Full wwPDB X-ray Structure Validation Report ⓘ

Nov 19, 2023 – 10:33 PM JST

PDB ID	:	7C1P
Title	:	Crystal structure of the starter condensation domain of the rhizomide synthetase RzmA mutant H140V, R148A
Authors	:	Zhong, L.; Diao, X.; Zhang, N.; Li, F.W.; Zhou, H.B.; Chen, H.N.; Ren, X.; Zhang, Y.; Wu, D.
Deposited on	:	2020-05-05
Resolution	:	2.60 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:

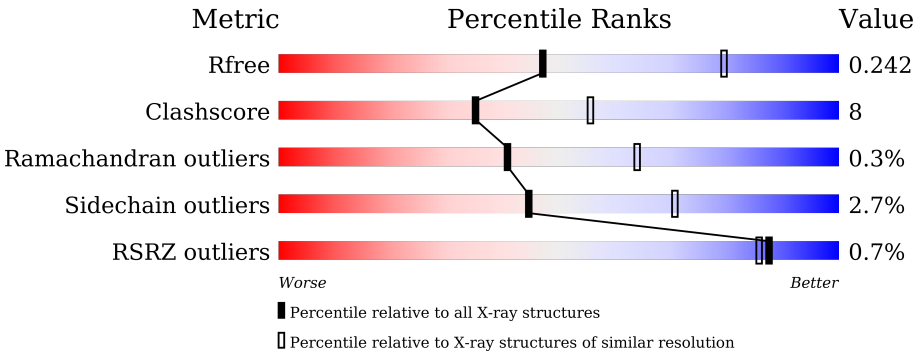
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.36
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

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	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 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 <=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	76% 18% 6%
1	B	434	2% 71% 21% 8%
1	C	434	74% 19% 6%
1	D	434	% 69% 22% 9%

2 Entry composition (i)

There are 2 unique types of molecules in this entry. The entry contains 13044 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	410	Total	C	N	O	S	0	0	0
			3236	2053	561	601	21			
1	B	399	Total	C	N	O	S	0	0	0
			3144	1996	542	585	21			
1	C	408	Total	C	N	O	S	0	0	0
			3224	2046	559	599	20			
1	D	395	Total	C	N	O	S	0	0	0
			3118	1982	538	578	20			

There are 20 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	140	VAL	HIS	engineered mutation	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	140	VAL	HIS	engineered mutation	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	140	VAL	HIS	engineered mutation	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	140	VAL	HIS	engineered mutation	UNP E5ATN9
D	148	ALA	ARG	engineered mutation	UNP E5ATN9

- Molecule 2 is water.

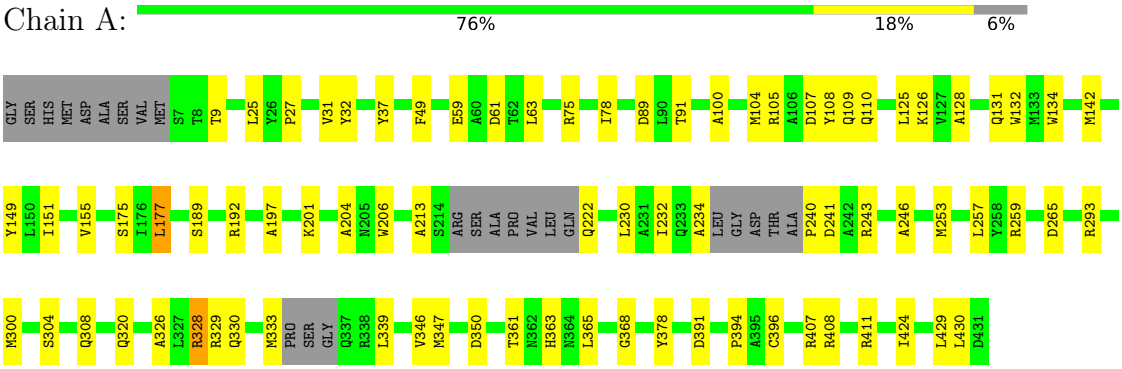
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	87	Total O 87 87	0	0
2	B	69	Total O 69 69	0	0
2	C	106	Total O 106 106	0	0
2	D	60	Total O 60 60	0	0

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.

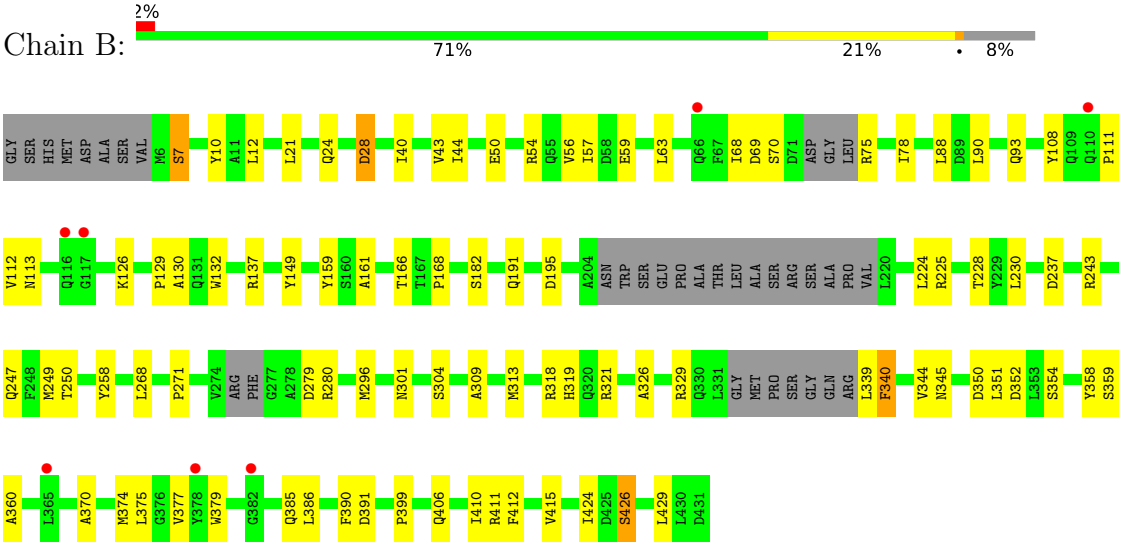
• Molecule 1: Non-ribosomal peptide synthetase modules

Chain A:



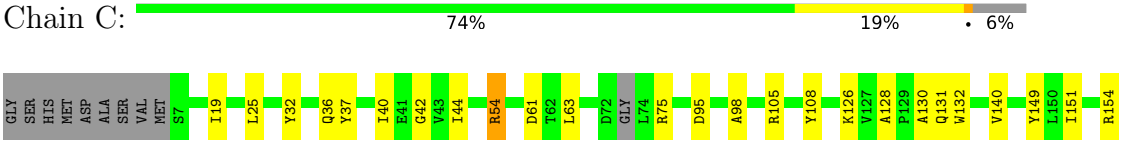
• Molecule 1: Non-ribosomal peptide synthetase modules

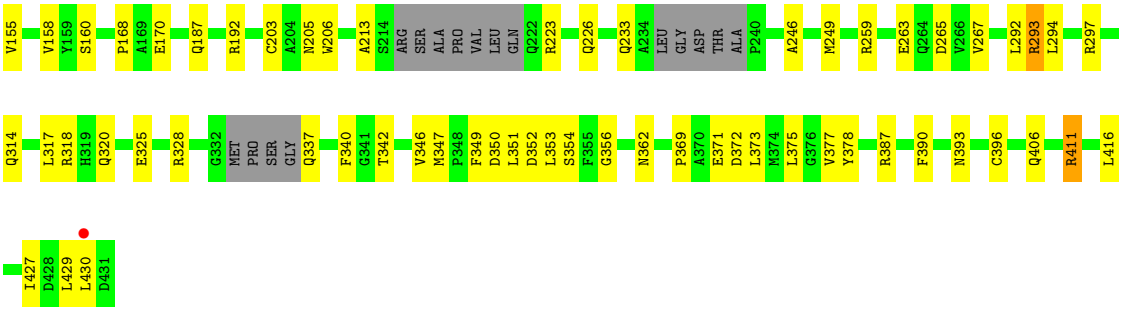
Chain B:



• Molecule 1: Non-ribosomal peptide synthetase modules

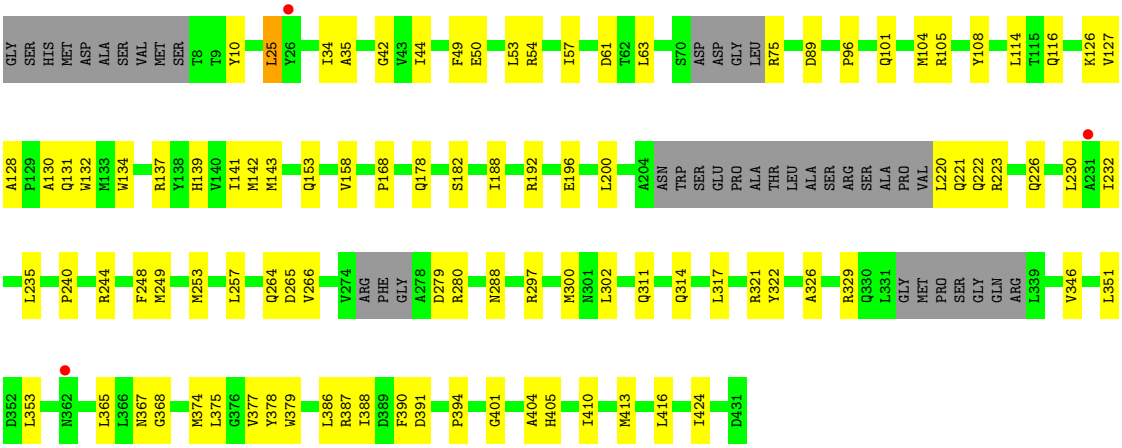
Chain C:





• Molecule 1: Non-ribosomal peptide synthetase modules

Chain D:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α, β, γ	60.64Å 89.65Å 98.07Å 66.89° 90.02° 90.25°	Depositor
Resolution (Å)	48.96 – 2.60 48.96 – 2.59	Depositor EDS
% Data completeness (in resolution range)	92.6 (48.96-2.60) 45.9 (48.96-2.59)	Depositor EDS
R_{merge}	0.04	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.62 (at 2.58Å)	Xtriage
Refinement program	PHENIX 1.14	Depositor
R, R_{free}	0.230 , 0.261 0.225 , 0.242	Depositor DCC
R_{free} test set	1050 reflections (3.68%)	wwPDB-VP
Wilson B-factor (Å^2)	35.3	Xtriage
Anisotropy	0.095	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.28 , 18.8	EDS
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	0.499 for h,-k,-l	Xtriage
Reported twinning fraction	0.480 for h,-k,-l	Depositor
Outliers	0 of 28504 reflections	Xtriage
F_o,F_c correlation	0.91	EDS
Total number of atoms	13044	wwPDB-VP
Average B, all atoms (Å^2)	45.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 7.48% of the height of the origin peak. No significant pseudotranslation is detected.*

[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

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	A	0.32	1/3312 (0.0%)	0.44	0/4507
1	B	0.26	0/3215	0.44	0/4375
1	C	0.25	0/3299	0.41	0/4489
1	D	0.27	0/3189	0.45	0/4341
All	All	0.28	1/13015 (0.0%)	0.44	0/17712

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	59	GLU	CD-OE1	-6.04	1.19	1.25

There are no bond angle outliers.

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	A	3236	0	3152	45	0
1	B	3144	0	3068	53	0
1	C	3224	0	3139	52	0
1	D	3118	0	3047	58	1
2	A	87	0	0	2	1
2	B	69	0	0	2	0
2	C	106	0	0	8	0
2	D	60	0	0	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
All	All	13044	0	12406	206	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 8.

All (206) 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:C:128:ALA:HB3	1:C:131:GLN:HB2	1.51	0.91
1:A:89:ASP:HA	1:A:126:LYS:HB2	1.59	0.85
1:D:302:LEU:HD12	1:D:416:LEU:HG	1.60	0.81
1:D:89:ASP:HA	1:D:126:LYS:HG2	1.66	0.76
1:A:222:GLN:N	2:A:501:HOH:O	2.18	0.76
1:B:249:MET:HG3	1:B:377:VAL:HG21	1.70	0.73
1:C:249:MET:HG2	1:C:377:VAL:HG21	1.69	0.73
1:B:12:LEU:HD13	1:B:75:ARG:HB3	1.70	0.72
1:A:326:ALA:O	1:A:330:GLN:HB2	1.91	0.71
1:A:259:ARG:HB3	1:A:429:LEU:HD11	1.74	0.69
1:D:379:TRP:HB2	1:D:386:LEU:HD12	1.75	0.68
1:C:259:ARG:NH1	1:C:427:ILE:O	2.23	0.67
1:B:10:TYR:O	1:B:75:ARG:N	2.28	0.67
1:D:401:GLY:O	1:D:405:HIS:N	2.27	0.66
1:C:205:ASN:O	2:C:501:HOH:O	2.14	0.64
1:D:249:MET:HG3	1:D:377:VAL:HG21	1.80	0.63
1:D:326:ALA:HA	1:D:329:ARG:HG3	1.80	0.63
1:B:228:THR:HG21	1:B:410:ILE:HG13	1.83	0.61
1:A:128:ALA:HB3	1:A:131:GLN:HB3	1.82	0.60
1:B:385:GLN:NE2	2:B:505:HOH:O	2.34	0.60
1:B:43:VAL:HA	1:B:132:TRP:CD1	2.36	0.60
1:D:288:ASN:ND2	1:D:322:TYR:O	2.36	0.59
1:C:126:LYS:HG3	1:C:132:TRP:CE2	2.37	0.59
1:C:267:VAL:HG22	1:C:293:ARG:HD3	1.84	0.59
1:B:191:GLN:OE1	1:B:318:ARG:NH2	2.35	0.59
1:D:314:GLN:HA	1:D:317:LEU:HB2	1.83	0.59
1:C:223:ARG:NH2	1:C:371:GLU:O	2.31	0.59
1:A:149:TYR:CZ	1:A:350:ASP:HB3	2.38	0.58
1:D:128:ALA:HB3	1:D:131:GLN:HB3	1.84	0.58
1:A:78:ILE:HG13	1:A:177:LEU:HD11	1.85	0.58
1:A:105:ARG:NH1	1:A:109:GLN:OE1	2.36	0.58
1:C:411:ARG:NH1	2:C:502:HOH:O	2.21	0.58
1:B:50:GLU:OE2	1:B:54:ARG:NH1	2.37	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:44:ILE:HD12	1:D:132:TRP:HB2	1.85	0.57
1:D:257:LEU:HG	1:D:266:VAL:HG21	1.86	0.57
1:D:153:GLN:HA	1:D:353:LEU:HD23	1.87	0.57
1:D:50:GLU:OE1	1:D:54:ARG:NH1	2.36	0.57
1:B:426:SER:OG	1:B:426:SER:O	2.23	0.56
1:A:213:ALA:HB1	1:A:396:CYS:HB3	1.88	0.56
1:D:192:ARG:NH2	2:D:503:HOH:O	2.38	0.56
1:C:411:ARG:HD3	1:C:430:LEU:HD21	1.88	0.56
1:D:240:PRO:HD2	1:D:244:ARG:HG2	1.86	0.56
1:A:9:THR:HB	1:A:75:ARG:HD3	1.86	0.55
1:C:342:THR:HG23	1:C:373:LEU:HG	1.89	0.55
1:A:100:ALA:HB1	1:A:125:LEU:HD13	1.88	0.55
1:B:195:ASP:OD1	1:B:319:HIS:ND1	2.27	0.55
1:C:151:ILE:O	1:C:155:VAL:HG23	2.07	0.54
1:C:406:GLN:NE2	2:C:503:HOH:O	2.33	0.54
1:C:54:ARG:NH2	2:C:515:HOH:O	2.40	0.54
1:B:161:ALA:HB3	1:B:168:PRO:HG3	1.90	0.54
1:A:222:GLN:HG2	2:A:501:HOH:O	2.07	0.53
1:C:265:ASP:HB2	1:C:293:ARG:NE	2.23	0.53
1:B:68:ILE:HG22	1:B:69:ASP:H	1.71	0.53
1:D:10:TYR:O	1:D:75:ARG:N	2.41	0.53
1:C:353:LEU:CD1	1:C:362:ASN:HD21	2.21	0.53
1:D:230:LEU:HD12	1:D:410:ILE:HG23	1.90	0.53
1:B:44:ILE:HG23	1:B:159:TYR:CZ	2.44	0.53
1:A:253:MET:O	1:A:257:LEU:HG	2.08	0.53
1:A:408:ARG:HA	1:A:430:LEU:HD22	1.90	0.53
1:D:96:PRO:HB2	1:D:127:VAL:HG12	1.92	0.52
1:A:329:ARG:HH21	1:B:318:ARG:HG3	1.74	0.52
1:C:292:LEU:HD23	1:C:294:LEU:HD21	1.92	0.52
1:C:154:ARG:NH2	2:C:507:HOH:O	2.37	0.52
1:D:137:ARG:NH1	2:D:506:HOH:O	2.42	0.52
1:D:178:GLN:O	1:D:182:SER:OG	2.24	0.52
1:C:25:LEU:HD21	1:D:311:GLN:HG2	1.92	0.52
1:C:325:GLU:HG3	1:C:328:ARG:HH11	1.74	0.52
1:D:141:ILE:HG23	1:D:142:MET:HG3	1.91	0.52
1:A:300:MET:HG3	1:A:304:SER:HB3	1.91	0.52
1:B:370:ALA:HB1	1:B:374:MET:SD	2.50	0.52
1:B:243:ARG:O	1:B:247:GLN:HG3	2.10	0.52
1:B:309:ALA:O	1:B:313:MET:HG2	2.10	0.52
1:B:379:TRP:HB2	1:B:386:LEU:HD12	1.91	0.52
1:C:32:TYR:CE1	1:C:369:PRO:HG3	2.45	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:88:LEU:HB3	1:B:90:LEU:HD11	1.91	0.51
1:A:25:LEU:O	1:A:27:PRO:HD3	2.11	0.51
1:B:350:ASP:N	1:B:350:ASP:OD1	2.43	0.51
1:B:258:TYR:CD2	1:B:424:ILE:HD11	2.46	0.51
1:D:139:HIS:HB3	1:D:141:ILE:HG22	1.92	0.51
1:B:40:ILE:HG23	1:B:360:ALA:HB2	1.94	0.50
1:B:7:SER:HB3	1:B:78:ILE:HB	1.92	0.50
1:A:63:LEU:HD23	1:A:142:MET:HE1	1.93	0.50
1:A:265:ASP:HB3	1:A:293:ARG:CZ	2.40	0.50
1:A:246:ALA:HA	1:A:346:VAL:HG21	1.93	0.50
1:C:61:ASP:N	1:C:61:ASP:OD1	2.36	0.50
1:B:161:ALA:HA	1:B:166:THR:OG1	2.12	0.50
1:D:367:ASN:ND2	1:D:368:GLY:O	2.45	0.50
1:C:293:ARG:NH1	2:C:501:HOH:O	2.45	0.49
1:D:375:LEU:HD13	1:D:390:PHE:HE1	1.77	0.49
1:B:44:ILE:HG23	1:B:159:TYR:CE1	2.47	0.49
1:D:220:LEU:HD13	1:D:221:GLN:N	2.28	0.49
1:D:297:ARG:HG2	1:D:300:MET:HG3	1.95	0.49
1:C:351:LEU:HD12	1:C:352:ASP:H	1.78	0.49
1:A:126:LYS:HG2	1:A:132:TRP:CZ2	2.47	0.49
1:A:232:ILE:HG22	1:A:234:ALA:H	1.77	0.49
1:B:90:LEU:HB3	1:B:93:GLN:HG3	1.95	0.49
1:D:57:ILE:HG23	1:D:63:LEU:HB2	1.95	0.49
1:A:49:PHE:HZ	1:A:134:TRP:CD2	2.31	0.48
1:A:408:ARG:HG3	1:A:430:LEU:HB2	1.94	0.48
1:D:374:MET:HB2	1:D:391:ASP:HB3	1.94	0.48
1:D:401:GLY:HA2	1:D:404:ALA:HB3	1.95	0.48
1:A:206:TRP:CZ2	1:A:293:ARG:HB2	2.48	0.48
1:D:223:ARG:NH2	1:D:391:ASP:O	2.47	0.48
1:A:37:TYR:HD2	1:A:365:LEU:HG	1.78	0.48
1:B:374:MET:HB2	1:B:391:ASP:HB3	1.95	0.48
1:B:57:ILE:HA	1:B:63:LEU:HD12	1.95	0.47
1:A:91:THR:CG2	1:A:126:LYS:HD2	2.44	0.47
1:B:250:THR:HG23	1:B:268:LEU:HD12	1.96	0.47
1:A:105:ARG:HA	1:A:108:TYR:CZ	2.49	0.47
1:D:57:ILE:HG12	1:D:63:LEU:HD13	1.96	0.47
1:B:271:PRO:HG2	1:B:345:ASN:ND2	2.29	0.47
1:C:267:VAL:HA	1:C:292:LEU:O	2.14	0.47
1:B:301:ASN:OD1	1:B:304:SER:OG	2.26	0.47
1:C:44:ILE:HB	1:C:132:TRP:CD2	2.50	0.47
1:D:42:GLY:N	1:D:130:ALA:O	2.48	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:182:SER:CB	1:D:321:ARG:HH22	2.28	0.47
1:D:188:ILE:O	1:D:188:ILE:HG22	2.15	0.47
1:A:61:ASP:OD2	1:A:175:SER:OG	2.23	0.47
1:D:377:VAL:HG22	1:D:388:ILE:HD13	1.97	0.47
1:B:230:LEU:HB3	1:B:386:LEU:HD23	1.97	0.46
1:B:411:ARG:O	1:B:415:VAL:HG23	2.15	0.46
1:A:149:TYR:CE1	1:A:350:ASP:HB3	2.50	0.46
1:A:361:THR:HB	1:A:363:HIS:HE1	1.81	0.46
1:C:63:LEU:HD11	1:C:151:ILE:HD13	1.97	0.46
1:A:411:ARG:HB3	1:A:430:LEU:HD21	1.96	0.46
1:C:372:ASP:HA	1:C:393:ASN:HB2	1.98	0.46
1:A:329:ARG:NH1	1:A:333:MET:SD	2.89	0.46
1:C:246:ALA:HA	1:C:346:VAL:HG21	1.98	0.45
1:A:107:ASP:HA	1:A:110:GLN:HE21	1.81	0.45
1:C:213:ALA:HB1	1:C:396:CYS:HB3	1.98	0.45
1:D:196:GLU:HG2	1:D:200:LEU:HD12	1.98	0.45
1:A:31:VAL:O	1:A:368:GLY:HA3	2.17	0.45
1:C:317:LEU:O	1:C:320:GLN:HG2	2.16	0.45
1:C:105:ARG:HA	1:C:108:TYR:CZ	2.51	0.45
1:D:232:ILE:HG22	1:D:235:LEU:H	1.81	0.45
1:A:104:MET:HE3	1:A:125:LEU:HD11	1.97	0.45
1:B:243:ARG:HE	1:B:243:ARG:HB2	1.63	0.45
1:C:375:LEU:HD13	1:C:390:PHE:HE1	1.82	0.45
1:D:158:VAL:HG12	1:D:168:PRO:HB3	1.99	0.45
1:B:326:ALA:HA	1:B:329:ARG:HG2	1.98	0.45
1:C:158:VAL:HG13	1:C:168:PRO:HG3	1.97	0.45
1:A:189:SER:HB3	1:A:192:ARG:H	1.82	0.44
1:B:225:ARG:HA	1:B:390:PHE:O	2.16	0.44
1:D:346:VAL:HG22	1:D:377:VAL:HB	1.99	0.44
1:D:49:PHE:HZ	1:D:134:TRP:CD2	2.35	0.44
1:B:21:LEU:HA	1:B:24:GLN:HG3	2.00	0.44
1:B:149:TYR:CE1	1:B:350:ASP:HB3	2.52	0.44
1:B:228:THR:OG1	1:B:406:GLN:OE1	2.35	0.44
1:B:258:TYR:HB2	1:B:296:MET:HG3	1.99	0.44
1:C:203:CYS:HA	1:C:206:TRP:CD1	2.53	0.44
1:D:35:ALA:HB3	1:D:365:LEU:HB2	1.99	0.44
1:B:112:VAL:HG21	1:B:137:ARG:HH12	1.82	0.44
1:B:279:ASP:OD1	1:B:279:ASP:N	2.51	0.44
1:B:224:LEU:HD21	1:B:399:PRO:HG3	1.99	0.44
1:C:160:SER:OG	1:C:356:GLY:N	2.40	0.44
1:C:353:LEU:HD11	1:C:362:ASN:HD21	1.83	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:105:ARG:HA	1:D:108:TYR:CZ	2.52	0.44
1:C:19:ILE:HD13	1:C:140:VAL:HG23	2.00	0.44
1:D:279:ASP:OD1	1:D:280:ARG:N	2.51	0.44
1:D:114:LEU:HD21	1:D:139:HIS:CE1	2.53	0.43
1:B:182:SER:HB3	1:B:321:ARG:HH22	1.83	0.43
1:B:351:LEU:HD23	1:B:351:LEU:HA	1.63	0.43
1:A:222:GLN:O	1:A:394:PRO:HG3	2.18	0.43
1:B:126:LYS:HE3	1:B:126:LYS:HB2	1.83	0.43
1:B:56:VAL:HA	1:B:59:GLU:HB2	2.00	0.43
1:D:101:GLN:HA	1:D:104:MET:HE2	2.00	0.43
1:D:253:MET:O	1:D:257:LEU:HD23	2.19	0.43
1:C:75:ARG:NH2	2:C:514:HOH:O	2.39	0.42
1:B:344:VAL:HA	1:B:375:LEU:HB3	2.00	0.42
1:B:354:SER:HA	1:B:358:TYR:O	2.19	0.42
1:C:263:GLU:OE2	1:C:265:ASP:N	2.48	0.42
1:D:34:ILE:HD11	1:D:143:MET:HG2	2.02	0.42
1:D:230:LEU:HB3	1:D:386:LEU:HD23	2.02	0.42
1:B:412:PHE:CD1	1:B:429:LEU:HD11	2.55	0.42
1:A:240:PRO:HB2	1:A:241:ASP:H	1.64	0.42
1:C:40:ILE:HD13	1:C:44:ILE:HD11	2.01	0.42
1:C:126:LYS:HE2	1:C:132:TRP:CZ2	2.55	0.42
1:D:300:MET:O	1:D:424:ILE:HG12	2.20	0.42
1:C:337:GLN:N	2:C:523:HOH:O	2.51	0.42
1:C:347:MET:O	1:C:378:TYR:HA	2.20	0.42
1:B:130:ALA:N	2:B:510:HOH:O	2.46	0.42
1:C:36:GLN:HG2	1:C:37:TYR:N	2.34	0.42
1:C:149:TYR:CZ	1:C:350:ASP:HB3	2.55	0.41
1:D:53:LEU:O	1:D:57:ILE:HG13	2.20	0.41
1:B:339:LEU:HD12	1:B:340:PHE:CD2	2.55	0.41
1:D:25:LEU:HD23	1:D:25:LEU:HA	1.92	0.41
1:A:328:ARG:NE	1:A:339:LEU:HG	2.35	0.41
1:A:300:MET:O	1:A:424:ILE:HG12	2.21	0.41
1:C:95:ASP:HB3	1:C:98:ALA:HB3	2.02	0.41
1:C:416:LEU:HD23	1:C:416:LEU:HA	1.90	0.41
1:D:300:MET:O	1:D:424:ILE:N	2.35	0.41
1:A:126:LYS:HG2	1:A:132:TRP:CE2	2.56	0.41
1:D:96:PRO:HB2	1:D:127:VAL:CG1	2.50	0.41
1:C:349:PHE:HZ	1:C:387:ARG:HD3	1.85	0.41
1:C:42:GLY:N	1:C:130:ALA:O	2.53	0.41
1:C:187:GLN:HA	1:C:192:ARG:HD2	2.03	0.41
1:D:248:PHE:HE2	1:D:413:MET:HE3	1.85	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:197:ALA:O	1:A:201:LYS:HG2	2.21	0.41
1:B:28:ASP:HA	1:B:111:PRO:HG2	2.02	0.41
1:D:230:LEU:HD21	1:D:232:ILE:HG13	2.03	0.41
1:C:36:GLN:NE2	1:C:362:ASN:OD1	2.54	0.40
1:D:221:GLN:NE2	1:D:394:PRO:HD2	2.36	0.40
1:D:378:TYR:HB2	1:D:387:ARG:HB3	2.03	0.40
1:A:151:ILE:O	1:A:155:VAL:HG23	2.22	0.40
1:A:347:MET:O	1:A:378:TYR:HA	2.22	0.40
1:C:126:LYS:HG3	1:C:132:TRP:CD2	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:D:116:GLN:OE1	2:A:508:HOH:O[1_654]	2.17	0.03

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	402/434 (93%)	383 (95%)	18 (4%)	1 (0%)	47	71
1	B	389/434 (90%)	371 (95%)	17 (4%)	1 (0%)	41	64
1	C	398/434 (92%)	386 (97%)	10 (2%)	2 (0%)	29	52
1	D	385/434 (89%)	372 (97%)	12 (3%)	1 (0%)	41	64
All	All	1574/1736 (91%)	1512 (96%)	57 (4%)	5 (0%)	41	64

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	25	LEU

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Mol	Chain	Res	Type
1	B	129	PRO
1	C	429	LEU
1	A	204	ALA
1	C	233	GLN

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	335/353 (95%)	326 (97%)	9 (3%)	44	71
1	B	326/353 (92%)	315 (97%)	11 (3%)	37	63
1	C	334/353 (95%)	324 (97%)	10 (3%)	41	67
1	D	323/353 (92%)	317 (98%)	6 (2%)	57	79
All	All	1318/1412 (93%)	1282 (97%)	36 (3%)	44	71

All (36) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	32	TYR
1	A	177	LEU
1	A	230	LEU
1	A	243	ARG
1	A	308	GLN
1	A	320	GLN
1	A	328	ARG
1	A	391	ASP
1	A	407	ARG
1	B	7	SER
1	B	28	ASP
1	B	70	SER
1	B	108	TYR
1	B	113	ASN
1	B	237	ASP
1	B	280	ARG
1	B	340	PHE

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Mol	Chain	Res	Type
1	B	352	ASP
1	B	359	SER
1	B	426	SER
1	C	54	ARG
1	C	170	GLU
1	C	226	GLN
1	C	293	ARG
1	C	297	ARG
1	C	314	GLN
1	C	318	ARG
1	C	340	PHE
1	C	354	SER
1	C	411	ARG
1	D	61	ASP
1	D	222	GLN
1	D	226	GLN
1	D	264	GLN
1	D	265	ASP
1	D	351	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	320	GLN
1	B	385	GLN
1	D	281	HIS

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

There are no ligands in this entry.

5.7 Other polymers

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^{th} 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	A	410/434 (94%)	-0.38	0 100 100	20, 36, 69, 90	0
1	B	399/434 (91%)	-0.18	7 (1%) 68 64	25, 50, 77, 102	0
1	C	408/434 (94%)	-0.34	1 (0%) 95 95	17, 36, 67, 89	0
1	D	395/434 (91%)	-0.20	3 (0%) 86 84	26, 50, 78, 95	0
All	All	1612/1736 (92%)	-0.27	11 (0%) 87 86	17, 44, 75, 102	0

All (11) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	231	ALA	5.7
1	B	116	GLN	4.4
1	B	117	GLY	3.2
1	B	66	GLN	2.5
1	B	365	LEU	2.5
1	B	378	TYR	2.3
1	D	362	ASN	2.2
1	C	430	LEU	2.1
1	B	110	GLN	2.1
1	B	382	GLY	2.0
1	D	26	TYR	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 monosaccharides 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.