



Full wwPDB X-ray Structure Validation Report ⓘ

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PDB ID : 3U1V / pdb_00003u1v
Title : X-ray Structure of De Novo design cysteine esterase FR29, Northeast Structural Genomics Consortium Target OR52
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Deposited on : 2011-09-30
Resolution : 2.80 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
Mogul	:	2022.3.0, CSD as543be (2022)
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)

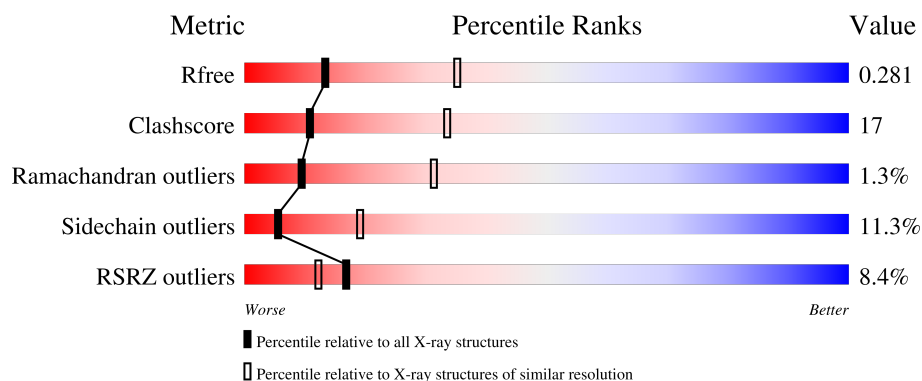
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.80 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	3866 (2.80-2.80)
Clashscore	190562	4276 (2.80-2.80)
Ramachandran outliers	187476	4196 (2.80-2.80)
Sidechain outliers	187428	4198 (2.80-2.80)
RSRZ outliers	180081	3869 (2.80-2.80)

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	338	2% 65% 27% • •
1	B	338	3% 54% 37% 5% •
1	C	338	14% 59% 35% • •
1	D	338	12% 48% 24% 8% 20%

Validation Pipeline (wwPDB-VP) : 2.49

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 9968 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 De Novo design cysteine esterase FR29.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	327	Total	C	N	O	S	Se	0	0	0
			2597	1653	443	487	4	10			
1	B	327	Total	C	N	O	S	Se	0	0	0
			2597	1653	443	487	4	10			
1	C	327	Total	C	N	O	S	Se	0	0	0
			2597	1653	443	487	4	10			
1	D	269	Total	C	N	O	S	Se	0	0	0
			2145	1371	368	393	4	9			

- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	9	Total	O	0	0
			9	9		
2	B	12	Total	O	0	0
			12	12		
2	C	6	Total	O	0	0
			6	6		
2	D	5	Total	O	0	0
			5	5		

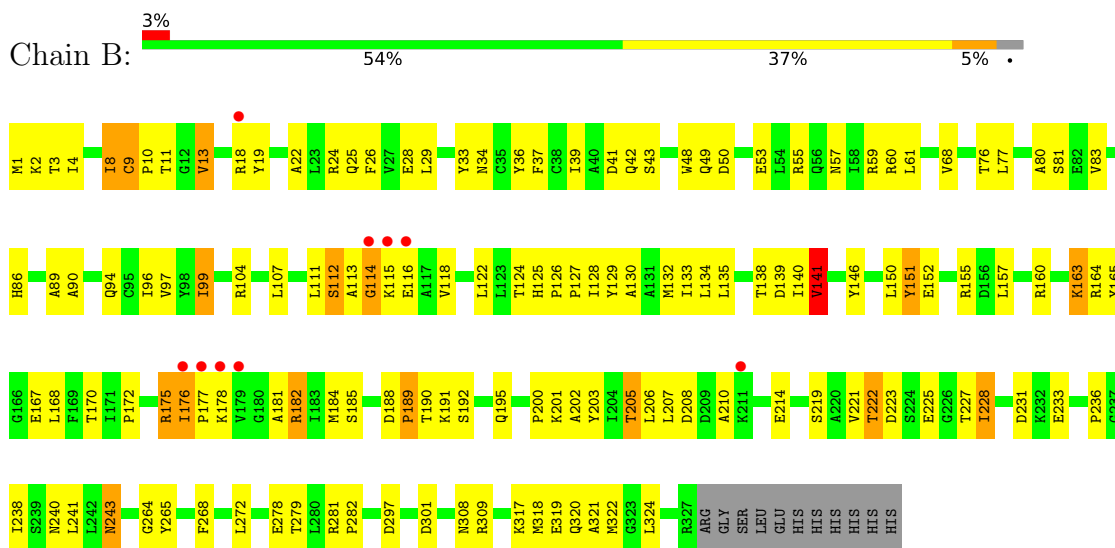
3 Residue-property plots

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.

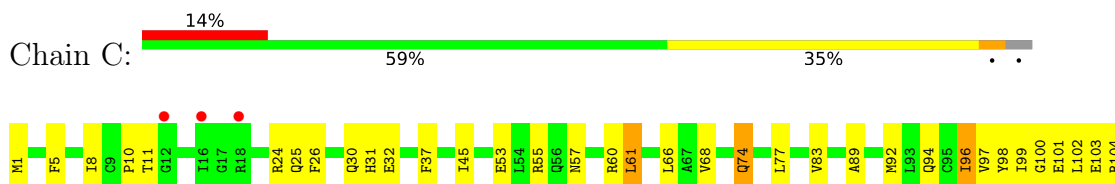
• Molecule 1: De Novo design cysteine esterase FR29



• Molecule 1: De Novo design cysteine esterase FR29



• Molecule 1: De Novo design cysteine esterase FR29



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	97.75Å 100.76Å 188.22Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	42.82 – 2.80 42.82 – 2.80	Depositor EDS
% Data completeness (in resolution range)	90.7 (42.82-2.80) 90.8 (42.82-2.80)	Depositor EDS
R_{merge}	0.12	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.45 (at 2.81Å)	Xtriage
Refinement program	PHENIX 1.7.1_743	Depositor
R, R_{free}	0.214 , 0.290 0.206 , 0.281	Depositor DCC
R_{free} test set	2117 reflections (4.54%)	wwPDB-VP
Wilson B-factor (Å ²)	39.8	Xtriage
Anisotropy	0.729	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 56.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	0.000 for k,h,-l	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	9968	wwPDB-VP
Average B, all atoms (Å ²)	48.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 35.62 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 5.6741e-04. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

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	0.56	0/2638	0.94	6/3554 (0.2%)
1	B	0.59	0/2638	0.91	5/3554 (0.1%)
1	C	0.49	0/2638	0.86	1/3554 (0.0%)
1	D	0.55	0/2177	0.91	2/2933 (0.1%)
All	All	0.55	0/10091	0.91	14/13595 (0.1%)

There are no bond length outliers.

All (14) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	176	ILE	CA-C-N	7.15	127.19	119.89
1	B	176	ILE	C-N-CA	7.15	127.19	119.89
1	C	326	ARG	N-CA-C	7.14	118.93	108.86
1	A	197	ASP	CA-C-N	7.06	127.37	119.32
1	A	197	ASP	C-N-CA	7.06	127.37	119.32
1	A	222	THR	CB-CA-C	-6.82	107.25	117.07
1	B	170	THR	CA-C-N	-6.31	118.31	122.60
1	B	170	THR	C-N-CA	-6.31	118.31	122.60
1	D	197	ASP	CA-C-N	5.48	125.31	119.28
1	D	197	ASP	C-N-CA	5.48	125.31	119.28
1	A	222	THR	CA-C-O	5.35	121.05	117.94
1	A	83	VAL	CA-C-N	5.29	125.61	119.47
1	A	83	VAL	C-N-CA	5.29	125.61	119.47
1	B	141	VAL	N-CA-C	5.04	113.61	107.61

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	2597	0	2620	73	0
1	B	2597	0	2620	99	0
1	C	2597	0	2620	93	0
1	D	2145	0	2171	87	0
2	A	9	0	0	0	0
2	B	12	0	0	2	0
2	C	6	0	0	1	0
2	D	5	0	0	0	0
All	All	9968	0	10031	332	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 17.

All (332) 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:205:THR:HG22	1:D:207:LEU:H	1.12	1.12
1:B:188:ASP:OD1	1:B:190:THR:HG22	1.61	1.01
1:D:213:ILE:HG21	1:D:277:ILE:HG23	1.39	0.98
1:B:175:ARG:HG2	1:B:175:ARG:HH11	1.33	0.93
1:C:205:THR:HG22	1:C:207:LEU:H	1.39	0.88
1:D:276:VAL:HB	1:D:277:ILE:HD12	1.57	0.86
1:C:162:ASN:HA	1:C:166:GLY:O	1.75	0.85
1:D:277:ILE:HD12	1:D:277:ILE:H	1.39	0.84
1:A:205:THR:HG22	1:A:207:LEU:H	1.44	0.81
1:C:215:LYS:O	1:C:219:SER:OG	2.01	0.77
1:C:129:TYR:CZ	1:C:133:ILE:HD11	2.19	0.77
1:D:96:ILE:HG23	1:D:160:ARG:HD2	1.65	0.77
1:D:277:ILE:HD12	1:D:277:ILE:N	2.00	0.77
1:B:222:THR:OG1	1:B:223:ASP:N	2.18	0.76
1:D:176:ILE:HG13	1:D:177:PRO:HD2	1.66	0.76
1:B:155:ARG:NH1	1:B:172:PRO:O	2.17	0.75
1:A:107:LEU:O	1:A:111:LEU:HD23	1.87	0.75
1:B:205:THR:HG22	1:B:207:LEU:H	1.52	0.74
1:C:60:ARG:HG2	1:C:291:MSE:HE2	1.68	0.74
1:A:205:THR:HB	1:A:208:ASP:OD1	1.88	0.73
1:B:43:SER:HB3	1:B:125:HIS:NE2	2.06	0.71
1:C:107:LEU:O	1:C:111:LEU:HD22	1.91	0.71
1:B:1:MSE:HE2	1:B:33:TYR:C	2.16	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:60:ARG:HG2	1:C:291:MSE:CE	2.21	0.70
1:C:225:GLU:HG2	1:C:226:GLY:H	1.55	0.69
1:A:116:GLU:H	1:A:116:GLU:CD	2.00	0.69
1:D:83:VAL:HG13	1:D:308:ASN:OD1	1.94	0.68
1:D:203:TYR:C	1:D:204:ILE:HD12	2.18	0.68
1:B:324:LEU:HD21	1:D:45:ILE:HD13	1.76	0.68
1:B:86:HIS:CE1	1:B:132:MSE:HG2	2.29	0.67
1:D:14:ILE:HD13	1:D:64:LEU:HG	1.74	0.67
1:D:205:THR:HG22	1:D:207:LEU:N	1.98	0.67
1:C:220:ALA:O	1:C:269:LYS:NZ	2.29	0.66
1:D:66:LEU:CD2	1:D:72:PRO:HG3	2.25	0.66
1:D:96:ILE:CG2	1:D:160:ARG:HD2	2.25	0.66
1:D:115:LYS:H	1:D:115:LYS:HD3	1.61	0.66
1:A:163:LYS:HD2	1:A:163:LYS:C	2.20	0.66
1:D:162:ASN:HA	1:D:166:GLY:O	1.96	0.66
1:A:126:PRO:HB2	1:A:127:PRO:HD3	1.77	0.66
1:D:184:MSE:HG2	1:D:185:SER:H	1.60	0.65
1:B:13:VAL:HG23	1:B:195:GLN:HB2	1.79	0.65
1:A:98:TYR:HD1	1:A:101:GLU:OE2	1.79	0.64
1:A:225:GLU:HG2	1:A:226:GLY:H	1.62	0.64
1:B:205:THR:CG2	1:B:207:LEU:H	2.10	0.64
1:A:184:MSE:HE3	1:A:191:LYS:C	2.23	0.64
1:A:133:ILE:HD13	1:A:141:VAL:HG21	1.80	0.63
1:D:276:VAL:HB	1:D:277:ILE:CD1	2.28	0.63
1:A:175:ARG:O	1:A:177:PRO:HD3	1.98	0.63
1:B:190:THR:HG23	1:B:191:LYS:HG3	1.80	0.63
1:B:115:LYS:HG3	1:B:116:GLU:H	1.63	0.63
1:B:10:PRO:HG3	1:B:41:ASP:HA	1.79	0.63
1:C:104:ARG:HA	1:C:109:LYS:HE3	1.80	0.62
1:A:26:PHE:HA	1:A:29:LEU:HB2	1.81	0.62
1:D:89:ALA:HA	1:D:92:MSE:HE3	1.80	0.62
1:B:26:PHE:HA	1:B:29:LEU:HB2	1.82	0.62
1:B:55:ARG:NH2	1:D:324:LEU:O	2.33	0.61
1:C:126:PRO:HB2	1:C:127:PRO:HD3	1.83	0.60
1:A:104:ARG:NH2	1:B:113:ALA:H	1.99	0.60
1:C:97:VAL:HG21	1:C:102:LEU:HD21	1.83	0.60
1:B:115:LYS:HD3	1:C:116:GLU:HB2	1.82	0.60
1:D:108:PHE:O	1:D:112:SER:HB3	2.01	0.60
1:D:277:ILE:H	1:D:277:ILE:CD1	2.13	0.60
1:B:133:ILE:HD13	1:B:141:VAL:HG21	1.84	0.60
1:C:205:THR:HG22	1:C:207:LEU:N	2.12	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:9:CYS:HB3	1:B:11:THR:HG22	1.83	0.60
1:B:94:GLN:OE1	1:B:124:THR:HB	2.02	0.59
1:B:126:PRO:HB2	1:B:127:PRO:HD3	1.82	0.59
1:A:108:PHE:CZ	1:A:123:LEU:HD13	2.38	0.59
1:B:39:ILE:HG12	1:B:61:LEU:HD23	1.83	0.59
1:B:129:TYR:CZ	1:B:133:ILE:HD11	2.37	0.59
1:D:171:ILE:N	1:D:171:ILE:HD12	2.18	0.59
1:D:239:SER:O	1:D:241:LEU:N	2.36	0.59
1:B:11:THR:HG23	1:B:11:THR:O	2.03	0.59
1:D:64:LEU:HD11	1:D:206:LEU:HD12	1.84	0.59
1:A:92:MSE:HE1	1:A:319:GLU:HG3	1.84	0.59
1:B:319:GLU:C	1:B:321:ALA:H	2.11	0.58
1:B:99:ILE:HG13	1:D:118:VAL:O	2.04	0.57
1:A:43:SER:CB	1:A:125:HIS:HE2	2.17	0.57
1:D:246:SER:O	1:D:249:SER:OG	2.22	0.57
1:A:324:LEU:O	1:C:55:ARG:NH2	2.38	0.57
1:D:16:ILE:HD12	1:D:17:GLY:H	1.68	0.57
1:D:25:GLN:HE21	1:D:178:LYS:HD3	1.70	0.57
1:D:197:ASP:HB3	1:D:203:TYR:CE2	2.40	0.57
1:C:89:ALA:HA	1:C:92:MSE:HE3	1.85	0.57
1:A:162:ASN:HA	1:A:166:GLY:O	2.04	0.56
1:B:80:ALA:HB1	2:B:516:HOH:O	2.04	0.56
1:D:183:ILE:HG23	1:D:240:ASN:HD21	1.70	0.56
1:A:104:ARG:HH21	1:B:113:ALA:H	1.53	0.56
1:B:4:ILE:HG12	1:B:140:ILE:HB	1.86	0.56
1:B:241:LEU:HD22	1:B:272:LEU:HD23	1.88	0.56
1:B:175:ARG:HG2	1:B:175:ARG:NH1	2.09	0.56
1:A:222:THR:OG1	1:A:223:ASP:N	2.38	0.56
1:D:13:VAL:HG11	1:D:205:THR:OG1	2.06	0.56
1:C:77:LEU:O	1:C:303:GLY:HA3	2.05	0.55
1:D:276:VAL:CB	1:D:277:ILE:HD12	2.34	0.55
1:A:183:ILE:HD13	1:A:183:ILE:N	2.21	0.55
1:A:301:ASP:OD1	1:C:326:ARG:NH2	2.39	0.55
1:B:115:LYS:HD3	1:C:116:GLU:CB	2.36	0.55
1:C:284:GLN:HA	1:C:287:TYR:HB3	1.88	0.55
1:B:112:SER:O	1:B:113:ALA:HB3	2.06	0.54
1:C:282:PRO:HB2	1:C:286:ARG:NH1	2.21	0.54
1:C:155:ARG:HB2	1:C:155:ARG:NH1	2.22	0.54
1:C:100:GLY:O	1:C:104:ARG:HG3	2.07	0.54
1:B:25:GLN:NE2	1:B:178:LYS:HE2	2.22	0.54
1:B:3:THR:HA	1:B:34:ASN:O	2.08	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:175:ARG:HH11	1:B:175:ARG:CG	2.12	0.54
1:C:97:VAL:HG22	1:C:98:TYR:N	2.23	0.54
1:D:245:TYR:O	1:D:245:TYR:HD1	1.90	0.53
1:C:24:ARG:HH22	1:C:247:THR:HB	1.72	0.53
1:C:245:TYR:CD2	1:C:272:LEU:HD13	2.43	0.53
1:C:83:VAL:HG22	1:C:308:ASN:ND2	2.24	0.53
1:C:185:SER:HB3	1:C:188:ASP:O	2.09	0.53
1:C:222:THR:OG1	1:C:223:ASP:N	2.39	0.53
1:D:317:LYS:O	1:D:320:GLN:HB3	2.09	0.53
1:A:129:TYR:CD2	1:A:150:LEU:HG	2.43	0.53
1:D:243:ASN:OD1	1:D:244:ILE:HG13	2.09	0.53
1:D:184:MSE:SE	1:D:184:MSE:N	2.92	0.53
1:A:225:GLU:HG2	1:A:226:GLY:N	2.22	0.53
1:D:13:VAL:HG22	1:D:14:ILE:H	1.74	0.53
1:A:14:ILE:HG13	1:A:64:LEU:HD23	1.90	0.52
1:A:281:ARG:NH1	1:A:282:PRO:HD3	2.24	0.52
1:B:138:THR:HG21	1:B:141:VAL:HG23	1.90	0.52
1:D:100:GLY:O	1:D:104:ARG:HG3	2.10	0.52
1:B:59:ARG:NH2	1:B:297:ASP:OD2	2.43	0.52
1:B:112:SER:HB3	1:B:118:VAL:HG21	1.91	0.52
1:A:59:ARG:NH1	1:A:296:LEU:HD23	2.25	0.51
1:B:231:ASP:C	1:B:231:ASP:OD1	2.52	0.51
1:B:181:ALA:HB3	1:B:243:ASN:OD1	2.10	0.51
1:D:137:ASN:OD1	1:D:314:MSE:HE3	2.10	0.51
1:A:116:GLU:CD	1:A:116:GLU:N	2.68	0.51
1:A:225:GLU:OE2	1:A:227:THR:OG1	2.29	0.51
1:A:36:TYR:CD1	1:A:76:THR:HB	2.46	0.51
1:C:222:THR:HA	1:C:237:GLY:HA3	1.92	0.51
1:D:199:ASN:HB3	1:D:202:ALA:HB2	1.93	0.51
1:C:103:GLU:HG3	1:C:123:LEU:HD11	1.91	0.51
1:A:99:ILE:HD11	1:C:118:VAL:HB	1.93	0.51
1:D:108:PHE:CZ	1:D:123:LEU:HD13	2.45	0.51
1:B:160:ARG:O	1:B:163:LYS:HD2	2.10	0.51
1:C:26:PHE:O	1:C:30:GLN:HG2	2.11	0.50
1:D:105:MSE:O	1:D:106:THR:C	2.54	0.50
1:C:225:GLU:HG2	1:C:226:GLY:N	2.25	0.50
1:A:98:TYR:HB2	1:A:101:GLU:HG3	1.93	0.50
1:D:19:TYR:HA	1:D:23:LEU:HB3	1.92	0.50
1:D:115:LYS:H	1:D:115:LYS:CD	2.24	0.50
1:C:225:GLU:CG	1:C:226:GLY:H	2.23	0.50
1:A:59:ARG:NH2	1:A:297:ASP:OD1	2.45	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:107:LEU:O	1:C:107:LEU:HD13	2.12	0.50
1:C:198:PRO:O	1:C:200:PRO:HD3	2.12	0.50
1:B:175:ARG:NH1	1:B:175:ARG:CG	2.74	0.49
1:B:97:VAL:HG23	1:B:157:LEU:HD21	1.93	0.49
1:B:2:LYS:HE3	1:B:139:ASP:HB3	1.95	0.49
1:B:42:GLN:NE2	2:B:440:HOH:O	2.35	0.49
1:B:210:ALA:O	1:B:214:GLU:HG2	2.13	0.49
1:B:319:GLU:HG2	1:B:324:LEU:HB2	1.94	0.49
1:A:112:SER:OG	1:A:113:ALA:N	2.46	0.49
1:B:150:LEU:HD12	1:B:150:LEU:O	2.11	0.49
1:A:164:ARG:HD2	1:A:165:TYR:CE1	2.48	0.49
1:B:96:ILE:HG22	1:B:160:ARG:HD2	1.94	0.48
1:B:164:ARG:HD2	1:B:165:TYR:CE2	2.48	0.48
1:A:210:ALA:O	1:A:214:GLU:HG2	2.14	0.48
1:C:271:ASP:O	1:C:275:VAL:HG23	2.13	0.48
1:A:125:HIS:O	1:A:128:ILE:HB	2.13	0.48
1:C:129:TYR:OH	1:C:133:ILE:HD11	2.13	0.48
1:C:148:LYS:O	1:C:152:GLU:HB2	2.13	0.48
1:B:319:GLU:C	1:B:321:ALA:N	2.71	0.48
1:C:53:GLU:HA	1:C:53:GLU:OE1	2.13	0.48
1:A:119:SER:HA	1:C:97:VAL:O	2.13	0.48
1:B:124:THR:HG21	1:D:124:THR:HG21	1.94	0.48
1:B:264:GLY:O	1:B:265:TYR:C	2.57	0.48
1:B:205:THR:HG22	1:B:207:LEU:N	2.26	0.48
1:C:155:ARG:HH11	1:C:155:ARG:CB	2.27	0.47
1:B:188:ASP:O	1:B:190:THR:N	2.47	0.47
1:C:83:VAL:HA	1:C:308:ASN:HD21	1.80	0.47
1:A:14:ILE:HG21	1:A:206:LEU:HD22	1.97	0.47
1:B:1:MSE:HE2	1:B:33:TYR:O	2.14	0.47
1:B:125:HIS:N	1:B:126:PRO:CD	2.78	0.47
1:D:183:ILE:HG23	1:D:240:ASN:ND2	2.30	0.47
1:D:184:MSE:HG2	1:D:185:SER:N	2.29	0.47
1:A:94:GLN:OE1	1:A:124:THR:HB	2.14	0.47
1:B:86:HIS:ND1	1:B:132:MSE:HG2	2.28	0.47
1:B:114:GLY:HA2	1:B:115:LYS:HA	1.55	0.47
1:C:184:MSE:HA	1:C:192:SER:HA	1.97	0.47
1:C:205:THR:CG2	1:C:207:LEU:H	2.21	0.47
1:D:15:THR:HG23	1:D:18:ARG:H	1.80	0.47
1:A:41:ASP:OD2	1:A:81:SER:HB3	2.15	0.46
1:C:98:TYR:O	1:C:101:GLU:N	2.46	0.46
1:D:186:LEU:HD11	1:D:204:ILE:CD1	2.44	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:208:ASP:O	1:C:284:GLN:NE2	2.41	0.46
1:D:186:LEU:HB3	1:D:187:VAL:H	1.53	0.46
1:A:14:ILE:HG13	1:A:64:LEU:CD2	2.45	0.46
1:D:213:ILE:CG2	1:D:277:ILE:HG23	2.27	0.46
1:D:239:SER:N	1:D:241:LEU:HD12	2.31	0.46
1:C:140:ILE:HD13	2:C:466:HOH:O	2.16	0.46
1:D:206:LEU:O	1:D:284:GLN:NE2	2.41	0.45
1:C:5:PHE:CD1	1:C:5:PHE:C	2.94	0.45
1:A:164:ARG:O	1:A:166:GLY:N	2.49	0.45
1:B:83:VAL:HA	1:B:308:ASN:HD21	1.80	0.45
1:D:176:ILE:HG13	1:D:177:PRO:CD	2.43	0.45
1:D:204:ILE:HD12	1:D:204:ILE:N	2.31	0.45
1:B:125:HIS:N	1:B:126:PRO:HD2	2.31	0.45
1:C:25:GLN:NE2	1:C:178:LYS:HE2	2.32	0.45
1:C:228:ILE:HG13	1:C:260:TYR:HB3	1.98	0.45
1:D:21:GLY:C	1:D:25:GLN:HE22	2.24	0.45
1:B:130:ALA:O	1:B:134:LEU:HG	2.15	0.45
1:B:205:THR:HB	1:B:208:ASP:OD1	2.16	0.45
1:C:136:TYR:CZ	1:C:311:ALA:HB2	2.51	0.45
1:C:155:ARG:HB2	1:C:155:ARG:HH11	1.81	0.45
1:C:221:VAL:O	1:C:237:GLY:HA3	2.17	0.45
1:A:136:TYR:OH	1:A:307:ALA:HB1	2.17	0.45
1:D:56:GLN:O	1:D:59:ARG:N	2.50	0.45
1:A:319:GLU:C	1:A:321:ALA:H	2.25	0.45
1:B:90:ALA:O	1:B:94:GLN:HB2	2.17	0.45
1:D:276:VAL:HG12	1:D:277:ILE:HG13	1.99	0.45
1:A:125:HIS:N	1:A:126:PRO:CD	2.80	0.45
1:B:19:TYR:O	1:B:24:ARG:HB2	2.17	0.45
1:B:48:TRP:C	1:B:49:GLN:HG2	2.42	0.44
1:C:114:GLY:HA2	1:C:115:LYS:HA	1.70	0.44
1:D:96:ILE:HD12	1:D:96:ILE:HA	1.85	0.44
1:B:168:LEU:CD1	1:B:317:LYS:HD3	2.47	0.44
1:B:176:ILE:HA	1:B:177:PRO:HD2	1.73	0.44
1:C:66:LEU:HD12	1:C:296:LEU:HD12	1.99	0.44
1:C:134:LEU:HB3	1:C:169:PHE:CD1	2.53	0.44
1:C:256:LEU:O	1:C:260:TYR:HB2	2.17	0.44
1:B:57:ASN:OD1	1:B:60:ARG:NH1	2.50	0.44
1:B:281:ARG:N	1:B:282:PRO:HD2	2.32	0.44
1:A:124:THR:O	1:A:127:PRO:HD2	2.17	0.44
1:A:124:THR:HG21	1:C:124:THR:HG21	1.98	0.44
1:C:282:PRO:HA	1:C:285:GLU:HB2	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:105:MSE:O	1:D:108:PHE:N	2.45	0.44
1:B:29:LEU:HD23	1:B:29:LEU:HA	1.77	0.44
1:B:168:LEU:HD11	1:B:317:LYS:HD3	1.99	0.44
1:B:189:PRO:HB2	1:B:236:PRO:HB2	1.98	0.44
1:C:248:LEU:HD23	1:C:248:LEU:HA	1.86	0.44
1:B:308:ASN:O	1:B:309:ARG:C	2.61	0.44
1:B:318:MSE:O	1:B:322:MSE:HG3	2.18	0.44
1:C:155:ARG:HG2	1:C:156:ASP:N	2.32	0.44
1:C:168:LEU:HD12	1:C:168:LEU:HA	1.66	0.44
1:D:66:LEU:HD21	1:D:72:PRO:HG3	1.98	0.44
1:D:279:THR:O	1:D:282:PRO:HD2	2.17	0.44
1:A:99:ILE:HG13	1:C:118:VAL:O	2.18	0.43
1:A:168:LEU:HD11	1:A:317:LYS:CD	2.47	0.43
1:B:37:PHE:O	1:B:77:LEU:HD12	2.18	0.43
1:C:140:ILE:HA	1:C:173:GLU:O	2.18	0.43
1:A:188:ASP:C	1:A:190:THR:H	2.25	0.43
1:C:180:GLY:O	1:C:181:ALA:C	2.60	0.43
1:C:207:LEU:HD21	1:C:287:TYR:CD2	2.53	0.43
1:D:14:ILE:H	1:D:14:ILE:HD12	1.83	0.43
1:D:79:ILE:HB	1:D:82:GLU:HG3	2.00	0.43
1:C:31:HIS:ND1	1:C:74:GLN:OE1	2.49	0.43
1:C:37:PHE:HB2	1:C:77:LEU:CD1	2.49	0.43
1:C:107:LEU:HD13	1:C:107:LEU:C	2.43	0.43
1:C:112:SER:OG	1:C:113:ALA:N	2.48	0.43
1:D:316:ARG:HD2	1:D:327:ARG:NH1	2.33	0.43
1:C:227:THR:O	1:C:235:LYS:HE2	2.18	0.43
1:A:10:PRO:HA	1:A:61:LEU:HD22	2.01	0.43
1:D:124:THR:O	1:D:127:PRO:HD2	2.17	0.43
1:A:101:GLU:HG2	1:B:113:ALA:HA	2.00	0.43
1:B:49:GLN:O	1:B:50:ASP:C	2.61	0.43
1:B:185:SER:OG	1:B:202:ALA:HB1	2.19	0.43
1:D:155:ARG:NH1	1:D:155:ARG:HB2	2.34	0.43
1:A:38:CYS:HB2	1:A:78:PHE:CE1	2.54	0.43
1:A:278:GLU:OE1	1:A:278:GLU:HA	2.18	0.43
1:A:324:LEU:HD21	1:C:45:ILE:HD13	2.00	0.43
1:B:8:ILE:CG2	1:B:61:LEU:HD21	2.49	0.43
1:B:200:PRO:HA	1:B:203:TYR:CE2	2.54	0.43
1:B:241:LEU:HD22	1:B:272:LEU:CD2	2.49	0.43
1:C:10:PRO:HA	1:C:61:LEU:HD22	2.01	0.43
1:B:43:SER:CB	1:B:125:HIS:NE2	2.79	0.43
1:C:189:PRO:HB3	1:C:236:PRO:C	2.44	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:129:TYR:CE2	1:C:133:ILE:CD1	3.02	0.42
1:A:60:ARG:HG2	1:A:287:TYR:OH	2.19	0.42
1:A:96:ILE:HD13	1:A:96:ILE:HA	1.72	0.42
1:C:60:ARG:HG2	1:C:291:MSE:HE1	2.00	0.42
1:D:168:LEU:HD11	1:D:317:LYS:HB3	2.02	0.42
1:D:4:ILE:HG12	1:D:140:ILE:HB	1.99	0.42
1:A:164:ARG:C	1:A:166:GLY:H	2.27	0.42
1:C:96:ILE:HD13	1:C:96:ILE:HA	1.81	0.42
1:C:115:LYS:H	1:C:115:LYS:HG3	1.67	0.42
1:C:260:TYR:HA	1:C:263:LYS:HD2	2.01	0.42
1:D:18:ARG:O	1:D:22:ALA:HB3	2.20	0.42
1:D:104:ARG:HE	1:D:104:ARG:HB2	1.54	0.42
1:D:186:LEU:HA	1:D:186:LEU:HD23	1.75	0.42
1:A:37:PHE:O	1:A:77:LEU:HD12	2.20	0.42
1:B:36:TYR:CD1	1:B:76:THR:HB	2.55	0.42
1:C:104:ARG:HE	1:C:104:ARG:HB2	1.52	0.42
1:B:182:ARG:HD2	1:B:192:SER:OG	2.19	0.41
1:D:96:ILE:HG23	1:D:160:ARG:CD	2.44	0.41
1:B:151:TYR:CD2	1:B:151:TYR:C	2.98	0.41
1:C:274:GLN:O	1:C:278:GLU:HB2	2.20	0.41
1:A:217:ILE:HD13	1:A:217:ILE:HA	1.90	0.41
1:D:130:ALA:O	1:D:134:LEU:HG	2.20	0.41
1:D:281:ARG:N	1:D:282:PRO:HD2	2.35	0.41
1:B:184:MSE:HB2	1:B:240:ASN:CG	2.46	0.41
1:C:131:ALA:O	1:C:135:LEU:HG	2.21	0.41
1:D:104:ARG:HA	1:D:109:LYS:HE2	2.02	0.41
1:D:239:SER:OG	1:D:240:ASN:N	2.53	0.41
1:B:28:GLU:O	1:B:29:LEU:C	2.64	0.41
1:C:37:PHE:HB2	1:C:77:LEU:HD12	2.02	0.41
1:A:161:PHE:CD1	1:A:161:PHE:C	2.98	0.41
1:D:284:GLN:HA	1:D:287:TYR:HB3	2.01	0.41
1:A:59:ARG:HH22	1:A:297:ASP:CG	2.28	0.41
1:B:228:ILE:HD12	1:B:268:PHE:CG	2.56	0.41
1:B:89:ALA:HB3	1:B:135:LEU:HD11	2.01	0.41
1:B:301:ASP:OD1	1:D:326:ARG:NH2	2.52	0.41
1:C:125:HIS:N	1:C:126:PRO:CD	2.84	0.41
1:C:129:TYR:CE2	1:C:133:ILE:HD11	2.55	0.41
1:C:313:GLU:OE1	1:C:313:GLU:HA	2.20	0.41
1:A:41:ASP:HB3	1:A:58:ILE:HD11	2.02	0.40
1:A:281:ARG:HB3	1:A:282:PRO:HD3	2.03	0.40
1:B:97:VAL:O	1:D:119:SER:HA	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:57:ASN:OD1	1:C:60:ARG:NH1	2.54	0.40
1:D:125:HIS:N	1:D:126:PRO:CD	2.84	0.40
1:D:201:LYS:HD2	1:D:201:LYS:HA	1.48	0.40
1:A:123:LEU:HD22	1:C:99:ILE:HD13	2.03	0.40
1:A:225:GLU:OE2	1:A:229:ARG:NH1	2.54	0.40
1:A:320:GLN:O	1:A:320:GLN:HG3	2.21	0.40
1:B:200:PRO:C	1:B:202:ALA:H	2.29	0.40
1:C:210:ALA:HB1	1:C:277:ILE:HD13	2.02	0.40
1:D:8:ILE:CG2	1:D:61:LEU:HD21	2.51	0.40
1:A:43:SER:CB	1:A:125:HIS:NE2	2.83	0.40
1:A:56:GLN:OE1	1:A:56:GLN:HA	2.21	0.40
1:A:150:LEU:HD12	1:A:150:LEU:HA	1.63	0.40
1:D:183:ILE:CG2	1:D:240:ASN:HD21	2.34	0.40
1:A:111:LEU:HD23	1:A:111:LEU:H	1.86	0.40
1:B:41:ASP:OD2	1:B:81:SER:HB3	2.22	0.40
1:A:55:ARG:NH2	1:C:324:LEU:O	2.47	0.40
1:B:41:ASP:OD1	1:B:42:GLN:N	2.55	0.40
1:B:129:TYR:CZ	1:B:133:ILE:CD1	3.05	0.40
1:B:243:ASN:HD22	1:B:243:ASN:HA	1.62	0.40
1:C:265:TYR:N	1:C:265:TYR:CD1	2.89	0.40
1:D:36:TYR:CD1	1:D:76:THR:HB	2.57	0.40
1:D:176:ILE:HD12	1:D:176:ILE:HA	1.96	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	325/338 (96%)	299 (92%)	23 (7%)	3 (1%)	14	41
1	B	325/338 (96%)	303 (93%)	18 (6%)	4 (1%)	10	34
1	C	325/338 (96%)	288 (89%)	34 (10%)	3 (1%)	14	41

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	D	261/338 (77%)	233 (89%)	22 (8%)	6 (2%)	5	18
All	All	1236/1352 (91%)	1123 (91%)	97 (8%)	16 (1%)	9	31

All (16) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	165	TYR
1	D	178	LYS
1	D	179	VAL
1	D	240	ASN
1	A	147	GLY
1	C	225	GLU
1	D	208	ASP
1	D	278	GLU
1	C	145	GLU
1	B	189	PRO
1	A	110	GLU
1	B	22	ALA
1	B	320	GLN
1	B	114	GLY
1	C	226	GLY
1	D	45	ILE

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	276/276 (100%)	246 (89%)	30 (11%)	6	21
1	B	276/276 (100%)	241 (87%)	35 (13%)	4	15
1	C	276/276 (100%)	254 (92%)	22 (8%)	11	34
1	D	228/276 (83%)	196 (86%)	32 (14%)	3	12
All	All	1056/1104 (96%)	937 (89%)	119 (11%)	5	19

All (119) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1	MSE
1	A	8	ILE
1	A	9	CYS
1	A	13	VAL
1	A	14	ILE
1	A	53	GLU
1	A	68	VAL
1	A	92	MSE
1	A	94	GLN
1	A	96	ILE
1	A	97	VAL
1	A	116	GLU
1	A	118	VAL
1	A	119	SER
1	A	122	LEU
1	A	128	ILE
1	A	155	ARG
1	A	163	LYS
1	A	190	THR
1	A	206	LEU
1	A	218	LYS
1	A	219	SER
1	A	224	SER
1	A	227	THR
1	A	229	ARG
1	A	238	ILE
1	A	255	GLU
1	A	278	GLU
1	A	298	ARG
1	A	315	VAL
1	B	8	ILE
1	B	9	CYS
1	B	13	VAL
1	B	18	ARG
1	B	53	GLU
1	B	68	VAL
1	B	99	ILE
1	B	104	ARG
1	B	107	LEU
1	B	111	LEU
1	B	112	SER
1	B	122	LEU
1	B	128	ILE

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Mol	Chain	Res	Type
1	B	141	VAL
1	B	146	TYR
1	B	151	TYR
1	B	152	GLU
1	B	163	LYS
1	B	167	GLU
1	B	175	ARG
1	B	182	ARG
1	B	201	LYS
1	B	205	THR
1	B	206	LEU
1	B	219	SER
1	B	221	VAL
1	B	222	THR
1	B	225	GLU
1	B	227	THR
1	B	228	ILE
1	B	233	GLU
1	B	238	ILE
1	B	243	ASN
1	B	278	GLU
1	B	279	THR
1	C	1	MSE
1	C	8	ILE
1	C	11	THR
1	C	32	GLU
1	C	61	LEU
1	C	68	VAL
1	C	74	GLN
1	C	94	GLN
1	C	96	ILE
1	C	111	LEU
1	C	116	GLU
1	C	118	VAL
1	C	128	ILE
1	C	152	GLU
1	C	155	ARG
1	C	179	VAL
1	C	206	LEU
1	C	212	THR
1	C	233	GLU
1	C	279	THR

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Mol	Chain	Res	Type
1	C	299	VAL
1	C	327	ARG
1	D	6	SER
1	D	8	ILE
1	D	11	THR
1	D	13	VAL
1	D	15	THR
1	D	16	ILE
1	D	64	LEU
1	D	68	VAL
1	D	96	ILE
1	D	112	SER
1	D	115	LYS
1	D	118	VAL
1	D	146	TYR
1	D	155	ARG
1	D	183	ILE
1	D	184	MSE
1	D	187	VAL
1	D	199	ASN
1	D	201	LYS
1	D	203	TYR
1	D	239	SER
1	D	242	LEU
1	D	246	SER
1	D	277	ILE
1	D	279	THR
1	D	294	GLU
1	D	302	GLU
1	D	309	ARG
1	D	312	SER
1	D	314	MSE
1	D	315	VAL
1	D	326	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
1	C	199	ASN
1	D	74	GLN
1	D	240	ASN
1	D	243	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 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	317/338 (93%)	-0.14	6 (1%) 66 57	15, 36, 68, 98	0
1	B	317/338 (93%)	-0.19	9 (2%) 55 45	11, 32, 63, 117	0
1	C	317/338 (93%)	0.65	48 (15%) 5 4	14, 54, 141, 162	0
1	D	260/338 (76%)	0.36	39 (15%) 5 4	12, 41, 102, 121	0
All	All	1211/1352 (89%)	0.16	102 (8%) 17 12	11, 38, 114, 162	0

All (102) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	179	VAL	5.9
1	D	276	VAL	5.7
1	D	185	SER	5.7
1	D	213	ILE	5.3
1	D	242	LEU	5.1
1	D	187	VAL	4.8
1	D	277	ILE	4.7
1	C	218	LYS	4.5
1	D	245	TYR	4.3
1	A	176	ILE	4.1
1	D	146	TYR	3.8
1	C	117	ALA	3.8
1	C	269	LYS	3.8
1	B	178	LYS	3.7
1	C	217	ILE	3.7
1	C	18	ARG	3.7
1	C	221	VAL	3.7
1	C	219	SER	3.7
1	B	176	ILE	3.6
1	A	177	PRO	3.6
1	C	12	GLY	3.6

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Mol	Chain	Res	Type	RSRZ
1	C	230	TYR	3.6
1	C	242	LEU	3.5
1	C	179	VAL	3.5
1	C	119	SER	3.5
1	A	179	VAL	3.5
1	C	234	ALA	3.4
1	C	268	PHE	3.4
1	D	183	ILE	3.3
1	B	115	LYS	3.3
1	C	229	ARG	3.3
1	D	215	LYS	3.3
1	C	265	TYR	3.2
1	D	182	ARG	3.1
1	D	240	ASN	3.0
1	C	228	ILE	3.0
1	C	224	SER	3.0
1	C	194	TYR	2.9
1	C	267	VAL	2.9
1	A	182	ARG	2.9
1	D	244	ILE	2.8
1	C	241	LEU	2.8
1	D	243	ASN	2.8
1	C	272	LEU	2.8
1	D	180	GLY	2.8
1	D	210	ALA	2.7
1	C	187	VAL	2.7
1	D	117	ALA	2.7
1	D	16	ILE	2.7
1	A	115	LYS	2.6
1	C	220	ALA	2.6
1	C	240	ASN	2.6
1	D	181	ALA	2.6
1	C	209	ASP	2.6
1	C	258	ARG	2.6
1	C	145	GLU	2.6
1	D	186	LEU	2.5
1	C	182	ARG	2.5
1	C	203	TYR	2.5
1	C	226	GLY	2.5
1	C	236	PRO	2.5
1	C	227	THR	2.5
1	B	177	PRO	2.4

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Mol	Chain	Res	Type	RSRZ
1	C	114	GLY	2.4
1	D	179	VAL	2.4
1	C	222	THR	2.4
1	C	186	LEU	2.4
1	D	248	LEU	2.4
1	C	116	GLU	2.4
1	D	116	GLU	2.4
1	D	246	SER	2.4
1	C	178	LYS	2.4
1	B	114	GLY	2.4
1	C	262	GLY	2.4
1	C	264	GLY	2.4
1	D	239	SER	2.3
1	D	144	GLY	2.3
1	C	212	THR	2.3
1	D	203	TYR	2.3
1	B	116	GLU	2.3
1	D	13	VAL	2.3
1	D	12	GLY	2.2
1	C	266	GLY	2.2
1	D	178	LYS	2.2
1	D	113	ALA	2.2
1	B	18	ARG	2.2
1	D	212	THR	2.1
1	D	114	GLY	2.1
1	A	116	GLU	2.1
1	D	15	THR	2.1
1	C	253	ILE	2.1
1	C	270	ALA	2.1
1	C	198	PRO	2.1
1	C	213	ILE	2.1
1	D	249	SER	2.0
1	B	211	LYS	2.0
1	D	148	LYS	2.0
1	D	211	LYS	2.0
1	C	16	ILE	2.0
1	D	118	VAL	2.0
1	C	281	ARG	2.0
1	D	202	ALA	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.