



# Full wwPDB X-ray Structure Validation Report ⓘ

Nov 17, 2020 – 10:16 AM JST

PDB ID : 7C1K  
Title : Crystal structure of the starter condensation domain of rhizomide synthetase RzmA mutant R148A  
Authors : Zhong, L.; Diao, X.; Zhang, N.; Li, F.W.; Zhou, H.B.; Chen, H.N.; Ren, X.; Zhang, Y.; Wu, D.; Bian, X.  
Deposited on : 2020-05-04  
Resolution : 2.75 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
Xtriage (Phenix)	:	1.13
EDS	:	2.14.6
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)	:	2.14.6

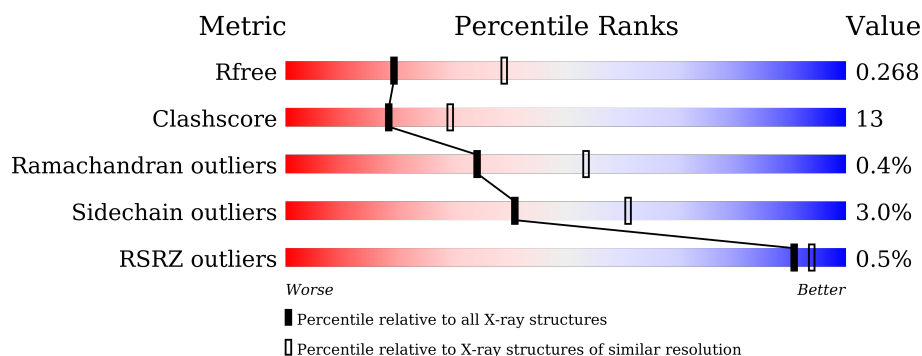
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.75 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	1235 (2.78-2.74)
Clashscore	141614	1277 (2.78-2.74)
Ramachandran outliers	138981	1257 (2.78-2.74)
Sidechain outliers	138945	1257 (2.78-2.74)
RSRZ outliers	127900	1207 (2.78-2.74)

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	434	<div> <div>69%</div> <div>24%</div> <div>• 6%</div> </div>
1	B	434	<div> <div>%</div> <div>65%</div> <div>26%</div> <div>• 9%</div> </div>
1	C	434	<div> <div>70%</div> <div>24%</div> <div>6%</div> </div>
1	D	434	<div> <div>%</div> <div>61%</div> <div>30%</div> <div>• 8%</div> </div>

## 2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 13032 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 Non-ribosomal peptide synthetase modules.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	409	Total	C	N	O	S	0	0	0
			3231	2049	562	600	20			
1	B	397	Total	C	N	O	S	0	0	0
			3133	1992	539	581	21			
1	C	409	Total	C	N	O	S	0	0	0
			3231	2049	562	600	20			
1	D	399	Total	C	N	O	S	0	0	0
			3147	1995	544	587	21			

There are 16 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-2	GLY	-	expression tag	UNP E5ATN9
A	-1	SER	-	expression tag	UNP E5ATN9
A	0	HIS	-	expression tag	UNP E5ATN9
A	148	ALA	ARG	engineered mutation	UNP E5ATN9
B	-2	GLY	-	expression tag	UNP E5ATN9
B	-1	SER	-	expression tag	UNP E5ATN9
B	0	HIS	-	expression tag	UNP E5ATN9
B	148	ALA	ARG	engineered mutation	UNP E5ATN9
C	-2	GLY	-	expression tag	UNP E5ATN9
C	-1	SER	-	expression tag	UNP E5ATN9
C	0	HIS	-	expression tag	UNP E5ATN9
C	148	ALA	ARG	engineered mutation	UNP E5ATN9
D	-2	GLY	-	expression tag	UNP E5ATN9
D	-1	SER	-	expression tag	UNP E5ATN9
D	0	HIS	-	expression tag	UNP E5ATN9
D	148	ALA	ARG	engineered mutation	UNP E5ATN9

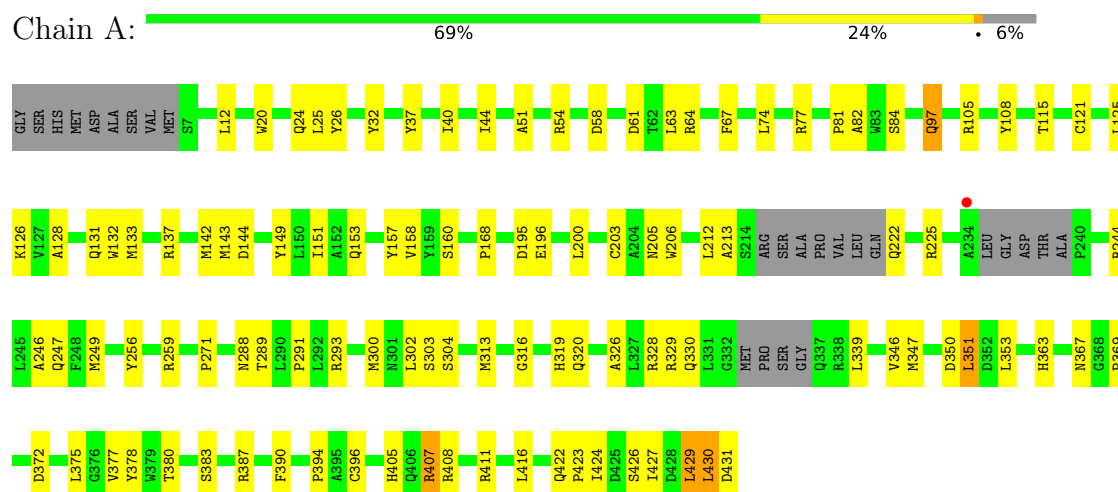
- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	86	Total 86	O 86	0	0
2	B	55	Total 55	O 55	0	0
2	C	84	Total 84	O 84	0	0
2	D	65	Total 65	O 65	0	0

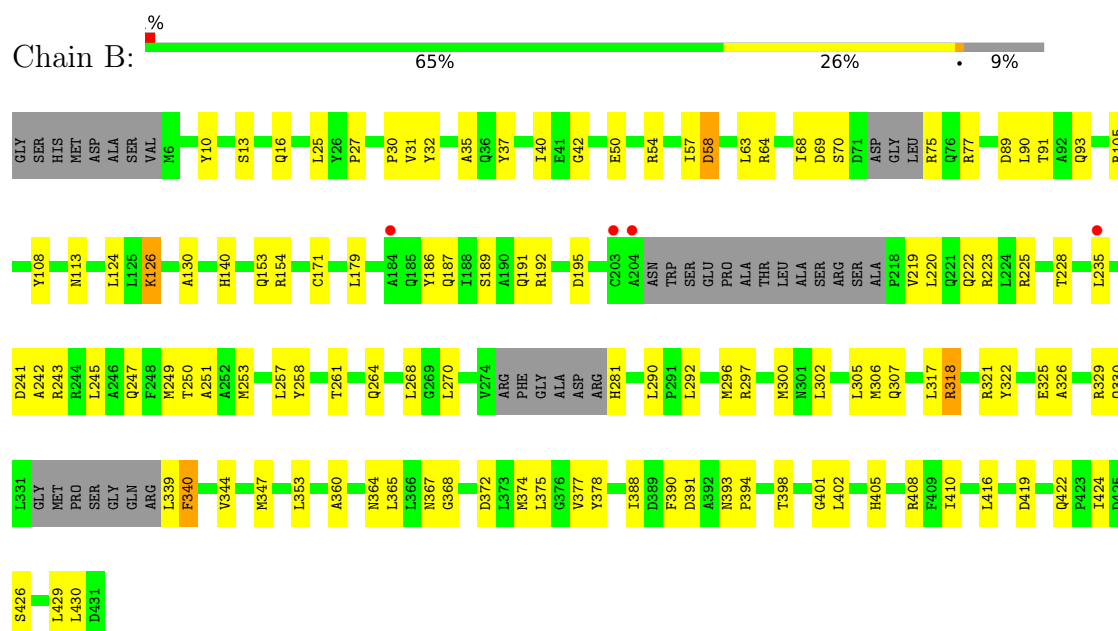
### 3 Residue-property plots

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: Non-ribosomal peptide synthetase modules

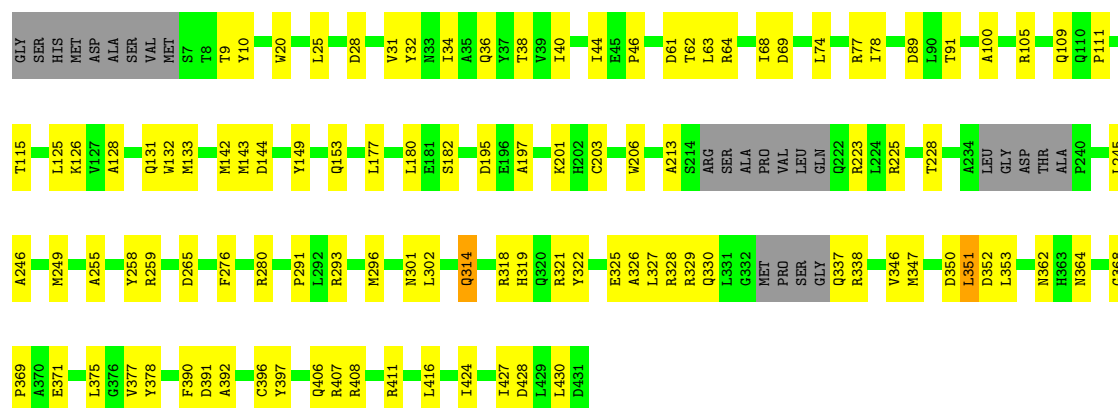


- Molecule 1: Non-ribosomal peptide synthetase modules



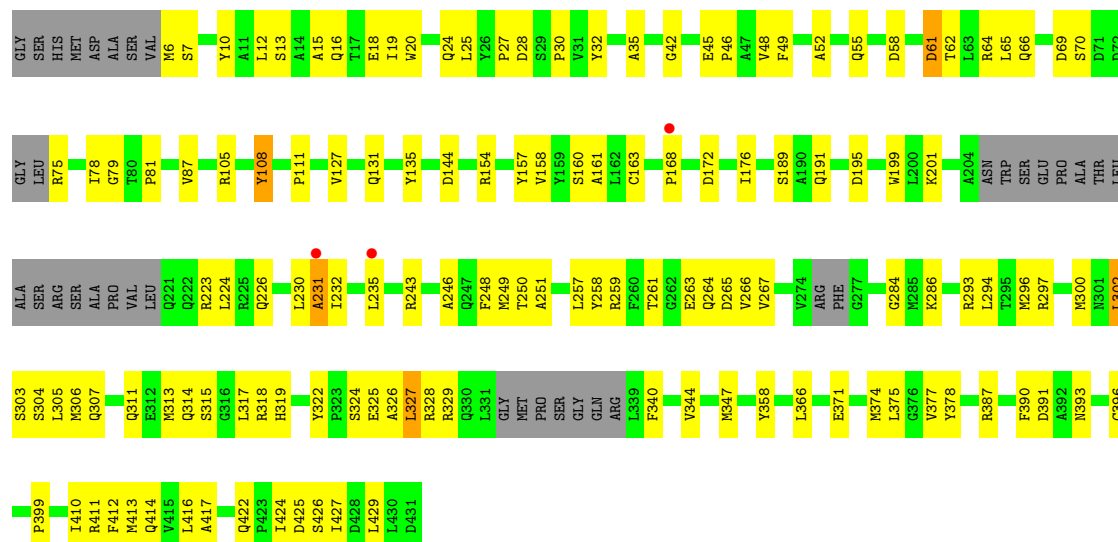
- Molecule 1: Non-ribosomal peptide synthetase modules

Chain C:  70% 24% 6%



• Molecule 1: Non-ribosomal peptide synthetase modules

Chain D:  61% 30% 8%



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	59.97Å 89.70Å 98.34Å 113.22° 90.09° 89.92°	Depositor
Resolution (Å)	39.12 – 2.75 39.12 – 2.76	Depositor EDS
% Data completeness (in resolution range)	89.3 (39.12-2.75) 44.1 (39.12-2.76)	Depositor EDS
$R_{merge}$	0.07	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	3.68 (at 2.77Å)	Xtriage
Refinement program	PHENIX 1.14	Depositor
R, $R_{free}$	0.237 , 0.275 0.232 , 0.268	Depositor DCC
$R_{free}$ test set	1012 reflections (4.52%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	37.3	Xtriage
Anisotropy	0.034	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.25 , 5.8	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.489 for h,-k,-l	Xtriage
Reported twinning fraction	0.500 for h,-k,-l	Depositor
Outliers	0 of 22370 reflections	Xtriage
$F_o, F_c$ correlation	0.89	EDS
Total number of atoms	13032	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	40.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 7.32% 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	A	0.27	0/3308	0.44	0/4502
1	B	0.30	0/3206	0.48	0/4364
1	C	0.27	0/3308	0.43	1/4502 (0.0%)
1	D	0.31	0/3219	0.48	0/4380
All	All	0.29	0/13041	0.46	1/17748 (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	C	352	ASP	CB-CA-C	5.07	120.54	110.40

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	3231	0	3141	75	1
1	B	3133	0	3058	82	0
1	C	3231	0	3141	77	1
1	D	3147	0	3059	110	0
2	A	86	0	0	7	0
2	B	55	0	0	3	0
2	C	84	0	0	2	0
2	D	65	0	0	5	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
All	All	13032	0	12399	335	1

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 13.

All (335) 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:D:302:LEU:HD11	1:D:306:MET:SD	1.66	1.35
1:C:63:LEU:HA	1:C:142:MET:HE1	1.14	1.13
1:D:302:LEU:CD1	1:D:306:MET:SD	2.43	1.05
1:C:326:ALA:O	1:C:330:GLN:HB2	1.58	1.03
1:C:351:LEU:HD12	1:C:351:LEU:H	1.24	0.98
1:D:264:GLN:CD	1:D:297:ARG:NH2	2.17	0.98
1:D:199:TRP:HB3	1:D:327:LEU:CD1	1.98	0.93
1:D:264:GLN:OE1	1:D:297:ARG:NH2	2.01	0.93
1:C:128:ALA:HB3	1:C:131:GLN:HB3	1.57	0.87
1:A:128:ALA:HB3	1:A:131:GLN:HB3	1.58	0.86
1:C:63:LEU:HA	1:C:142:MET:CE	2.01	0.85
1:D:58:ASP:OD1	1:D:64:ARG:NH2	2.09	0.84
1:B:290:LEU:HD22	1:B:317:LEU:HD21	1.59	0.84
1:D:302:LEU:HD12	1:D:302:LEU:O	1.78	0.83
1:B:339:LEU:HD22	1:B:340:PHE:CD2	2.14	0.83
1:D:413:MET:HA	1:D:416:LEU:HB2	1.60	0.82
1:D:259:ARG:HE	1:D:425:ASP:HA	1.46	0.80
1:D:300:MET:HG2	1:D:304:SER:OG	1.81	0.80
1:B:401:GLY:O	1:B:405:HIS:N	2.14	0.80
1:C:249:MET:HG2	1:C:377:VAL:HG21	1.63	0.79
1:D:264:GLN:NE2	1:D:297:ARG:NH2	2.30	0.78
1:A:249:MET:HG2	1:A:377:VAL:HG21	1.67	0.76
1:D:35:ALA:N	1:D:366:LEU:O	2.13	0.76
1:D:264:GLN:CD	1:D:297:ARG:HH22	1.89	0.76
1:C:25:LEU:O	1:D:307:GLN:NE2	2.19	0.75
1:A:158:VAL:HG13	1:A:168:PRO:HG3	1.69	0.75
1:A:222:GLN:HG3	1:A:394:PRO:HG2	1.70	0.74
1:C:36:GLN:HG2	1:C:364:ASN:HA	1.71	0.73
1:C:351:LEU:N	1:C:351:LEU:HD12	2.03	0.72
1:A:329:ARG:HH11	1:B:318:ARG:HD3	1.54	0.72
1:D:267:VAL:HG22	1:D:293:ARG:HD2	1.71	0.72
1:B:10:TYR:O	1:B:75:ARG:N	2.23	0.71
1:A:259:ARG:NH1	1:A:427:ILE:O	2.21	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:231:ALA:O	2:D:501:HOH:O	2.09	0.70
1:B:31:VAL:HG11	1:B:219:VAL:HB	1.72	0.70
1:D:261:THR:HG23	1:D:263:GLU:H	1.57	0.69
1:A:54:ARG:HH22	1:D:231:ALA:HB2	1.57	0.69
1:A:302:LEU:HD22	1:A:416:LEU:HB3	1.73	0.69
1:A:422:GLN:OE1	1:A:423:PRO:O	2.12	0.67
1:B:187:GLN:HA	1:B:192:ARG:HD2	1.76	0.67
1:D:264:GLN:NE2	1:D:297:ARG:HH22	1.90	0.66
1:C:351:LEU:CD1	1:C:351:LEU:H	1.97	0.66
1:B:257:LEU:O	1:B:261:THR:N	2.17	0.66
1:A:32:TYR:HE1	1:A:369:PRO:HG3	1.60	0.65
1:D:65:LEU:HD23	1:D:78:ILE:HG12	1.77	0.65
1:D:48:VAL:HG11	1:D:163:CYS:HB2	1.77	0.65
1:D:302:LEU:HD12	1:D:302:LEU:C	2.17	0.65
1:C:325:GLU:HG3	1:C:328:ARG:HH11	1.62	0.65
1:C:9:THR:HG22	1:C:77:ARG:HB3	1.79	0.65
1:D:249:MET:HG3	1:D:377:VAL:HG21	1.80	0.64
1:C:314:GLN:OE1	1:C:318:ARG:NH2	2.32	0.63
1:A:97:GLN:OE1	1:A:131:GLN:NE2	2.31	0.63
1:D:18:GLU:HG3	1:D:329:ARG:HH22	1.64	0.63
1:B:113:ASN:ND2	2:B:502:HOH:O	2.30	0.63
1:B:223:ARG:NE	1:B:391:ASP:OD1	2.24	0.63
1:C:353:LEU:HD12	1:C:362:ASN:HD21	1.65	0.62
1:A:246:ALA:HA	1:A:346:VAL:HG21	1.82	0.62
1:A:51:ALA:O	1:A:54:ARG:HB2	2.00	0.62
1:B:353:LEU:O	1:B:360:ALA:N	2.24	0.62
1:B:154:ARG:HH12	1:B:171:CYS:HA	1.65	0.62
1:B:258:TYR:HD2	1:B:424:ILE:HD11	1.65	0.62
1:D:230:LEU:HD22	1:D:410:ILE:HD12	1.80	0.62
1:A:411:ARG:HD2	1:A:430:LEU:HD21	1.82	0.61
1:B:50:GLU:OE2	1:B:54:ARG:NH1	2.33	0.61
1:B:13:SER:H	1:B:16:GLN:HB2	1.66	0.61
1:B:258:TYR:CD2	1:B:424:ILE:HD11	2.36	0.60
1:C:259:ARG:NH1	1:C:424:ILE:O	2.34	0.60
1:A:408:ARG:O	1:A:429:LEU:HD22	2.01	0.60
1:C:302:LEU:HD22	1:C:416:LEU:HB3	1.84	0.60
1:D:199:TRP:HB3	1:D:327:LEU:HD13	1.78	0.60
1:A:25:LEU:O	1:B:307:GLN:NE2	2.23	0.60
1:D:258:TYR:CD2	1:D:424:ILE:HD11	2.35	0.60
1:C:78:ILE:HG13	1:C:177:LEU:HD11	1.84	0.59
1:A:408:ARG:NH2	2:A:516:HOH:O	2.35	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:62:THR:O	1:C:142:MET:HE3	2.03	0.58
1:D:161:ALA:HB3	1:D:168:PRO:HG3	1.84	0.58
1:B:191:GLN:NE2	1:B:195:ASP:OD1	2.37	0.58
1:D:257:LEU:O	1:D:261:THR:N	2.35	0.58
1:D:411:ARG:HA	1:D:414:GLN:HG3	1.83	0.58
1:A:367:ASN:ND2	2:A:521:HOH:O	2.37	0.58
1:B:398:THR:OG1	1:B:401:GLY:N	2.32	0.58
1:B:250:THR:HG23	1:B:268:LEU:HD12	1.86	0.58
1:D:264:GLN:CD	1:D:297:ARG:HH21	2.02	0.57
1:D:127:VAL:HG23	1:D:131:GLN:HB3	1.86	0.57
1:D:324:SER:OG	1:D:328:ARG:NH2	2.36	0.57
1:A:329:ARG:NH2	2:A:523:HOH:O	2.37	0.57
1:B:374:MET:HB2	1:B:391:ASP:HB3	1.85	0.57
1:D:6:MET:O	1:D:6:MET:HG2	2.05	0.57
1:D:326:ALA:N	2:D:504:HOH:O	2.31	0.57
1:D:58:ASP:OD1	1:D:64:ARG:HD2	2.04	0.57
1:D:374:MET:HB2	1:D:391:ASP:HB3	1.87	0.57
1:B:419:ASP:HB3	1:B:422:GLN:HE21	1.68	0.56
1:D:10:TYR:O	1:D:75:ARG:N	2.37	0.56
1:B:93:GLN:NE2	2:B:505:HOH:O	2.37	0.56
1:A:149:TYR:CZ	1:A:350:ASP:HB3	2.40	0.56
1:D:199:TRP:NE1	1:D:319:HIS:O	2.31	0.56
1:A:407:ARG:NH2	2:A:524:HOH:O	2.38	0.56
1:C:407:ARG:NH2	2:C:511:HOH:O	2.37	0.56
1:A:203:CYS:HA	1:A:206:TRP:CD1	2.40	0.56
1:A:407:ARG:NH1	2:A:525:HOH:O	2.38	0.56
1:A:408:ARG:O	1:A:429:LEU:CD2	2.53	0.55
1:C:61:ASP:N	1:C:61:ASP:OD1	2.39	0.55
1:A:271:PRO:HA	1:A:289:THR:HA	1.88	0.55
1:A:375:LEU:HD13	1:A:390:PHE:HE1	1.70	0.55
1:C:411:ARG:HE	1:C:430:LEU:HD11	1.71	0.55
1:D:195:ASP:HB3	1:D:322:TYR:HB2	1.88	0.55
1:B:249:MET:HG3	1:B:377:VAL:HG21	1.88	0.55
1:B:281:HIS:N	2:B:506:HOH:O	2.39	0.55
1:D:258:TYR:HD2	1:D:424:ILE:HD11	1.71	0.55
1:D:223:ARG:NH1	1:D:371:GLU:O	2.36	0.55
1:C:89:ASP:OD1	1:C:91:THR:OG1	2.19	0.55
1:A:408:ARG:HG3	1:A:429:LEU:HD23	1.88	0.55
1:D:265:ASP:HB3	1:D:293:ARG:HH11	1.73	0.54
1:B:300:MET:O	1:B:424:ILE:N	2.41	0.54
1:C:10:TYR:CD2	1:C:180:LEU:HB3	2.42	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:422:GLN:HE22	1:A:427:ILE:N	2.06	0.54
1:C:206:TRP:CZ2	1:C:293:ARG:HB2	2.43	0.54
1:B:364:ASN:OD1	1:B:367:ASN:ND2	2.41	0.53
1:C:408:ARG:HG3	1:C:430:LEU:HD13	1.91	0.53
1:D:65:LEU:HD21	1:D:176:ILE:HG21	1.89	0.53
1:A:20:TRP:CD1	1:A:74:LEU:HD21	2.44	0.53
1:C:38:THR:O	1:C:133:MET:HA	2.08	0.53
1:C:25:LEU:HD22	1:D:314:GLN:HG2	1.90	0.53
1:B:195:ASP:HB3	1:B:322:TYR:HB2	1.90	0.53
1:A:143:MET:HE3	1:A:144:ASP:N	2.24	0.53
1:C:126:LYS:HG3	1:C:132:TRP:CE2	2.44	0.53
1:B:89:ASP:HA	1:B:126:LYS:HG2	1.91	0.52
1:C:195:ASP:OD1	1:C:319:HIS:ND1	2.39	0.52
1:D:257:LEU:C	1:D:261:THR:HG22	2.29	0.52
1:A:429:LEU:HG	1:A:430:LEU:HG	1.92	0.52
1:D:154:ARG:O	1:D:158:VAL:HG22	2.10	0.52
1:B:372:ASP:HA	1:B:393:ASN:HB2	1.91	0.52
1:C:246:ALA:HA	1:C:346:VAL:HG21	1.91	0.52
1:C:63:LEU:HD23	1:C:142:MET:HE2	1.92	0.52
1:B:90:LEU:HB3	1:B:93:GLN:HG3	1.92	0.51
1:C:255:ALA:O	1:C:259:ARG:HG2	2.11	0.51
1:D:266:VAL:HG12	1:D:296:MET:HE1	1.93	0.51
1:C:337:GLN:N	2:C:515:HOH:O	2.43	0.51
1:B:339:LEU:HD22	1:B:340:PHE:CE2	2.44	0.51
1:C:31:VAL:O	1:C:368:GLY:HA2	2.11	0.51
1:C:69:ASP:OD2	1:D:243:ARG:NH1	2.44	0.51
1:D:19:ILE:HG12	1:D:32:TYR:CE1	2.46	0.51
1:D:259:ARG:NE	1:D:425:ASP:HA	2.22	0.51
1:B:339:LEU:CD2	1:B:340:PHE:CD2	2.91	0.50
1:A:300:MET:HG2	1:A:304:SER:HB3	1.94	0.50
1:C:20:TRP:HH2	1:C:115:THR:HG1	1.58	0.50
1:B:408:ARG:HD3	1:B:430:LEU:O	2.12	0.50
1:C:347:MET:O	1:C:378:TYR:HA	2.12	0.50
1:A:259:ARG:NH1	1:A:424:ILE:O	2.44	0.50
1:D:246:ALA:O	1:D:250:THR:OG1	2.29	0.50
1:D:311:GLN:NE2	1:D:315:SER:OG	2.41	0.50
1:D:66:GLN:NE2	1:D:79:GLY:HA3	2.26	0.50
1:A:61:ASP:OD1	1:A:61:ASP:N	2.40	0.50
1:D:144:ASP:HB3	1:D:286:LYS:NZ	2.26	0.49
1:A:54:ARG:HH12	1:D:231:ALA:CB	2.25	0.49
1:D:313:MET:O	1:D:317:LEU:HB2	2.11	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:121:CYS:HB2	1:A:137:ARG:HH21	1.77	0.49
1:D:15:ALA:O	1:D:19:ILE:HG13	2.12	0.49
1:A:256:TYR:HE1	1:A:408:ARG:HG2	1.78	0.49
1:B:37:TYR:CD1	1:B:365:LEU:HD21	2.47	0.49
1:B:37:TYR:CE1	1:B:365:LEU:HD21	2.47	0.49
1:A:153:GLN:HG3	1:A:353:LEU:CD2	2.43	0.49
1:A:244:ARG:HA	1:A:247:GLN:HG2	1.94	0.49
1:B:154:ARG:HH22	1:B:171:CYS:HB2	1.78	0.49
1:B:251:ALA:HB1	1:B:305:LEU:HB2	1.95	0.49
1:C:225:ARG:HB3	1:C:225:ARG:HH11	1.78	0.49
1:A:153:GLN:HG3	1:A:353:LEU:HD22	1.95	0.48
1:D:232:ILE:HG21	1:D:417:ALA:HB3	1.95	0.48
1:C:182:SER:OG	1:C:321:ARG:NH2	2.46	0.48
1:A:430:LEU:H	1:A:430:LEU:HG	1.28	0.48
1:B:250:THR:OG1	1:B:270:LEU:HD21	2.14	0.48
1:B:377:VAL:HG22	1:B:388:ILE:HD13	1.95	0.48
1:D:393:ASN:HB3	1:D:396:CYS:SG	2.54	0.48
1:B:40:ILE:HG12	1:B:360:ALA:HB2	1.96	0.48
1:C:197:ALA:O	1:C:201:LYS:HG2	2.13	0.48
1:D:25:LEU:O	1:D:27:PRO:HD3	2.13	0.48
1:D:258:TYR:CD2	1:D:296:MET:HB3	2.48	0.48
1:C:245:LEU:HG	1:C:346:VAL:HG11	1.95	0.48
1:C:301:ASN:HA	1:C:424:ILE:HG12	1.96	0.48
1:D:224:LEU:HD21	1:D:399:PRO:HG3	1.95	0.48
1:C:326:ALA:O	1:C:330:GLN:CB	2.48	0.47
1:D:422:GLN:NE2	1:D:426:SER:O	2.28	0.47
1:D:69:ASP:OD1	1:D:70:SER:N	2.47	0.47
1:A:25:LEU:HD23	1:A:26:TYR:CE2	2.49	0.47
1:A:206:TRP:HH2	1:A:291:PRO:HB2	1.79	0.47
1:A:380:THR:HB	1:A:383:SER:HB3	1.97	0.47
1:A:54:ARG:HH22	1:D:231:ALA:CB	2.25	0.47
1:C:411:ARG:NH2	1:C:428:ASP:O	2.47	0.47
1:C:100:ALA:HB1	1:C:125:LEU:HD13	1.96	0.47
1:D:248:PHE:HE2	1:D:413:MET:HE3	1.80	0.47
1:D:65:LEU:CD2	1:D:78:ILE:HG12	2.44	0.47
1:C:149:TYR:OH	1:C:351:LEU:HD13	2.15	0.47
1:C:408:ARG:HA	1:C:430:LEU:HD13	1.95	0.47
1:B:253:MET:O	1:B:257:LEU:HD12	2.14	0.47
1:D:65:LEU:HD11	1:D:176:ILE:HD13	1.97	0.47
1:B:264:GLN:HG3	1:B:296:MET:O	2.15	0.47
1:B:68:ILE:HD11	1:B:77:ARG:HD2	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:243:ARG:NH2	2:D:510:HOH:O	2.48	0.47
1:A:212:LEU:HD22	1:A:405:HIS:CE1	2.49	0.47
1:C:213:ALA:HB1	1:C:396:CYS:HB3	1.97	0.47
1:D:61:ASP:OD1	1:D:176:ILE:HG22	2.14	0.47
1:C:20:TRP:CE2	1:C:74:LEU:HD22	2.50	0.47
1:C:371:GLU:OE1	1:C:371:GLU:N	2.36	0.46
1:C:329:ARG:O	1:D:318:ARG:NH2	2.49	0.46
1:D:422:GLN:NE2	2:D:511:HOH:O	2.49	0.46
1:B:344:VAL:HG13	1:B:375:LEU:HD13	1.96	0.46
1:C:78:ILE:HG12	1:C:177:LEU:HD21	1.98	0.46
1:D:226:GLN:HB2	1:D:390:PHE:HB2	1.98	0.46
1:A:247:GLN:NE2	2:A:501:HOH:O	2.39	0.46
1:B:228:THR:HG21	1:B:410:ILE:HD12	1.98	0.46
1:D:223:ARG:HH22	1:D:374:MET:HG3	1.80	0.46
1:A:82:ALA:HA	2:D:501:HOH:O	2.16	0.46
1:B:347:MET:O	1:B:378:TYR:HA	2.16	0.46
1:D:230:LEU:HD11	1:D:414:GLN:NE2	2.30	0.46
1:C:375:LEU:HD13	1:C:390:PHE:HE1	1.81	0.46
1:B:69:ASP:HA	1:B:75:ARG:HH11	1.81	0.46
1:D:257:LEU:O	1:D:261:THR:HG22	2.16	0.46
1:B:58:ASP:OD1	1:B:64:ARG:NH1	2.48	0.46
1:D:105:ARG:HA	1:D:108:TYR:CZ	2.51	0.45
1:A:387:ARG:NH1	2:A:513:HOH:O	2.49	0.45
1:B:344:VAL:HA	1:B:375:LEU:HB3	1.98	0.45
1:D:325:GLU:HG3	1:D:328:ARG:HH12	1.82	0.45
1:B:416:LEU:HA	1:B:416:LEU:HD23	1.81	0.45
1:D:412:PHE:CD1	1:D:429:LEU:HD21	2.52	0.45
1:C:28:ASP:HA	1:C:111:PRO:HG2	1.98	0.45
1:D:251:ALA:HB1	1:D:305:LEU:HB3	1.98	0.45
1:B:89:ASP:OD1	1:B:91:THR:HG23	2.16	0.45
1:C:228:THR:OG1	1:C:406:GLN:OE1	2.25	0.45
1:D:325:GLU:CD	1:D:325:GLU:H	2.20	0.45
1:A:213:ALA:HB1	1:A:396:CYS:HB3	1.98	0.45
1:D:317:LEU:HD12	1:D:317:LEU:HA	1.72	0.45
1:A:326:ALA:O	1:A:330:GLN:HG2	2.16	0.45
1:B:57:ILE:HA	1:B:63:LEU:HD12	1.99	0.45
1:A:195:ASP:OD1	1:A:319:HIS:ND1	2.38	0.45
1:C:203:CYS:HA	1:C:206:TRP:CD1	2.52	0.45
1:D:64:ARG:HA	1:D:81:PRO:HG3	1.98	0.44
1:A:121:CYS:HB3	1:A:137:ARG:HB3	1.98	0.44
1:B:325:GLU:H	1:B:325:GLU:CD	2.20	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:259:ARG:HH11	1:C:424:ILE:HG22	1.82	0.44
1:D:411:ARG:HA	1:D:414:GLN:CG	2.46	0.44
1:B:140:HIS:ND1	1:B:368:GLY:HA3	2.31	0.44
1:B:247:GLN:HB3	1:B:306:MET:HE3	1.99	0.44
1:B:296:MET:HB2	1:B:296:MET:HE2	1.73	0.44
1:B:408:ARG:HD2	1:B:429:LEU:HD23	1.99	0.44
1:A:37:TYR:CZ	1:A:363:HIS:HB2	2.53	0.44
1:B:242:ALA:O	1:B:245:LEU:HB3	2.17	0.44
1:A:105:ARG:HA	1:A:108:TYR:CZ	2.53	0.44
1:A:32:TYR:CE1	1:A:369:PRO:HG3	2.48	0.44
1:A:40:ILE:HG21	1:A:44:ILE:HD11	2.00	0.44
1:C:62:THR:O	1:C:142:MET:CE	2.66	0.44
1:C:105:ARG:O	1:C:109:GLN:HB2	2.17	0.44
1:C:153:GLN:HA	1:C:353:LEU:HD22	1.99	0.44
1:C:392:ALA:HB1	1:C:397:TYR:CD1	2.53	0.43
1:D:412:PHE:O	1:D:416:LEU:N	2.51	0.43
1:B:426:SER:OG	1:B:426:SER:O	2.36	0.43
1:C:64:ARG:HB3	1:C:64:ARG:HE	1.66	0.43
1:A:288:ASN:ND2	1:A:320:GLN:O	2.41	0.43
1:C:206:TRP:CH2	1:C:291:PRO:HB2	2.53	0.43
1:D:264:GLN:HE22	1:D:297:ARG:HH22	1.62	0.43
1:D:52:ALA:O	1:D:55:GLN:HB3	2.18	0.43
1:A:196:GLU:O	1:A:200:LEU:HD12	2.19	0.43
1:B:32:TYR:O	1:B:140:HIS:N	2.45	0.43
1:D:144:ASP:HB3	1:D:286:LYS:HZ3	1.82	0.43
1:D:412:PHE:CZ	1:D:416:LEU:HD21	2.53	0.43
1:A:12:LEU:HD11	1:A:67:PHE:HD2	1.83	0.43
1:B:105:ARG:HA	1:B:108:TYR:CZ	2.53	0.43
1:B:186:TYR:CZ	1:B:192:ARG:HG3	2.54	0.43
1:C:68:ILE:HG21	1:C:77:ARG:CZ	2.49	0.43
1:A:206:TRP:NE1	1:A:293:ARG:HD2	2.34	0.43
1:A:328:ARG:HG2	1:A:339:LEU:HD13	2.01	0.43
1:C:40:ILE:HG21	1:C:44:ILE:HD11	2.01	0.43
1:D:12:LEU:HD13	1:D:75:ARG:HB2	2.00	0.43
1:A:380:THR:HB	1:A:383:SER:CB	2.48	0.43
1:A:20:TRP:CH2	1:A:115:THR:HG22	2.54	0.43
1:C:265:ASP:HB3	1:C:293:ARG:CZ	2.49	0.43
1:C:258:TYR:HB2	1:C:296:MET:HG3	2.01	0.43
1:D:157:TYR:O	1:D:160:SER:HB3	2.18	0.43
1:D:45:GLU:HA	1:D:46:PRO:HD3	1.91	0.42
1:B:35:ALA:HB3	1:B:365:LEU:HB2	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:13:SER:H	1:D:16:GLN:HB2	1.83	0.42
1:A:351:LEU:HD22	1:A:351:LEU:HA	1.63	0.42
1:B:339:LEU:HD22	1:B:340:PHE:HD2	1.78	0.42
1:D:46:PRO:HB3	1:D:87:VAL:HG21	2.02	0.42
1:B:390:PHE:HD2	1:B:402:LEU:HG	1.85	0.42
1:A:203:CYS:HA	1:A:206:TRP:NE1	2.34	0.42
1:D:344:VAL:HA	1:D:375:LEU:HB3	2.00	0.42
1:D:410:ILE:O	1:D:414:GLN:HG2	2.19	0.42
1:B:222:GLN:O	1:B:394:PRO:HG3	2.19	0.42
1:B:300:MET:O	1:B:424:ILE:HG23	2.19	0.42
1:B:302:LEU:O	1:B:306:MET:HG3	2.20	0.42
1:C:259:ARG:HH12	1:C:427:ILE:HB	1.85	0.42
1:D:199:TRP:HB3	1:D:327:LEU:HD12	1.94	0.42
1:B:326:ALA:O	1:B:330:GLN:HG3	2.20	0.42
1:C:44:ILE:O	1:C:46:PRO:HD3	2.20	0.42
1:B:124:LEU:HA	1:B:124:LEU:HD23	1.91	0.41
1:B:297:ARG:HB2	1:B:300:MET:HE3	2.01	0.41
1:D:412:PHE:CE1	1:D:416:LEU:HD21	2.55	0.41
1:B:219:VAL:O	1:B:219:VAL:HG23	2.21	0.41
1:B:225:ARG:HA	1:B:390:PHE:O	2.21	0.41
1:C:32:TYR:CE1	1:C:369:PRO:HG3	2.55	0.41
1:D:265:ASP:CB	1:D:293:ARG:HH11	2.32	0.41
1:A:347:MET:O	1:A:378:TYR:HA	2.19	0.41
1:B:25:LEU:O	1:B:27:PRO:HD3	2.20	0.41
1:A:225:ARG:HA	1:A:390:PHE:O	2.20	0.41
1:A:126:LYS:HD2	1:A:132:TRP:CZ2	2.55	0.41
1:D:108:TYR:HB3	1:D:135:TYR:OH	2.21	0.41
1:A:429:LEU:HG	1:A:430:LEU:H	1.86	0.41
1:B:250:THR:HG21	1:B:292:LEU:HD22	2.03	0.41
1:D:201:LYS:HB2	1:D:201:LYS:HE2	1.91	0.41
1:D:235:LEU:HD21	1:D:248:PHE:CE2	2.56	0.41
1:D:422:GLN:HG2	1:D:427:ILE:HG12	2.03	0.41
1:A:64:ARG:HA	1:A:81:PRO:HG3	2.03	0.41
1:C:144:ASP:N	1:C:144:ASP:OD1	2.52	0.41
1:C:34:ILE:HD11	1:C:143:MET:HB3	2.03	0.41
1:D:302:LEU:CD1	1:D:302:LEU:C	2.84	0.41
1:B:42:GLY:N	1:B:130:ALA:O	2.53	0.41
1:B:235:LEU:HA	1:B:235:LEU:HD12	1.91	0.41
1:B:353:LEU:HD23	1:B:353:LEU:HA	1.94	0.41
1:A:125:LEU:HB2	1:A:133:MET:HB2	2.03	0.41
1:A:142:MET:O	1:A:143:MET:HG2	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:186:TYR:HA	1:B:189:SER:HB2	2.03	0.41
1:D:28:ASP:HA	1:D:111:PRO:HG2	2.03	0.40
1:C:225:ARG:NE	1:C:391:ASP:OD2	2.54	0.40
1:D:378:TYR:HB2	1:D:387:ARG:HB3	2.01	0.40
1:A:157:TYR:O	1:A:160:SER:OG	2.27	0.40
1:A:63:LEU:HD11	1:A:151:ILE:HD13	2.02	0.40
1:B:223:ARG:HH21	1:B:374:MET:HG3	1.85	0.40
1:D:266:VAL:HG12	1:D:294:LEU:HB2	2.03	0.40
1:D:62:THR:HG21	1:D:284:GLY:HA3	2.03	0.40
1:C:206:TRP:HH2	1:C:291:PRO:HB2	1.85	0.40
1:C:322:TYR:CE2	1:C:327:LEU:HB2	2.57	0.40
1:C:338:ARG:NH1	1:C:371:GLU:HA	2.36	0.40
1:B:219:VAL:O	1:B:220:LEU:HB3	2.22	0.40
1:C:149:TYR:CZ	1:C:350:ASP:HB3	2.57	0.40
1:D:42:GLY:HA3	1:D:358:TYR:CD1	2.57	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:426:SER:OG	1:C:276:PHE:O[1_444]	2.18	0.02

## 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	A	401/434 (92%)	377 (94%)	22 (6%)	2 (0%)	29	47
1	B	387/434 (89%)	364 (94%)	21 (5%)	2 (0%)	29	47
1	C	401/434 (92%)	387 (96%)	14 (4%)	0	100	100
1	D	389/434 (90%)	369 (95%)	17 (4%)	3 (1%)	19	34

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
All	All	1578/1736 (91%)	1497 (95%)	74 (5%)	7 (0%)	34	53

All (7) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	70	SER
1	D	231	ALA
1	A	372	ASP
1	B	30	PRO
1	D	61	ASP
1	A	316	GLY
1	D	30	PRO

### 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	334/353 (95%)	321 (96%)	13 (4%)	32	52
1	B	326/353 (92%)	316 (97%)	10 (3%)	40	60
1	C	334/353 (95%)	330 (99%)	4 (1%)	71	82
1	D	326/353 (92%)	313 (96%)	13 (4%)	31	51
All	All	1320/1412 (94%)	1280 (97%)	40 (3%)	41	61

All (40) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	24	GLN
1	A	58	ASP
1	A	77	ARG
1	A	84	SER
1	A	97	GLN
1	A	205	ASN
1	A	303	SER
1	A	313	MET

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Mol	Chain	Res	Type
1	A	351	LEU
1	A	407	ARG
1	A	429	LEU
1	A	430	LEU
1	A	431	ASP
1	B	58	ASP
1	B	126	LYS
1	B	153	GLN
1	B	179	LEU
1	B	241	ASP
1	B	243	ARG
1	B	318	ARG
1	B	321	ARG
1	B	329	ARG
1	B	340	PHE
1	C	223	ARG
1	C	280	ARG
1	C	314	GLN
1	C	351	LEU
1	D	7	SER
1	D	20	TRP
1	D	24	GLN
1	D	49	PHE
1	D	108	TYR
1	D	172	ASP
1	D	189	SER
1	D	191	GLN
1	D	302	LEU
1	D	303	SER
1	D	327	LEU
1	D	340	PHE
1	D	347	MET

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (7) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	55	GLN
1	A	97	GLN
1	A	131	GLN
1	B	264	GLN
1	C	55	GLN
1	C	362	ASN

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Mol	Chain	Res	Type
1	C	364	ASN

### 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](#)

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 [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, 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	409/434 (94%)	-0.43	1 (0%) 95 97	18, 34, 63, 91	0
1	B	397/434 (91%)	-0.31	4 (1%) 82 87	24, 43, 66, 81	0
1	C	409/434 (94%)	-0.51	0 100 100	13, 30, 58, 73	0
1	D	399/434 (91%)	-0.31	3 (0%) 86 90	26, 48, 70, 82	0
All	All	1614/1736 (92%)	-0.39	8 (0%) 91 94	13, 39, 65, 91	0

All (8) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	234	ALA	5.0
1	B	235	LEU	4.6
1	B	203	CYS	3.2
1	D	235	LEU	3.0
1	D	231	ALA	2.9
1	B	184	ALA	2.9
1	B	204	ALA	2.6
1	D	168	PRO	2.4

### 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](#)

There are no ligands in this entry.

## 6.5 Other polymers [i](#)

There are no such residues in this entry.