



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 05:05 PM UTC

PDB ID : 6JUY / pdb_00006juy
Title : Crystal Structure of ArgZ, apo structure, an Arginine Dihydrolase from the Ornithine-Ammonia Cycle in Cyanobacteria
Authors : Zhuang, N.; Li, L.; Wu, X.; Zhang, Y.
Deposited on : 2019-04-15
Resolution : 2.97 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

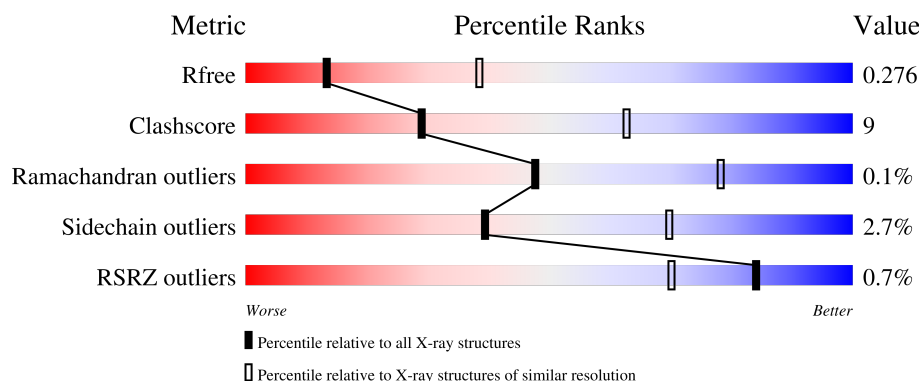
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.97 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	3580 (3.00-2.96)
Clashscore	190562	3904 (3.00-2.96)
Ramachandran outliers	187476	3761 (3.00-2.96)
Sidechain outliers	187428	3764 (3.00-2.96)
RSRZ outliers	180081	3579 (3.00-2.96)

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	A	707	% 73% 17% • 10%
1	B	707	72% 17% • 10%
1	C	707	72% 20% • 7%
1	D	707	% 70% 18% • 12%

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 18519 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 Sll1336 protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	639	Total	C	N	O	S	0	0	0
			4736	3005	812	889	30			
1	B	637	Total	C	N	O	S	0	0	0
			4722	2991	817	885	29			
1	C	656	Total	C	N	O	S	0	0	0
			4723	3000	803	893	27			
1	D	623	Total	C	N	O	S	0	0	0
			4333	2745	737	823	28			

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-1	GLY	-	expression tag	UNP P74535
A	0	ALA	-	expression tag	UNP P74535
B	-1	GLY	-	expression tag	UNP P74535
B	0	ALA	-	expression tag	UNP P74535
C	-1	GLY	-	expression tag	UNP P74535
C	0	ALA	-	expression tag	UNP P74535
D	-1	GLY	-	expression tag	UNP P74535
D	0	ALA	-	expression tag	UNP P74535

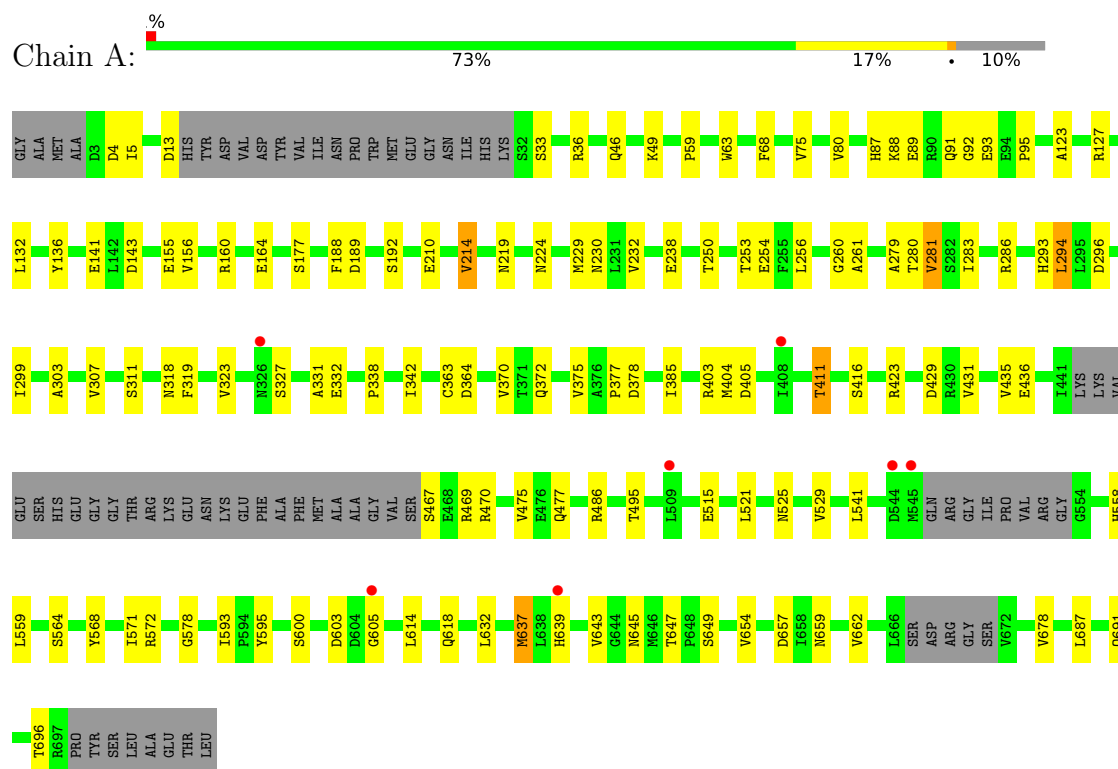
- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	5	Total	O	0	0
			5	5		

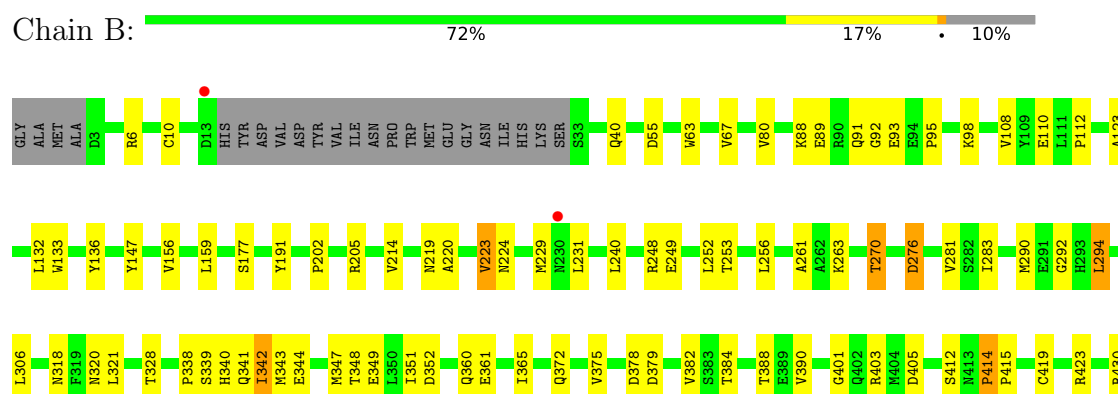
3 Residue-property plots

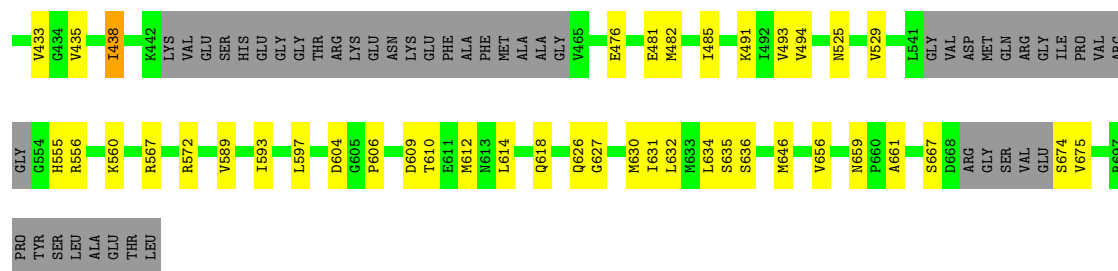
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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: Sll1336 protein



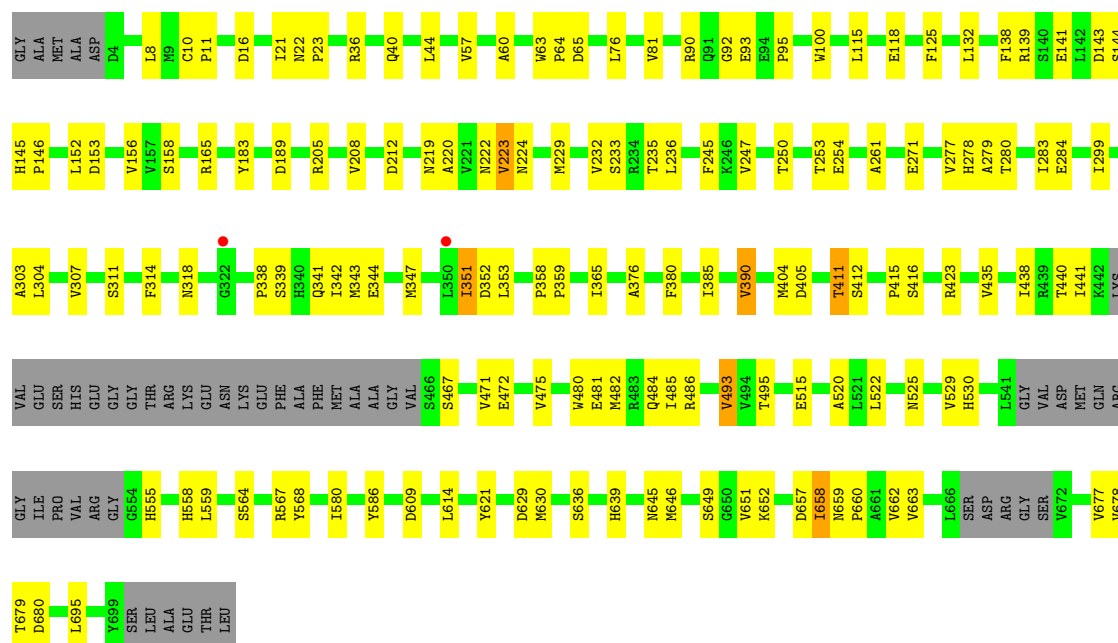
• Molecule 1: Sll1336 protein





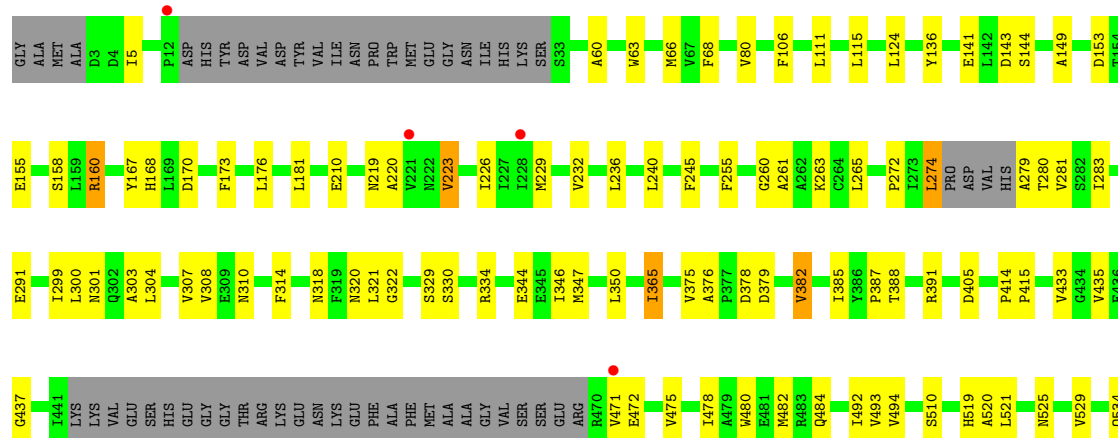
• Molecule 1: Sll1336 protein

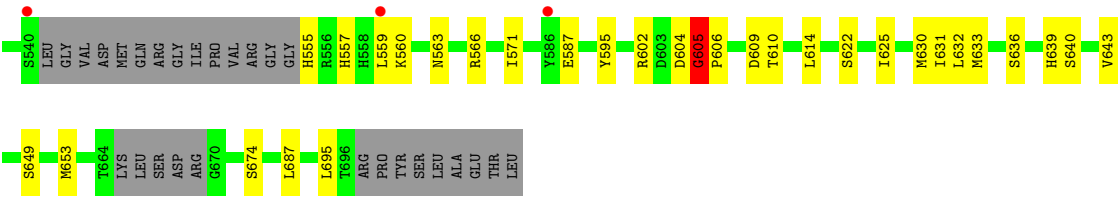
Chain C: 72% 20% 7%



• Molecule 1: Sll1336 protein

Chain D: 70% 18% 12%





4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	189.87Å 105.44Å 165.91Å 90.00° 113.18° 90.00°	Depositor
Resolution (Å)	41.06 – 2.97 41.06 – 2.97	Depositor EDS
% Data completeness (in resolution range)	97.1 (41.06-2.97) 97.1 (41.06-2.97)	Depositor EDS
R_{merge}	0.04	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.96 (at 2.96Å)	Xtriage
Refinement program	PHENIX 1.17_3644	Depositor
R, R_{free}	0.234 , 0.275 0.237 , 0.276	Depositor DCC
R_{free} test set	1990 reflections (3.19%)	wwPDB-VP
Wilson B-factor (Å ²)	109.2	Xtriage
Anisotropy	0.456	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 74.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.000 for 1/2*h-3/2*k,-1/2*h-1/2*k,-1/2*h +1/2*k-l 0.003 for 1/2*h+3/2*k,1/2*h-1/2*k,-1/2*h- 1/2*k-l	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	18519	wwPDB-VP
Average B, all atoms (Å ²)	109.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.46% 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 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	0.17	0/4825	0.45	0/6572
1	B	0.18	0/4814	0.48	4/6565 (0.1%)
1	C	0.24	1/4821 (0.0%)	0.50	3/6597 (0.0%)
1	D	0.19	0/4412	0.48	0/6041
All	All	0.19	1/18872 (0.0%)	0.48	7/25775 (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	1
1	B	0	2
1	C	0	2
1	D	0	1
All	All	0	6

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	341	GLN	CD-OE1	-6.26	1.11	1.23

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	659	ASN	CA-C-N	7.08	144.00	127.00
1	C	659	ASN	C-N-CA	7.08	144.00	127.00
1	C	659	ASN	C-N-CD	-6.81	105.61	120.60
1	B	414	PRO	CA-C-N	5.59	140.41	127.00
1	B	414	PRO	C-N-CA	5.59	140.41	127.00
1	B	414	PRO	C-N-CD	-5.40	108.73	120.60
1	B	626	GLN	N-CA-C	5.33	116.78	110.97

There are no chirality outliers.

All (6) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	605	GLY	Peptide
1	B	223	VAL	Peptide
1	B	634	LEU	Peptide
1	C	223	VAL	Peptide
1	C	277	VAL	Peptide
1	D	605	GLY	Peptide

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	4736	0	4513	71	2
1	B	4722	0	4477	82	1
1	C	4723	0	4314	93	1
1	D	4333	0	3874	85	0
2	A	5	0	0	0	0
All	All	18519	0	17178	311	2

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 9.

All (311) 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:659:ASN:HB3	1:A:662:VAL:HB	1.55	0.88
1:D:493:VAL:HG12	1:D:520:ALA:HB3	1.55	0.88
1:C:76:LEU:HB3	1:C:152:LEU:HD12	1.59	0.82
1:C:229:MET:HE2	1:C:232:VAL:HG12	1.61	0.82
1:B:338:PRO:HD2	1:B:342:ILE:HD11	1.63	0.80
1:B:340:HIS:O	1:B:341:GLN:NE2	2.13	0.79
1:A:155:GLU:HG3	1:A:280:THR:HB	1.66	0.78
1:A:294:LEU:HA	1:A:299:ILE:HG22	1.65	0.77
1:B:347:MET:HB3	1:B:435:VAL:HG11	1.64	0.77
1:D:636:SER:HB2	1:D:639:HIS:HB3	1.67	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:510:SER:HB2	1:D:587:GLU:HG3	1.67	0.76
1:C:153:ASP:HA	1:C:279:ALA:HB2	1.67	0.74
1:C:8:LEU:HD21	1:C:57:VAL:HG23	1.70	0.73
1:B:281:VAL:HG12	1:B:283:ILE:H	1.53	0.73
1:A:691:GLN:NE2	1:D:210:GLU:OE2	2.21	0.73
1:B:214:VAL:HG11	1:C:480:TRP:HE1	1.54	0.73
1:A:411:THR:OG1	1:A:416:SER:OG	2.05	0.73
1:C:219:ASN:HB3	1:C:261:ALA:HB3	1.72	0.72
1:A:219:ASN:HB3	1:A:261:ALA:HB3	1.72	0.72
1:B:339:SER:HB3	1:B:342:ILE:HG12	1.71	0.71
1:C:40:GLN:HE22	1:C:253:THR:HG22	1.56	0.70
1:C:423:ARG:HA	1:D:566:ARG:HH22	1.57	0.70
1:C:493:VAL:HG13	1:C:520:ALA:HB3	1.73	0.69
1:C:189:ASP:OD2	1:C:311:SER:OG	2.10	0.69
1:D:219:ASN:HB3	1:D:261:ALA:HB3	1.74	0.69
1:B:667:SER:HA	1:B:674:SER:HA	1.76	0.67
1:D:153:ASP:HA	1:D:279:ALA:HB2	1.77	0.66
1:B:343:MET:HE2	1:B:347:MET:HG2	1.75	0.66
1:A:403:ARG:NH2	1:A:404:MET:O	2.29	0.65
1:B:306:LEU:HD13	1:B:349:GLU:HG3	1.76	0.65
1:D:229:MET:HE2	1:D:232:VAL:HG11	1.78	0.65
1:A:68:PHE:CE1	1:A:260:GLY:HA3	2.31	0.65
1:C:365:ILE:HG12	1:C:390:VAL:HG13	1.79	0.65
1:C:385:ILE:HG23	1:C:649:SER:HB2	1.80	0.64
1:A:281:VAL:HG13	1:A:283:ILE:H	1.63	0.64
1:B:351:ILE:HD13	1:B:438:ILE:HG23	1.79	0.64
1:C:351:ILE:HD13	1:C:438:ILE:HB	1.79	0.64
1:D:493:VAL:HG23	1:D:631:ILE:HG23	1.80	0.64
1:A:89:GLU:N	1:A:89:GLU:OE1	2.30	0.64
1:C:380:PHE:O	1:D:560:LYS:NZ	2.24	0.64
1:A:296:ASP:O	1:D:301:ASN:ND2	2.30	0.63
1:C:232:VAL:HG11	1:C:247:VAL:HG11	1.79	0.62
1:D:310:ASN:HB3	1:D:346:ILE:HG12	1.80	0.62
1:D:365:ILE:HG22	1:D:437:GLY:HA3	1.81	0.62
1:D:115:LEU:HD21	1:D:144:SER:HA	1.81	0.62
1:D:636:SER:O	1:D:640:SER:N	2.19	0.62
1:A:318:ASN:ND2	1:A:332:GLU:OE1	2.33	0.62
1:A:229:MET:HE2	1:A:232:VAL:HG11	1.82	0.61
1:A:541:LEU:HA	1:A:558:HIS:HE1	1.63	0.61
1:C:411:THR:OG1	1:C:416:SER:OG	2.19	0.61
1:D:375:VAL:HG12	1:D:376:ALA:H	1.65	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:81:VAL:HG23	1:C:152:LEU:HD21	1.82	0.61
1:A:559:LEU:HD12	1:B:382:VAL:HG13	1.83	0.60
1:B:360:GLN:HG3	1:B:361:GLU:HG3	1.83	0.60
1:D:272:PRO:HB2	1:D:274:LEU:HD12	1.84	0.60
1:B:63:TRP:CZ2	1:B:92:GLY:HA3	2.38	0.58
1:B:253:THR:HA	1:B:256:LEU:HD12	1.83	0.58
1:A:132:LEU:HD23	1:A:156:VAL:HG22	1.85	0.58
1:B:344:GLU:O	1:B:348:THR:HG23	2.02	0.58
1:A:495:THR:HB	1:A:639:HIS:CE1	2.39	0.58
1:C:141:GLU:HG3	1:C:143:ASP:H	1.69	0.58
1:C:339:SER:HB3	1:C:342:ILE:HG13	1.85	0.58
1:C:467:SER:HA	1:C:678:VAL:HG12	1.86	0.57
1:A:286:ARG:NH1	1:A:436:GLU:OE2	2.38	0.57
1:C:567:ARG:HH22	1:D:378:ASP:CG	2.12	0.57
1:C:212:ASP:OD1	1:C:233:SER:OG	2.18	0.57
1:A:541:LEU:HA	1:A:558:HIS:CE1	2.38	0.57
1:D:320:ASN:O	1:D:329:SER:OG	2.11	0.57
1:C:16:ASP:H	1:C:64:PRO:HB2	1.69	0.57
1:C:404:MET:HE3	1:C:645:ASN:HA	1.86	0.57
1:A:4:ASP:OD1	1:A:5:ILE:N	2.34	0.57
1:B:494:VAL:HG22	1:B:632:LEU:HB2	1.87	0.57
1:A:323:VAL:N	1:A:327:SER:OG	2.39	0.56
1:B:379:ASP:HB3	1:B:433:VAL:HG13	1.86	0.56
1:A:63:TRP:CH2	1:A:92:GLY:HA3	2.40	0.56
1:B:177:SER:OG	1:B:224:ASN:O	2.14	0.56
1:C:283:ILE:HG13	1:C:338:PRO:HA	1.88	0.56
1:D:60:ALA:HB3	1:D:63:TRP:HD1	1.71	0.56
1:D:232:VAL:HB	1:D:236:LEU:HD23	1.88	0.56
1:D:471:VAL:HG12	1:D:472:GLU:HG3	1.87	0.56
1:C:658:ILE:HG23	1:C:679:THR:C	2.31	0.55
1:A:614:LEU:HD11	1:B:614:LEU:HD11	1.89	0.55
1:B:344:GLU:HG3	1:B:435:VAL:HG23	1.89	0.55
1:D:636:SER:CB	1:D:639:HIS:HB3	2.36	0.55
1:C:57:VAL:HG22	1:C:100:TRP:CD1	2.42	0.55
1:C:284:GLU:HG2	1:C:343:MET:HE3	1.88	0.55
1:C:481:GLU:O	1:C:485:ILE:HG12	2.07	0.55
1:D:124:LEU:HD21	1:D:263:LYS:HE2	1.89	0.55
1:D:482:MET:HG2	1:D:630:MET:HE1	1.89	0.55
1:A:486:ARG:NH2	1:A:515:GLU:O	2.39	0.54
1:B:98:LYS:HG3	1:B:108:VAL:HG11	1.88	0.54
1:B:659:ASN:C	1:B:661:ALA:H	2.15	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:255:PHE:HD2	1:D:265:LEU:HD11	1.71	0.54
1:A:657:ASP:O	1:A:678:VAL:HA	2.08	0.54
1:C:636:SER:HB3	1:C:639:HIS:ND1	2.23	0.54
1:D:220:ALA:O	1:D:263:LYS:HD2	2.08	0.54
1:B:318:ASN:ND2	1:B:320:ASN:OD1	2.39	0.54
1:B:132:LEU:HD23	1:B:156:VAL:HG22	1.90	0.53
1:D:158:SER:OG	1:D:283:ILE:HD11	2.09	0.53
1:B:604:ASP:O	1:B:606:PRO:HA	2.09	0.53
1:A:475:VAL:HG11	1:A:687:LEU:HB3	1.91	0.52
1:B:10:CYS:HB3	1:B:67:VAL:HA	1.91	0.52
1:C:614:LEU:HD11	1:D:614:LEU:HD11	1.90	0.52
1:C:660:PRO:HB3	1:C:678:VAL:CG1	2.38	0.52
1:C:677:VAL:HG12	1:C:679:THR:HG22	1.90	0.52
1:A:469:ARG:HG3	1:A:470:ARG:H	1.75	0.52
1:A:377:PRO:HD2	1:A:431:VAL:HG21	1.91	0.52
1:B:388:THR:HG21	1:B:438:ILE:HD11	1.90	0.52
1:C:358:PRO:HG2	1:C:359:PRO:HD3	1.92	0.52
1:C:405:ASP:C	1:D:559:LEU:HD11	2.34	0.52
1:A:632:LEU:HD23	1:A:654:VAL:HB	1.90	0.52
1:C:22:ASN:HB2	1:C:23:PRO:HD2	1.92	0.52
1:A:423:ARG:NH2	1:A:618:GLN:OE1	2.43	0.51
1:D:236:LEU:O	1:D:240:LEU:HG	2.11	0.51
1:C:138:PHE:HB3	1:C:139:ARG:HH21	1.76	0.51
1:C:486:ARG:NH1	1:C:515:GLU:O	2.42	0.51
1:C:660:PRO:HB3	1:C:678:VAL:HG13	1.91	0.51
1:C:482:MET:HG2	1:C:630:MET:HE1	1.91	0.51
1:D:255:PHE:CD2	1:D:265:LEU:HD11	2.45	0.51
1:A:404:MET:HE3	1:A:645:ASN:HA	1.92	0.51
1:C:158:SER:OG	1:C:283:ILE:HD11	2.11	0.51
1:A:33:SER:HB3	1:A:254:GLU:OE1	2.10	0.51
1:A:338:PRO:HD2	1:A:342:ILE:HG21	1.92	0.51
1:C:344:GLU:HG3	1:C:435:VAL:HG23	1.93	0.51
1:C:347:MET:HB3	1:C:435:VAL:HG11	1.93	0.50
1:B:219:ASN:HB3	1:B:261:ALA:HB3	1.94	0.50
1:B:556:ARG:HE	1:B:560:LYS:HE3	1.77	0.50
1:D:111:LEU:HD22	1:D:115:LEU:HD23	1.93	0.50
1:D:136:TYR:CZ	1:D:160:ARG:HB2	2.46	0.50
1:A:637:MET:HE3	1:A:662:VAL:HA	1.93	0.50
1:A:564:SER:O	1:A:568:TYR:HD1	1.94	0.50
1:D:344:GLU:HG3	1:D:435:VAL:HG23	1.94	0.50
1:B:220:ALA:O	1:B:263:LYS:HD2	2.12	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:292:GLY:H	1:B:328:THR:HB	1.77	0.50
1:C:405:ASP:OD1	1:D:555:HIS:HA	2.12	0.50
1:D:602:ARG:O	1:D:602:ARG:HG2	2.11	0.49
1:B:229:MET:HE1	1:B:240:LEU:HD13	1.93	0.49
1:B:414:PRO:HD2	1:B:415:PRO:HA	1.93	0.49
1:C:220:ALA:HB2	1:C:229:MET:HB3	1.94	0.49
1:D:347:MET:HB3	1:D:435:VAL:HG11	1.95	0.49
1:D:300:LEU:O	1:D:304:LEU:HG	2.12	0.49
1:D:314:PHE:HA	1:D:334:ARG:O	2.13	0.49
1:B:340:HIS:ND1	1:B:341:GLN:HG2	2.28	0.49
1:C:657:ASP:OD1	1:C:658:ILE:N	2.46	0.49
1:B:223:VAL:HG12	1:B:224:ASN:H	1.78	0.48
1:D:606:PRO:HB2	1:D:610:THR:OG1	2.12	0.48
1:B:525:ASN:O	1:B:529:VAL:HG13	2.13	0.48
1:C:411:THR:O	1:C:415:PRO:HA	2.12	0.48
1:B:347:MET:CB	1:B:435:VAL:HG11	2.37	0.48
1:C:132:LEU:HD23	1:C:156:VAL:HG22	1.95	0.48
1:A:63:TRP:HB3	1:A:93:GLU:HG2	1.95	0.48
1:A:363:CYS:SG	1:A:364:ASP:N	2.86	0.48
1:A:370:VAL:HG23	1:A:429:ASP:O	2.14	0.48
1:C:559:LEU:HD12	1:D:382:VAL:CG1	2.43	0.48
1:D:604:ASP:O	1:D:605:GLY:C	2.57	0.48
1:C:555:HIS:ND1	1:D:405:ASP:OD1	2.45	0.48
1:A:525:ASN:O	1:A:529:VAL:HG13	2.13	0.48
1:C:63:TRP:CH2	1:C:92:GLY:HA3	2.48	0.48
1:C:21:ILE:O	1:C:139:ARG:NH1	2.47	0.48
1:D:387:PRO:HD3	1:D:649:SER:OG	2.14	0.48
1:D:521:LEU:O	1:D:595:TYR:HA	2.14	0.48
1:A:385:ILE:HG13	1:A:649:SER:HB3	1.96	0.48
1:B:476:GLU:CD	1:C:165:ARG:HH12	2.22	0.48
1:D:346:ILE:O	1:D:350:LEU:HB2	2.13	0.48
1:A:495:THR:HG21	1:A:643:VAL:HG11	1.95	0.47
1:C:481:GLU:OE2	1:C:652:LYS:HE3	2.14	0.47
1:D:155:GLU:HA	1:D:280:THR:O	2.13	0.47
1:C:679:THR:OG1	1:C:680:ASP:N	2.47	0.47
1:A:210:GLU:O	1:A:214:VAL:HG13	2.13	0.47
1:A:378:ASP:OD1	1:B:567:ARG:NH1	2.47	0.47
1:C:36:ARG:HB3	1:C:254:GLU:HG3	1.95	0.47
1:C:92:GLY:O	1:C:95:PRO:HD2	2.14	0.47
1:A:13:ASP:CG	1:A:59:PRO:HG2	2.40	0.47
1:B:89:GLU:OE1	1:B:89:GLU:N	2.48	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:559:LEU:HD12	1:D:382:VAL:HG13	1.97	0.47
1:D:304:LEU:HD13	1:D:314:PHE:CE1	2.49	0.47
1:D:494:VAL:HG22	1:D:632:LEU:HB2	1.96	0.47
1:C:303:ALA:O	1:C:307:VAL:HG23	2.15	0.47
1:D:223:VAL:HG12	1:D:226:ILE:H	1.79	0.47
1:B:112:PRO:HG2	1:B:147:TYR:HE2	1.80	0.47
1:C:223:VAL:HG12	1:C:224:ASN:H	1.79	0.47
1:D:653:MET:N	1:D:674:SER:OG	2.41	0.47
1:B:423:ARG:NH2	1:B:618:GLN:OE1	2.39	0.46
1:B:491:LYS:HD2	1:B:627:GLY:C	2.41	0.46
1:D:149:ALA:O	1:D:153:ASP:N	2.48	0.46
1:D:379:ASP:HB3	1:D:433:VAL:HG13	1.95	0.46
1:B:412:SER:HB2	1:B:430:ARG:HH11	1.80	0.46
1:D:281:VAL:HG12	1:D:283:ILE:H	1.79	0.46
1:A:123:ALA:HB1	1:A:132:LEU:HD11	1.98	0.46
1:B:292:GLY:N	1:B:328:THR:HB	2.30	0.46
1:B:493:VAL:O	1:B:631:ILE:HA	2.16	0.46
1:C:564:SER:O	1:C:568:TYR:HD1	1.99	0.46
1:B:123:ALA:HB1	1:B:132:LEU:HD11	1.97	0.46
1:A:521:LEU:O	1:A:595:TYR:HA	2.15	0.46
1:B:88:LYS:HA	1:B:91:GLN:CD	2.41	0.46
1:C:376:ALA:N	1:D:563:ASN:OD1	2.44	0.46
1:D:375:VAL:HG12	1:D:376:ALA:N	2.30	0.46
1:B:283:ILE:HG12	1:B:338:PRO:HA	1.98	0.46
1:C:621:TYR:HB3	1:C:646:MET:SD	2.56	0.46
1:A:188:PHE:HB3	1:A:192:SER:HB2	1.98	0.46
1:B:481:GLU:O	1:B:485:ILE:HG13	2.16	0.46
1:A:495:THR:HB	1:A:639:HIS:HE1	1.80	0.45
1:B:63:TRP:HB3	1:B:93:GLU:HG2	1.97	0.45
1:B:98:LYS:NZ	1:B:110:GLU:OE2	2.40	0.45
1:C:118:GLU:HG3	1:C:139:ARG:HB3	1.98	0.45
1:C:663:VAL:HG21	1:C:678:VAL:HG22	1.98	0.45
1:D:571:ILE:HG12	1:D:609:ASP:OD2	2.16	0.45
1:B:401:GLY:O	1:B:419:CYS:HB2	2.15	0.45
1:A:469:ARG:CG	1:A:470:ARG:H	2.28	0.45
1:C:352:ASP:O	1:C:353:LEU:HD13	2.16	0.45
1:D:170:ASP:O	1:D:219:ASN:ND2	2.39	0.45
1:A:75:VAL:HG13	1:A:80:VAL:HG22	1.99	0.45
1:A:303:ALA:O	1:A:307:VAL:HG23	2.15	0.45
1:C:525:ASN:O	1:C:529:VAL:HG13	2.16	0.45
1:A:559:LEU:HD11	1:B:405:ASP:C	2.42	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:467:SER:HA	1:C:678:VAL:CG1	2.46	0.45
1:D:622:SER:O	1:D:625:ILE:HG22	2.17	0.45
1:A:253:THR:HA	1:A:256:LEU:HB2	1.98	0.45
1:B:191:TYR:OH	1:B:339:SER:HB2	2.16	0.45
1:C:376:ALA:O	1:D:563:ASN:ND2	2.27	0.45
1:D:303:ALA:O	1:D:307:VAL:HG23	2.17	0.45
1:D:321:LEU:HD23	1:D:322:GLY:O	2.16	0.45
1:D:525:ASN:O	1:D:529:VAL:HG13	2.16	0.45
1:B:6:ARG:HG2	1:B:270:THR:HG23	1.99	0.45
1:B:482:MET:HG2	1:B:630:MET:SD	2.57	0.44
1:D:68:PHE:CE1	1:D:260:GLY:HA3	2.52	0.44
1:D:141:GLU:HG3	1:D:143:ASP:H	1.82	0.44
1:D:304:LEU:HD22	1:D:314:PHE:CD1	2.52	0.44
1:A:230:ASN:HA	1:A:250:THR:O	2.17	0.44
1:B:6:ARG:NH2	1:B:55:ASP:OD2	2.50	0.44
1:A:127:ARG:HA	1:A:127:ARG:NE	2.32	0.44
1:A:46:GLN:O	1:A:49:LYS:HB3	2.18	0.44
1:B:609:ASP:OD1	1:B:609:ASP:N	2.51	0.44
1:C:183:TYR:HE1	1:C:205:ARG:HB3	1.83	0.44
1:C:471:VAL:HG12	1:C:475:VAL:HG23	2.00	0.44
1:D:63:TRP:HB2	1:D:66:MET:HE3	2.00	0.44
1:A:75:VAL:HG22	1:A:80:VAL:HG22	2.00	0.44
1:B:191:TYR:CZ	1:B:339:SER:HB2	2.53	0.44
1:B:306:LEU:HD22	1:B:349:GLU:HG2	1.99	0.44
1:B:606:PRO:HG3	1:B:612:MET:SD	2.58	0.44
1:C:580:ILE:HG22	1:C:586:TYR:HB2	2.00	0.44
1:A:141:GLU:HG3	1:A:143:ASP:H	1.83	0.43
1:B:133:TRP:CE3	1:B:159:LEU:HD11	2.53	0.43
1:C:125:PHE:CE1	1:C:132:LEU:HB2	2.53	0.43
1:C:44:LEU:HD23	1:C:250:THR:HG21	2.00	0.43
1:D:480:TRP:O	1:D:484:GLN:HG2	2.18	0.43
1:A:189:ASP:OD2	1:A:311:SER:OG	2.30	0.43
1:A:372:GLN:HB3	1:A:375:VAL:HB	2.00	0.43
1:C:657:ASP:O	1:C:678:VAL:HA	2.19	0.43
1:D:475:VAL:HG11	1:D:687:LEU:HB3	1.99	0.43
1:D:492:ILE:O	1:D:519:HIS:N	2.41	0.43
1:A:88:LYS:HA	1:A:91:GLN:CD	2.44	0.43
1:A:319:PHE:HD1	1:A:331:ALA:HB2	1.83	0.43
1:B:597:LEU:HB2	1:B:610:THR:HA	1.99	0.43
1:A:467:SER:HA	1:A:678:VAL:HG22	2.00	0.43
1:D:80:VAL:HG12	1:D:106:PHE:HB3	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:291:GLU:HA	1:D:330:SER:OG	2.19	0.43
1:B:92:GLY:O	1:B:95:PRO:HD2	2.19	0.43
1:B:341:GLN:HB3	1:B:344:GLU:HB2	2.01	0.43
1:B:403:ARG:NH2	1:B:646:MET:HG2	2.34	0.43
1:B:635:SER:HB2	1:B:656:VAL:O	2.19	0.42
1:C:65:ASP:O	1:C:90:ARG:NH2	2.52	0.42
1:D:633:MET:HE1	1:D:643:VAL:HB	2.00	0.42
1:A:405:ASP:OD1	1:B:555:HIS:ND1	2.53	0.42
1:B:136:TYR:OH	1:B:338:PRO:HG3	2.19	0.42
1:C:609:ASP:OD1	1:C:609:ASP:N	2.52	0.42
1:D:385:ILE:C	1:D:649:SER:HB3	2.44	0.42
1:D:414:PRO:HA	1:D:415:PRO:HD3	1.84	0.42
1:B:276:ASP:OD1	1:B:276:ASP:N	2.53	0.42
1:C:629:ASP:C	1:C:651:VAL:HG13	2.44	0.42
1:D:304:LEU:O	1:D:308:VAL:HG22	2.19	0.42
1:A:600:SER:HB3	1:A:603:ASP:OD1	2.20	0.42
1:B:321:LEU:HD23	1:B:321:LEU:HA	1.88	0.42
1:B:365:ILE:HG21	1:B:390:VAL:HB	2.02	0.42
1:C:145:HIS:N	1:C:146:PRO:HD2	2.33	0.42
1:A:571:ILE:HG13	1:A:572:ARG:N	2.34	0.42
1:C:115:LEU:HD21	1:C:144:SER:HA	2.01	0.42
1:D:609:ASP:N	1:D:609:ASP:OD1	2.52	0.42
1:A:177:SER:OG	1:A:224:ASN:O	2.30	0.42
1:B:231:LEU:HA	1:B:249:GLU:OE2	2.20	0.42
1:C:10:CYS:HA	1:C:11:PRO:HD3	1.91	0.42
1:C:233:SER:HB2	1:C:236:LEU:H	1.85	0.42
1:A:136:TYR:CZ	1:A:160:ARG:HB2	2.55	0.42
1:B:202:PRO:HA	1:B:205:ARG:HG3	2.00	0.42
1:C:343:MET:HE2	1:C:343:MET:HB2	1.95	0.42
1:C:495:THR:HA	1:C:522:LEU:O	2.19	0.42
1:C:222:ASN:HD21	1:C:245:PHE:HE1	1.67	0.41
1:C:299:ILE:HD12	1:C:299:ILE:HA	1.86	0.41
1:B:40:GLN:HB3	1:B:252:LEU:HD23	2.01	0.41
1:B:80:VAL:HG13	1:B:108:VAL:HA	2.02	0.41
1:C:530:HIS:HE2	1:C:558:HIS:CE1	2.38	0.41
1:D:173:PHE:CZ	1:D:181:LEU:HD21	2.54	0.41
1:D:176:LEU:HB3	1:D:245:PHE:CZ	2.55	0.41
1:B:290:MET:O	1:B:294:LEU:HD11	2.21	0.41
1:B:372:GLN:HB3	1:B:375:VAL:HB	2.03	0.41
1:C:304:LEU:HD22	1:C:314:PHE:CG	2.55	0.41
1:A:87:HIS:HB3	1:A:89:GLU:OE1	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:572:ARG:HG3	1:B:589:VAL:HG13	2.02	0.41
1:C:365:ILE:HG12	1:C:390:VAL:CG1	2.47	0.41
1:C:471:VAL:HG21	1:C:679:THR:HB	2.02	0.41
1:B:435:VAL:HG12	1:B:435:VAL:O	2.21	0.41
1:C:60:ALA:HB3	1:C:63:TRP:HD1	1.86	0.41
1:C:358:PRO:CG	1:C:359:PRO:HD3	2.51	0.41
1:D:478:ILE:O	1:D:482:MET:HG3	2.21	0.41
1:D:365:ILE:HG23	1:D:391:ARG:O	2.21	0.40
1:A:36:ARG:NH2	1:A:253:THR:OG1	2.54	0.40
1:A:92:GLY:O	1:A:95:PRO:HD2	2.21	0.40
1:C:90:ARG:O	1:C:93:GLU:HG2	2.21	0.40
1:D:167:TYR:HE1	1:D:168:HIS:CE1	2.39	0.40
1:D:557:HIS:O	1:D:560:LYS:N	2.51	0.40
1:B:352:ASP:OD2	1:B:384:THR:HG21	2.22	0.40

All (2) 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:279:ALA:O	1:C:412:SER:OG[1_565]	2.08	0.12
1:A:238:GLU:OE2	1:B:248:ARG:NH2[3_455]	2.13	0.07

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	629/707 (89%)	594 (94%)	34 (5%)	1 (0%)	43 73
1	B	627/707 (89%)	600 (96%)	27 (4%)	0	100 100
1	C	648/707 (92%)	619 (96%)	28 (4%)	1 (0%)	43 73
1	D	611/707 (86%)	580 (95%)	30 (5%)	1 (0%)	43 73

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
All	All	2515/2828 (89%)	2393 (95%)	119 (5%)	3 (0%)	48 78

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	278	HIS
1	D	605	GLY
1	A	578	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	A	483/601 (80%)	471 (98%)	12 (2%)	42 71
1	B	478/601 (80%)	469 (98%)	9 (2%)	50 75
1	C	452/601 (75%)	436 (96%)	16 (4%)	32 63
1	D	398/601 (66%)	387 (97%)	11 (3%)	38 69
All	All	1811/2404 (75%)	1763 (97%)	48 (3%)	39 70

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

Mol	Chain	Res	Type
1	A	164	GLU
1	A	214	VAL
1	A	281	VAL
1	A	293	HIS
1	A	294	LEU
1	A	411	THR
1	A	435	VAL
1	A	477	GLN
1	A	593	ILE
1	A	637	MET
1	A	647	THR
1	A	696	THR

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Mol	Chain	Res	Type
1	B	270	THR
1	B	276	ASP
1	B	294	LEU
1	B	342	ILE
1	B	378	ASP
1	B	438	ILE
1	B	593	ILE
1	B	636	SER
1	B	675	VAL
1	C	208	VAL
1	C	235	THR
1	C	271	GLU
1	C	280	THR
1	C	318	ASN
1	C	351	ILE
1	C	390	VAL
1	C	411	THR
1	C	440	THR
1	C	441	ILE
1	C	472	GLU
1	C	484	GLN
1	C	493	VAL
1	C	658	ILE
1	C	662	VAL
1	C	695	LEU
1	D	5	ILE
1	D	160	ARG
1	D	223	VAL
1	D	274	LEU
1	D	299	ILE
1	D	318	ASN
1	D	365	ILE
1	D	382	VAL
1	D	388	THR
1	D	534	GLN
1	D	695	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (14) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	477	GLN
1	A	508	HIS

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Mol	Chain	Res	Type
1	A	591	ASN
1	B	278	HIS
1	B	508	HIS
1	B	591	ASN
1	C	14	HIS
1	C	22	ASN
1	C	301	ASN
1	C	488	GLN
1	C	508	HIS
1	C	591	ASN
1	D	222	ASN
1	D	502	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 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	A	639/707 (90%)	-0.02	7 (1%) 78 61	68, 97, 133, 156	0
1	B	637/707 (90%)	-0.09	2 (0%) 90 82	68, 96, 132, 185	0
1	C	656/707 (92%)	0.09	2 (0%) 90 82	74, 116, 146, 185	0
1	D	623/707 (88%)	0.26	7 (1%) 78 61	85, 125, 151, 176	0
All	All	2555/2828 (90%)	0.06	18 (0%) 84 70	68, 108, 144, 185	0

All (18) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	322	GLY	2.9
1	D	471	VAL	2.7
1	A	544	ASP	2.6
1	A	509	LEU	2.5
1	A	326	ASN	2.5
1	D	559	LEU	2.4
1	D	221	VAL	2.4
1	B	13	ASP	2.3
1	B	230	ASN	2.3
1	A	639	HIS	2.3
1	D	12	PRO	2.2
1	D	586	TYR	2.2
1	A	605	GLY	2.1
1	A	408	ILE	2.1
1	D	228	ILE	2.1
1	D	540	SER	2.1
1	C	350	LEU	2.1
1	A	545	MET	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.