:A:106:LYS:O	1:A:109:GLU:HB3	2.21	0.40
1:A:611:TYR:CE1	1:A:632:ILE:HD11	2.55	0.40
1:A:828:PHE:O	1:A:829:ILE:HD13	2.20	0.40
1:A:1279:PHE:O	1:A:1283:VAL:HG23	2.20	0.40
1:A:611:TYR:CE1	1:A:662:THR:HG21	2.56	0.40
1:A:1150:LYS:O	1:A:1227:LEU:HD23	2.22	0.40
1:A:354:VAL:O	1:A:391:MET:HA	2.21	0.40
1:A:3:GLN:HE22	1:A:123:ARG:NH1	2.19	0.40
1:A:950:ASN:OD1	1:A:950:ASN:N	2.54	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	1265/1304 (97%)	1121 (89%)	109 (9%)	35 (3%)	5	7

All (35) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	569	GLN
1	A	642	MET
1	A	910	ARG
1	A	1015	LYS
1	A	1016	GLU
1	A	1045	ASP
1	A	1269	THR
1	A	75	VAL
1	A	222	GLN
1	A	223	LYS
1	A	346	PRO
1	A	461	HIS
1	A	618	THR
1	A	1058	GLU
1	A	1129	ALA
1	A	1272	VAL
1	A	1289	SER
1	A	951	LYS
1	A	1270	GLN
1	A	343	ALA
1	A	344	ASP
1	A	347	LYS
1	A	463	THR
1	A	775	SER
1	A	898	SER
1	A	953	LEU
1	A	1019	ILE
1	A	562	ALA
1	A	617	GLY
1	A	897	GLU
1	A	923	LYS
1	A	1022	PRO
1	A	1020	ASP
1	A	969	PRO
1	A	760	VAL

5.3.2 Protein sidechains (i)

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	1077/1124 (96%)	966 (90%)	111 (10%)	7 13

All (111) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	7	ASP
1	A	25	HIS
1	A	29	ASN
1	A	37	GLU
1	A	39	ILE
1	A	50	LYS
1	A	59	ILE
1	A	73	GLU
1	A	74	LYS
1	A	75	VAL
1	A	77	ARG
1	A	113	GLN
1	A	123	ARG
1	A	180	VAL
1	A	190	LEU
1	A	195	LYS
1	A	222	GLN
1	A	224	ASP
1	A	229	LYS
1	A	231	LEU
1	A	248	LYS
1	A	250	GLN
1	A	265	LEU
1	A	267	SER
1	A	271	GLN
1	A	280	VAL
1	A	287	GLU
1	A	292	GLU
1	A	306	VAL
1	A	309	SER
1	A	323	GLU
1	A	324	GLN
1	A	360	LEU
1	A	365	ASN
1	A	367	GLU
1	A	374	ASP
1	A	380	VAL
1	A	382	GLU

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Mol	Chain	Res	Type
1	A	384	SER
1	A	385	ASN
1	A	390	LEU
1	A	391	MET
1	A	399	LEU
1	A	406	GLU
1	A	414	ILE
1	A	421	LEU
1	A	430	GLN
1	A	448	GLU
1	A	454	LEU
1	A	461	HIS
1	A	483	LEU
1	A	547	LYS
1	A	551	ASP
1	A	557	LEU
1	A	573	GLU
1	A	581	THR
1	A	584	THR
1	A	587	ILE
1	A	588	ASP
1	A	590	GLN
1	A	615	THR
1	A	619	THR
1	A	635	LEU
1	A	642	MET
1	A	656	TYR
1	A	694	LEU
1	A	697	ASN
1	A	720	LYS
1	A	722	LEU
1	A	726	LEU
1	A	742	ARG
1	A	770	LEU
1	A	774	ILE
1	A	787	SER
1	A	794	GLN
1	A	823	LEU
1	A	826	GLU
1	A	829	ILE
1	A	845	LEU
1	A	859	ARG

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Mol	Chain	Res	Type
1	A	864	VAL
1	A	876	ILE
1	A	886	VAL
1	A	887	LYS
1	A	895	ARG
1	A	903	ILE
1	A	917	ASP
1	A	924	LYS
1	A	939	ASP
1	A	940	GLU
1	A	950	ASN
1	A	952	ARG
1	A	977	ILE
1	A	979	GLN
1	A	992	ILE
1	A	1011	SER
1	A	1019	ILE
1	A	1025	LEU
1	A	1031	THR
1	A	1035	ILE
1	A	1044	SER
1	A	1048	GLN
1	A	1051	THR
1	A	1165	ASP
1	A	1174	ARG
1	A	1239	ARG
1	A	1241	LYS
1	A	1254	GLU
1	A	1270	GLN
1	A	1285	GLN
1	A	1287	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (27) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	32	GLN
1	A	113	GLN
1	A	218	GLN
1	A	250	GLN
1	A	270	GLN
1	A	324	GLN
1	A	340	GLN

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Mol	Chain	Res	Type
1	A	342	GLN
1	A	345	GLN
1	A	365	ASN
1	A	426	GLN
1	A	434	GLN
1	A	459	GLN
1	A	475	ASN
1	A	507	GLN
1	A	569	GLN
1	A	607	ASN
1	A	633	GLN
1	A	671	ASN
1	A	751	ASN
1	A	785	ASN
1	A	1109	GLN
1	A	1136	GLN
1	A	1152	GLN
1	A	1171	ASN
1	A	1173	ASN
1	A	1207	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 monosaccharides in this entry.

5.6 Ligand geometry (i)

2 ligands are 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	LEU	A	2291	-	5,8,8	0.81	0	6,10,10	0.60	0
3	SO4	A	2292	-	4,4,4	0.14	0	6,6,6	0.11	0

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	LEU	A	2291	-	-	4/4/8/8	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	2291	LEU	CA-CB-CG-CD2
2	A	2291	LEU	CA-CB-CG-CD1
2	A	2291	LEU	C-CA-CB-CG
2	A	2291	LEU	N-CA-CB-CG

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 (i)

6.1 Protein, DNA and RNA chains (i)

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled 'Q< 0.9' lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å²)	Q<0.9
1	A	1273/1304 (97%)	0.63	152 (11%)	4	3	57, 70, 79, 110	0

All (152) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	1043	GLY	12.3
1	A	888	ASP	8.2
1	A	1021	LEU	6.6
1	A	1017	LEU	6.5
1	A	939	ASP	6.4
1	A	1174	ARG	6.4
1	A	1161	THR	6.2
1	A	1038	TYR	5.7
1	A	1196	TYR	5.6
1	A	942	PRO	5.3
1	A	1155	SER	5.3
1	A	1057	GLN	5.2
1	A	1153	GLY	5.2
1	A	1020	ASP	5.1
1	A	1190	GLN	5.1
1	A	1171	ASN	5.0
1	A	1152	GLN	4.9
1	A	943	LEU	4.9
1	A	1107	LYS	4.8
1	A	940	GLU	4.7
1	A	913	LEU	4.7
1	A	1244	PHE	4.7
1	A	1100	ARG	4.6
1	A	1199	TYR	4.6
1	A	1047	LEU	4.6
1	A	1016	GLU	4.5
1	A	947	GLY	4.4

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Mol	Chain	Res	Type	RSRZ
1	A	1056	ASP	4.4
1	A	1150	LYS	4.4
1	A	907	LEU	4.2
1	A	1055	GLN	4.2
1	A	1165	ASP	4.2
1	A	909	ASN	4.1
1	A	977	ILE	4.1
1	A	1091	PHE	4.1
1	A	911	THR	4.0
1	A	1169	LEU	3.8
1	A	577	GLU	3.8
1	A	1111	GLU	3.7
1	A	1221	PHE	3.5
1	A	1112	GLY	3.5
1	A	1187	GLY	3.5
1	A	654	SER	3.5
1	A	1164	SER	3.5
1	A	1026	LEU	3.5
1	A	948	LYS	3.5
1	A	1060	ILE	3.4
1	A	618	THR	3.4
1	A	887	LYS	3.4
1	A	882	GLU	3.4
1	A	1163	GLU	3.3
1	A	1059	GLN	3.3
1	A	897	GLU	3.3
1	A	889	ALA	3.2
1	A	908	VAL	3.2
1	A	952	ARG	3.2
1	A	1134	GLU	3.2
1	A	1262	ILE	3.2
1	A	585	LEU	3.2
1	A	652	SER	3.1
1	A	1109	GLN	3.1
1	A	973	MET	3.1
1	A	1058	GLU	3.1
1	A	880	LEU	3.1
1	A	1162	VAL	3.1
1	A	581	THR	3.1
1	A	941	LEU	3.0
1	A	1087	CYS	3.0
1	A	1252	GLN	3.0

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Mol	Chain	Res	Type	RSRZ
1	A	949	VAL	3.0
1	A	938	LEU	3.0
1	A	588	ASP	2.9
1	A	1090	ASP	2.9
1	A	361	GLN	2.9
1	A	886	VAL	2.9
1	A	661	PHE	2.9
1	A	1172	VAL	2.9
1	A	910	ARG	2.9
1	A	493	ARG	2.9
1	A	946	ASN	2.8
1	A	1023	VAL	2.8
1	A	1246	THR	2.8
1	A	980	ILE	2.8
1	A	578	LEU	2.8
1	A	881	GLN	2.8
1	A	576	ALA	2.7
1	A	662	THR	2.7
1	A	1108	LEU	2.7
1	A	1272	VAL	2.7
1	A	1039	LEU	2.7
1	A	955	PRO	2.7
1	A	665	PHE	2.7
1	A	1041	ASN	2.7
1	A	660	ALA	2.6
1	A	656	TYR	2.6
1	A	1018	GLY	2.6
1	A	1076	ASN	2.6
1	A	954	LEU	2.6
1	A	1192	THR	2.6
1	A	1072	LEU	2.6
1	A	937	PHE	2.6
1	A	1154	VAL	2.6
1	A	1046	GLY	2.6
1	A	1228	ALA	2.6
1	A	1086	LEU	2.6
1	A	976	THR	2.5
1	A	1009	ALA	2.5
1	A	557	LEU	2.5
1	A	920	ALA	2.5
1	A	919	LYS	2.5
1	A	1191	LYS	2.5

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Mol	Chain	Res	Type	RSRZ
1	A	769	ASP	2.5
1	A	950	ASN	2.5
1	A	1197	SER	2.4
1	A	883	TYR	2.4
1	A	1283	VAL	2.4
1	A	1186	HIS	2.4
1	A	1045	ASP	2.4
1	A	1240	MET	2.3
1	A	921	HIS	2.3
1	A	1110	PRO	2.3
1	A	531	ILE	2.3
1	A	653	VAL	2.3
1	A	912	GLN	2.3
1	A	944	THR	2.3
1	A	1075	GLN	2.3
1	A	1201	ASN	2.3
1	A	702	PHE	2.3
1	A	357	ASN	2.3
1	A	1013	ILE	2.2
1	A	1019	ILE	2.2
1	A	1070	TYR	2.2
1	A	896	HIS	2.2
1	A	925	GLN	2.2
1	A	1094	GLU	2.2
1	A	703	ALA	2.2
1	A	1044	SER	2.2
1	A	229	LYS	2.2
1	A	601	ALA	2.2
1	A	1225	GLU	2.1
1	A	669	MET	2.1
1	A	1232	GLU	2.1
1	A	1130	ALA	2.1
1	A	597	ALA	2.1
1	A	1183	ALA	2.1
1	A	701	MET	2.1
1	A	1250	MET	2.1
1	A	223	LYS	2.1
1	A	657	ALA	2.1
1	A	953	LEU	2.0
1	A	1274	VAL	2.0
1	A	569	GLN	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 monosaccharides 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, 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	B-factors(Å^2)	Q<0.9
2	LEU	A	2291	9/9	0.65	0.53	77,78,79,79	0
3	SO4	A	2292	5/5	0.90	0.19	122,122,122,123	0

6.5 Other polymers (i)

There are no such residues in this entry.