



Full wwPDB X-ray Structure Validation Report ⓘ

May 15, 2020 – 06:23 pm BST

PDB ID : 1NPP
Title : CRYSTAL STRUCTURE OF AQUIFEX AEOLICUS NUSG IN P2(1)
Authors : Knowlton, J.R.; Bubunenko, M.; Andrykovitch, M.; Guo, W.; Routzahn, K.M.; Waugh, D.S.; Court, D.L.; Ji, X.
Deposited on : 2003-01-18
Resolution : 2.00 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 following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.11
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) : 2.11

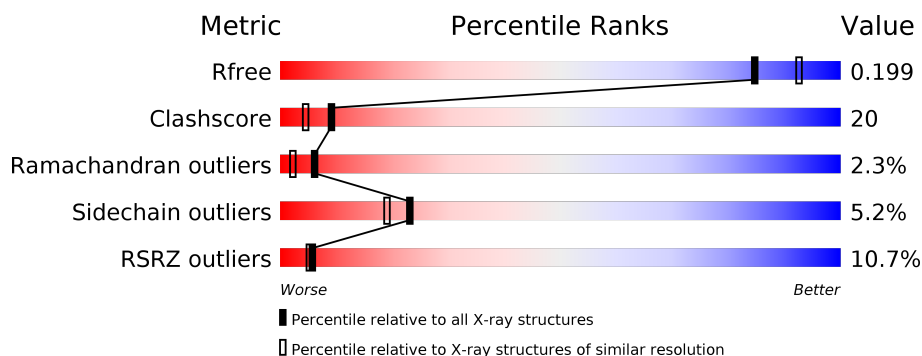
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.00 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	8085 (2.00-2.00)
Clashscore	141614	9178 (2.00-2.00)
Ramachandran outliers	138981	9054 (2.00-2.00)
Sidechain outliers	138945	9053 (2.00-2.00)
RSRZ outliers	127900	7900 (2.00-2.00)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. 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	248	<div> <div>14%</div> <div>80%</div> <div>16%</div> <div>..</div> </div>
1	B	248	<div> <div>14%</div> <div>56%</div> <div>37%</div> <div>...</div> </div>
1	C	248	<div> <div>13%</div> <div>61%</div> <div>30%</div> <div>..</div> </div>
1	D	248	<div> <div>13%</div> <div>71%</div> <div>21%</div> <div>...</div> </div>

2 Entry composition [i](#)

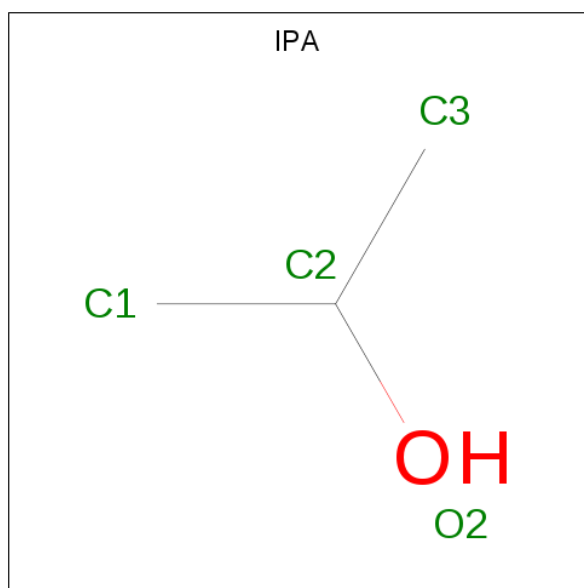
There are 3 unique types of molecules in this entry. The entry contains 8486 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 Transcription antitermination protein nusG.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	244	Total	C	N	O	S	0	0	0
			1933	1234	329	362	8			
1	B	241	Total	C	N	O	S	8	0	0
			1908	1219	324	357	8			
1	C	238	Total	C	N	O	S	8	0	0
			1882	1202	321	351	8			
1	D	240	Total	C	N	O	S	28	0	0
			1897	1212	323	354	8			

- Molecule 2 is ISOPROPYL ALCOHOL (three-letter code: IPA) (formula: C₃H₈O).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	D	1	Total	C	O	0	0
			4	3	1		
2	D	1	Total	C	O	0	0
			4	3	1		

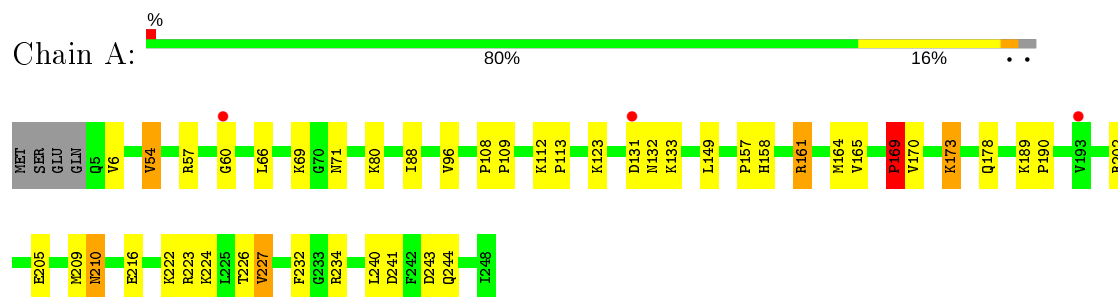
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	237	Total 237	O 237	0	0
3	B	199	Total 199	O 199	0	0
3	C	181	Total 181	O 181	0	0
3	D	241	Total 241	O 241	0	0

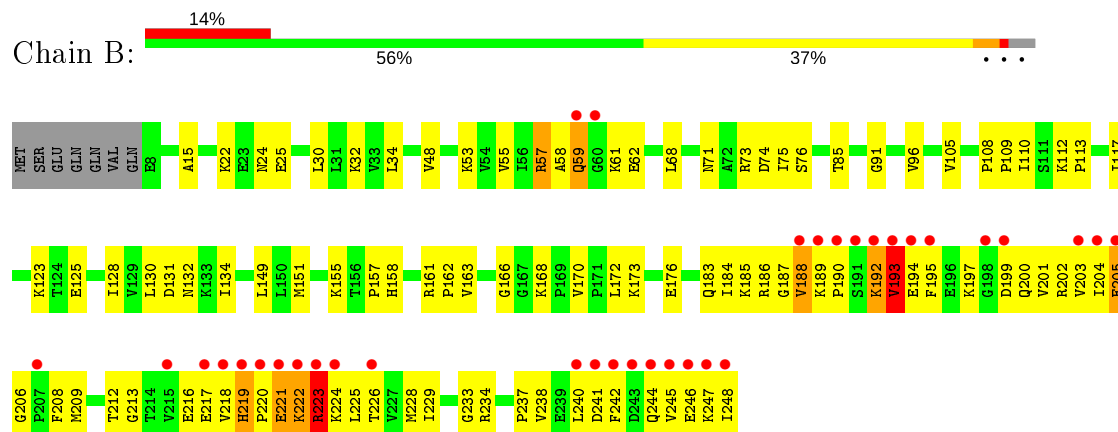
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA 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.

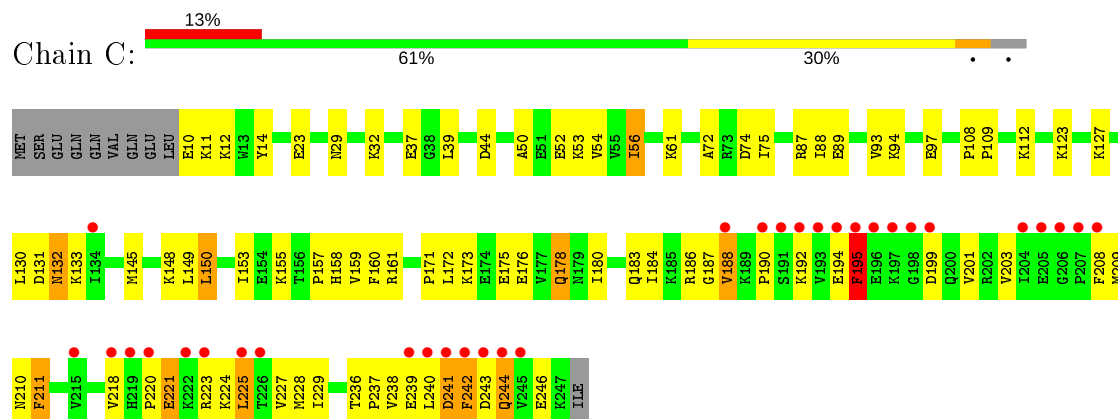
- Molecule 1: Transcription antitermination protein nusG



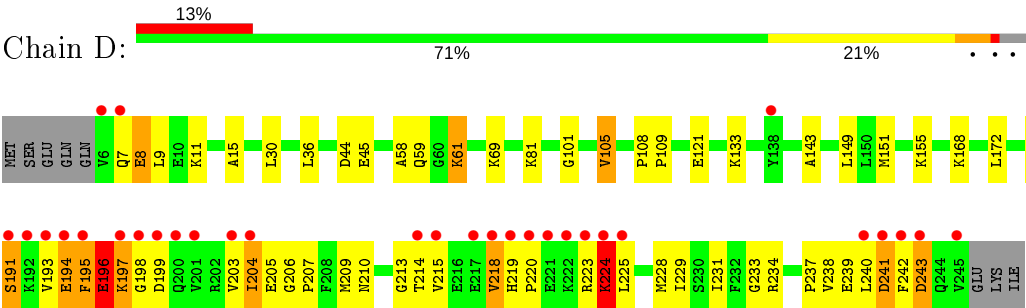
- Molecule 1: Transcription antitermination protein nusG



- Molecule 1: Transcription antitermination protein nusG



● Molecule 1: Transcription antitermination protein nusG



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	87.07Å 55.86Å 112.61Å 90.00° 90.39° 90.00°	Depositor
Resolution (Å)	19.98 – 2.00 36.02 – 1.92	Depositor EDS
% Data completeness (in resolution range)	76.1 (19.98-2.00) 87.3 (36.02-1.92)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	0.87 (at 1.92Å)	Xtriage
Refinement program	CNS 1.0	Depositor
R, R_{free}	0.219 , 0.279 0.199 , 0.199	Depositor DCC
R_{free} test set	2877 reflections (3.60%)	wwPDB-VP
Wilson B-factor (Å ²)	29.8	Xtriage
Anisotropy	0.210	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 61.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.029 for h,-k,-l	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	8486	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 12.28% 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](#)

Bond lengths and bond angles in the following residue types are not validated in this section: IPA

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	0.57	0/1962	0.79	1/2638 (0.0%)
1	B	0.60	0/1937	0.79	0/2604
1	C	0.54	0/1911	0.74	0/2570
1	D	0.59	0/1926	0.77	0/2592
All	All	0.57	0/7736	0.78	1/10404 (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	A	169	PRO	CA-N-CD	-13.97	91.94	111.50

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	1933	0	2025	62	0
1	B	1908	0	2000	105	0
1	C	1882	0	1972	104	0
1	D	1897	0	1987	66	0
2	D	8	0	16	1	0
3	A	237	0	0	12	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	B	199	0	0	17	0
3	C	181	0	0	11	0
3	D	241	0	0	8	0
All	All	8486	0	8000	310	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 20.

All (310) 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:224:LYS:HB3	1:D:241:ASP:HA	1.45	0.98
1:B:219:HIS:HB3	1:B:220:PRO:HD2	1.47	0.94
1:A:57:ARG:HD3	3:A:443:HOH:O	1.70	0.90
1:C:127:LYS:NZ	1:C:127:LYS:HB3	1.86	0.90
1:A:227:VAL:HG11	1:A:240:LEU:HD12	1.54	0.89
1:B:132:ASN:HB3	3:B:350:HOH:O	1.71	0.89
1:B:187:GLY:O	1:B:189:LYS:HE3	1.74	0.88
1:A:209:MET:HG2	1:A:210:ASN:ND2	1.90	0.87
1:D:190:PRO:O	1:D:191:SER:C	2.12	0.86
1:C:224:LYS:HA	1:C:241:ASP:HA	1.57	0.83
1:C:29:ASN:ND2	1:C:157:PRO:HG2	1.95	0.81
1:D:218:VAL:HA	1:D:225:LEU:HD23	1.62	0.81
1:A:222:LYS:HZ1	1:B:248:ILE:HG22	1.47	0.80
1:B:197:LYS:HD3	1:B:217:GLU:OE1	1.82	0.80
1:B:220:PRO:O	1:B:221:GLU:C	2.14	0.79
1:C:29:ASN:HD22	1:C:157:PRO:HG2	1.48	0.79
1:B:193:VAL:HG22	3:B:354:HOH:O	1.81	0.79
1:B:183:GLN:HG2	1:B:188:VAL:HG11	1.65	0.79
1:C:228:MET:HE2	1:C:237:PRO:HA	1.65	0.79
1:D:105:VAL:HG22	3:D:976:HOH:O	1.81	0.78
1:D:203:VAL:HG12	1:D:204:ILE:H	1.49	0.78
1:B:238:VAL:HG12	1:B:240:LEU:HG	1.66	0.77
1:B:205:GLU:HB3	1:B:244:GLN:HG2	1.65	0.76
1:C:173:LYS:HD3	1:D:234:ARG:HD3	1.68	0.76
1:C:132:ASN:HD22	1:C:132:ASN:H	1.32	0.76
1:C:195:PHE:HE2	1:C:225:LEU:HB3	1.51	0.76
1:D:206:GLY:O	1:D:209:MET:HG3	1.85	0.76
1:D:9:LEU:HG	3:D:1044:HOH:O	1.85	0.75
1:C:228:MET:CE	1:C:237:PRO:HA	2.17	0.74
1:D:219:HIS:O	1:D:223:ARG:HB2	1.88	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:242:PHE:O	1:D:243:ASP:HB2	1.87	0.74
1:A:222:LYS:HG2	1:A:224:LYS:HD3	1.70	0.73
1:B:76:SER:OG	1:B:85:THR:HG22	1.88	0.73
1:B:194:GLU:HG2	1:B:194:GLU:O	1.88	0.72
1:B:59:GLN:HB2	1:B:123:LYS:O	1.88	0.72
1:C:203:VAL:HA	1:C:244:GLN:HB3	1.71	0.72
1:A:173:LYS:NZ	1:A:173:LYS:HB2	2.05	0.72
1:B:155:LYS:HB2	3:B:375:HOH:O	1.89	0.72
1:D:203:VAL:HG12	1:D:204:ILE:N	2.04	0.72
1:C:12:LYS:HB2	1:C:14:TYR:CZ	2.24	0.72
1:B:219:HIS:HB3	1:B:220:PRO:CD	2.21	0.71
1:A:222:LYS:NZ	1:B:248:ILE:HG22	2.06	0.70
1:C:201:VAL:HB	1:C:244:GLN:HE21	1.54	0.70
1:B:220:PRO:O	1:B:221:GLU:O	2.09	0.70
1:A:165:VAL:HG23	1:A:170:VAL:HG21	1.73	0.69
1:B:188:VAL:O	1:B:190:PRO:HD3	1.92	0.69
1:A:234:ARG:HD3	3:A:407:HOH:O	1.92	0.69
1:D:205:GLU:HA	1:D:209:MET:HG2	1.73	0.69
1:A:173:LYS:HZ1	1:B:233:GLY:C	1.97	0.69
1:D:224:LYS:HB3	1:D:241:ASP:CA	2.22	0.68
1:B:155:LYS:HE3	3:B:331:HOH:O	1.93	0.68
1:C:127:LYS:HB3	1:C:127:LYS:HZ3	1.57	0.67
1:A:227:VAL:CG1	1:A:240:LEU:HD12	2.24	0.67
1:A:80:LYS:HD2	1:A:123:LYS:HD3	1.76	0.67
1:C:132:ASN:HD22	1:C:132:ASN:N	1.91	0.67
1:C:229:ILE:HD12	1:C:238:VAL:HG21	1.77	0.67
1:C:61:LYS:HB2	1:C:61:LYS:NZ	2.09	0.67
1:A:209:MET:O	1:A:210:ASN:HB2	1.95	0.67
1:C:208:PHE:O	1:C:211:PHE:HB2	1.95	0.66
1:C:145:MET:SD	1:C:150:LEU:HD13	2.35	0.66
1:C:224:LYS:HG2	1:C:241:ASP:CG	2.16	0.66
1:B:22:LYS:HE2	3:B:348:HOH:O	1.96	0.66
1:C:195:PHE:CD2	1:C:225:LEU:HD23	2.31	0.66
1:C:223:ARG:HH11	1:C:223:ARG:HG2	1.60	0.66
1:C:225:LEU:HD13	1:C:227:VAL:HG23	1.79	0.65
1:D:81:LYS:HD3	3:D:992:HOH:O	1.96	0.65
1:B:221:GLU:HG3	1:B:221:GLU:O	1.96	0.65
1:C:220:PRO:C	1:C:221:GLU:HG3	2.16	0.64
1:A:173:LYS:HE3	1:B:234:ARG:HA	1.80	0.64
1:A:222:LYS:HZ1	1:B:248:ILE:HA	1.62	0.64
1:B:217:GLU:HG3	1:B:218:VAL:N	2.14	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:224:LYS:HG2	1:C:241:ASP:OD2	1.99	0.63
1:A:205:GLU:HB2	1:C:186:ARG:HD3	1.80	0.63
1:C:195:PHE:O	1:C:218:VAL:HG11	1.98	0.63
1:D:196:GLU:HB2	1:D:199:ASP:OD2	1.99	0.63
1:C:175:GLU:HG2	3:C:325:HOH:O	1.98	0.63
1:A:173:LYS:NZ	1:B:233:GLY:C	2.52	0.63
1:B:183:GLN:HE21	1:B:188:VAL:HG11	1.63	0.63
1:D:193:VAL:O	1:D:194:GLU:HB2	1.99	0.62
1:D:61:LYS:H	1:D:61:LYS:HD3	1.64	0.62
1:B:151:MET:HE2	3:B:329:HOH:O	1.98	0.62
1:A:173:LYS:HZ2	1:A:173:LYS:HB2	1.65	0.62
1:B:213:GLY:HA3	1:B:228:MET:O	2.00	0.61
1:C:161:ARG:HH21	1:D:207:PRO:HG3	1.65	0.61
1:C:127:LYS:CB	1:C:127:LYS:NZ	2.61	0.61
1:C:89:GLU:HA	3:C:427:HOH:O	2.01	0.61
1:C:176:GLU:HG2	1:D:233:GLY:CA	2.31	0.61
1:B:188:VAL:HB	3:B:385:HOH:O	2.01	0.60
1:A:165:VAL:HG23	1:A:170:VAL:CG2	2.30	0.60
1:A:190:PRO:HG3	1:C:72:ALA:HB2	1.82	0.60
1:D:205:GLU:CA	1:D:209:MET:HG2	2.32	0.59
1:B:203:VAL:HB	1:B:208:PHE:O	2.03	0.59
1:C:132:ASN:H	1:C:132:ASN:ND2	1.99	0.59
1:A:71:ASN:HD21	1:C:87:ARG:HH12	1.51	0.59
1:C:157:PRO:O	1:C:158:HIS:HB2	2.02	0.58
1:C:194:GLU:O	1:C:195:PHE:HB3	2.03	0.58
1:B:206:GLY:O	1:B:209:MET:HG3	2.03	0.58
1:C:223:ARG:O	1:C:224:LYS:HG3	2.04	0.58
1:A:6:VAL:HG22	3:A:473:HOH:O	2.04	0.58
1:B:217:GLU:HG3	1:B:218:VAL:H	1.69	0.58
1:B:134:ILE:HD12	1:B:184:ILE:HD13	1.85	0.57
1:D:190:PRO:O	1:D:191:SER:O	2.21	0.57
1:D:203:VAL:CG1	1:D:204:ILE:H	2.16	0.57
1:B:32:LYS:HD2	3:B:326:HOH:O	2.03	0.57
1:C:32:LYS:HE2	3:C:316:HOH:O	2.04	0.56
1:C:12:LYS:HB2	1:C:14:TYR:OH	2.05	0.56
1:D:199:ASP:O	1:D:214:THR:HG23	2.04	0.56
1:C:199:ASP:HB3	1:C:246:GLU:OE2	2.04	0.56
1:C:127:LYS:HB3	1:C:127:LYS:HZ2	1.69	0.56
1:B:225:LEU:HG	1:B:242:PHE:HE1	1.70	0.56
1:D:101:GLY:C	1:D:121:GLU:HG3	2.26	0.56
1:C:203:VAL:HG11	1:C:208:PHE:HB2	1.87	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:196:GLU:O	1:D:218:VAL:HG21	2.07	0.55
1:B:188:VAL:HG13	1:B:188:VAL:O	2.06	0.55
1:A:205:GLU:HG3	1:C:186:ARG:NH1	2.22	0.55
1:B:204:ILE:O	1:B:209:MET:HG2	2.07	0.55
1:B:85:THR:HG23	3:B:276:HOH:O	2.06	0.55
1:C:131:ASP:OD2	1:C:133:LYS:HE2	2.07	0.55
1:A:205:GLU:HG3	1:C:186:ARG:HH11	1.72	0.55
1:A:210:ASN:N	1:A:210:ASN:HD22	2.05	0.54
1:D:44:ASP:C	1:D:45:GLU:HG2	2.26	0.54
1:C:171:PRO:HG2	1:D:234:ARG:NH2	2.21	0.54
1:B:197:LYS:CD	1:B:217:GLU:OE1	2.54	0.54
1:C:241:ASP:O	1:C:242:PHE:HB2	2.08	0.54
1:C:10:GLU:HG2	3:C:298:HOH:O	2.07	0.54
1:C:209:MET:O	1:C:210:ASN:HB2	2.08	0.54
1:A:80:LYS:HD2	1:A:123:LYS:CD	2.38	0.54
1:A:216:GLU:HB3	1:A:226:THR:O	2.08	0.54
1:A:210:ASN:OD1	1:C:178:GLN:HG2	2.08	0.53
1:D:198:GLY:H	1:D:215:VAL:HG13	1.74	0.53
1:A:131:ASP:O	1:A:132:ASN:HB2	2.06	0.53
1:B:216:GLU:HB2	1:B:226:THR:O	2.09	0.53
1:B:71:ASN:O	1:B:73:ARG:HD3	2.09	0.53
1:B:183:GLN:O	1:B:188:VAL:HG12	2.08	0.53
1:C:176:GLU:HA	1:C:176:GLU:OE1	2.09	0.53
1:A:205:GLU:HA	1:A:209:MET:HE2	1.89	0.53
1:D:203:VAL:CG1	1:D:204:ILE:N	2.72	0.52
1:A:69:LYS:HG2	3:A:272:HOH:O	2.08	0.52
1:A:222:LYS:HZ1	1:B:248:ILE:CG2	2.21	0.52
1:A:222:LYS:NZ	1:B:248:ILE:HA	2.24	0.52
1:C:180:ILE:O	1:C:184:ILE:HG13	2.10	0.52
1:A:54:VAL:HG21	1:A:88:ILE:HD11	1.92	0.52
1:B:189:LYS:HE2	1:B:189:LYS:HA	1.90	0.52
1:A:60:GLY:C	3:A:443:HOH:O	2.49	0.52
1:C:61:LYS:HB2	1:C:61:LYS:HZ2	1.73	0.52
1:C:195:PHE:CE2	1:C:225:LEU:HD23	2.45	0.52
1:D:155:LYS:HE3	2:D:860:IPA:H33	1.92	0.52
1:A:209:MET:HG2	1:A:210:ASN:HD22	1.75	0.51
1:B:229:ILE:CD1	1:B:238:VAL:HG21	2.40	0.51
1:B:85:THR:OG1	1:B:96:VAL:HG23	2.10	0.51
1:B:192:LYS:HB2	1:B:194:GLU:OE1	2.10	0.51
1:C:23:GLU:HG2	3:C:354:HOH:O	2.09	0.51
1:B:201:VAL:HA	1:B:248:ILE:HG12	1.93	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:225:LEU:O	1:C:225:LEU:HD12	2.11	0.51
1:B:59:GLN:NE2	3:B:306:HOH:O	2.44	0.51
1:A:210:ASN:HD21	1:C:178:GLN:HG2	1.76	0.51
1:D:133:LYS:NZ	1:D:133:LYS:HB2	2.27	0.50
1:D:209:MET:O	1:D:210:ASN:HB2	2.11	0.50
1:B:204:ILE:HG13	1:B:205:GLU:N	2.26	0.50
3:A:253:HOH:O	1:B:170:VAL:HG13	2.11	0.50
1:C:239:GLU:O	1:C:240:LEU:HD23	2.12	0.49
1:D:204:ILE:HD12	1:D:205:GLU:H	1.76	0.49
1:C:112:LYS:HD3	3:C:394:HOH:O	2.12	0.49
1:C:53:LYS:NZ	3:C:267:HOH:O	2.44	0.49
1:A:178:GLN:HA	1:A:178:GLN:OE1	2.12	0.49
1:B:187:GLY:O	1:B:189:LYS:N	2.45	0.49
1:C:225:LEU:HD13	1:C:227:VAL:CG2	2.43	0.49
1:C:195:PHE:CE1	1:C:242:PHE:CZ	3.01	0.49
1:A:164:MET:SD	1:A:169:PRO:HD3	2.52	0.49
1:A:96:VAL:HG21	3:A:476:HOH:O	2.12	0.49
1:C:39:LEU:HD21	1:C:148:LYS:HD3	1.95	0.49
1:C:195:PHE:CE2	1:C:225:LEU:HB3	2.40	0.49
1:D:204:ILE:HD12	1:D:205:GLU:N	2.26	0.49
1:C:94:LYS:HG2	3:C:416:HOH:O	2.12	0.49
1:D:191:SER:C	1:D:193:VAL:H	2.14	0.49
1:D:243:ASP:HB3	3:D:990:HOH:O	2.13	0.49
1:A:209:MET:O	1:A:210:ASN:CB	2.61	0.48
1:C:201:VAL:CB	1:C:244:GLN:HE21	2.22	0.48
1:C:132:ASN:HB3	3:C:388:HOH:O	2.13	0.48
1:C:127:LYS:CB	1:C:127:LYS:HZ2	2.22	0.48
1:B:194:GLU:CG	1:B:194:GLU:O	2.61	0.48
1:D:195:PHE:O	1:D:196:GLU:HB3	2.13	0.48
1:B:192:LYS:N	1:B:192:LYS:HD3	2.28	0.48
1:D:231:ILE:HB	1:D:234:ARG:HB2	1.95	0.48
1:D:242:PHE:O	1:D:243:ASP:CB	2.59	0.48
1:A:202:ARG:NH1	3:A:347:HOH:O	2.47	0.48
1:C:188:VAL:O	1:C:190:PRO:HD3	2.12	0.48
1:B:161:ARG:HB2	1:B:162:PRO:HD2	1.96	0.47
1:C:12:LYS:HB2	1:C:14:TYR:CE2	2.48	0.47
1:C:97:GLU:HG2	3:C:355:HOH:O	2.14	0.47
1:D:168:LYS:HG2	3:D:986:HOH:O	2.13	0.47
1:A:157:PRO:O	1:A:158:HIS:HB2	2.14	0.47
1:B:134:ILE:HA	1:B:190:PRO:HG3	1.95	0.47
1:B:225:LEU:HG	1:B:242:PHE:CE1	2.48	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:203:VAL:O	1:D:204:ILE:HG23	2.13	0.47
1:C:201:VAL:HG11	1:C:244:GLN:NE2	2.30	0.47
1:B:223:ARG:HA	1:B:242:PHE:CZ	2.49	0.47
1:B:200:GLN:O	1:B:248:ILE:HG12	2.15	0.47
1:D:69:LYS:NZ	3:D:934:HOH:O	2.47	0.47
1:A:161:ARG:HH11	1:A:161:ARG:HB3	1.80	0.47
1:B:59:GLN:HB2	1:B:123:LYS:HB3	1.96	0.47
1:B:61:LYS:HE2	3:B:440:HOH:O	2.15	0.47
1:B:108:PRO:HA	1:B:109:PRO:HD3	1.76	0.47
1:B:201:VAL:HG12	1:B:247:LYS:HA	1.97	0.47
1:B:68:LEU:HD11	1:B:91:GLY:O	2.15	0.47
1:A:170:VAL:CG1	1:B:234:ARG:HG2	2.45	0.46
1:C:228:MET:HE1	1:C:237:PRO:HA	1.97	0.46
1:D:225:LEU:O	1:D:239:GLU:HA	2.15	0.46
1:B:74:ASP:O	1:B:75:ILE:HD13	2.15	0.46
1:D:213:GLY:HA3	1:D:229:ILE:HA	1.98	0.46
1:C:236:THR:HA	1:C:237:PRO:HD3	1.73	0.46
1:D:191:SER:C	1:D:193:VAL:N	2.69	0.46
1:B:134:ILE:HD13	1:B:188:VAL:HG13	1.98	0.46
1:B:183:GLN:NE2	1:B:188:VAL:HG11	2.31	0.46
1:B:58:ALA:O	1:B:59:GLN:C	2.54	0.46
1:B:222:LYS:O	1:B:224:LYS:HG3	2.15	0.46
1:B:59:GLN:HA	1:B:59:GLN:OE1	2.16	0.46
1:D:15:ALA:HB2	1:D:172:LEU:HD11	1.97	0.46
1:C:132:ASN:N	1:C:132:ASN:ND2	2.61	0.46
1:C:56:ILE:N	1:C:56:ILE:CD1	2.78	0.46
1:D:61:LYS:N	1:D:61:LYS:HD3	2.30	0.46
3:A:253:HOH:O	1:B:163:VAL:HB	2.16	0.45
1:A:173:LYS:HZ3	1:A:173:LYS:HB2	1.81	0.45
1:A:6:VAL:O	1:A:6:VAL:HG23	2.17	0.45
1:B:112:LYS:O	1:B:113:PRO:C	2.55	0.45
1:C:224:LYS:CG	1:C:241:ASP:OD2	2.64	0.45
1:D:213:GLY:HA3	1:D:228:MET:O	2.17	0.45
1:C:50:ALA:HB1	1:C:131:ASP:O	2.16	0.45
1:D:197:LYS:HZ3	1:D:198:GLY:CA	2.30	0.45
1:B:134:ILE:HD13	1:B:188:VAL:CG1	2.47	0.45
1:B:117:ILE:O	1:B:125:GLU:HB2	2.17	0.45
1:B:186:ARG:HD2	3:B:385:HOH:O	2.16	0.45
1:B:185:LYS:HG3	3:B:394:HOH:O	2.16	0.45
1:C:160:PHE:O	1:C:161:ARG:HB3	2.16	0.45
1:B:134:ILE:HG12	1:B:190:PRO:HD3	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:224:LYS:CB	1:D:241:ASP:HA	2.31	0.45
1:B:188:VAL:O	1:B:190:PRO:CD	2.64	0.44
1:B:217:GLU:CG	1:B:218:VAL:N	2.80	0.44
1:D:168:LYS:NZ	3:D:1043:HOH:O	2.38	0.44
1:D:59:GLN:O	1:D:61:LYS:HD3	2.17	0.44
1:B:217:GLU:HG3	1:B:219:HIS:H	1.82	0.44
1:C:238:VAL:HG12	1:C:239:GLU:N	2.31	0.44
1:D:185:LYS:HE2	3:D:1068:HOH:O	2.16	0.44
1:B:24:ASN:HB2	1:B:130:LEU:HD12	1.99	0.44
1:B:173:LYS:HE3	3:B:349:HOH:O	2.17	0.44
1:D:219:HIS:CE1	1:D:223:ARG:HG3	2.52	0.44
1:B:218:VAL:O	1:B:219:HIS:HB2	2.18	0.44
1:C:183:GLN:HA	1:C:186:ARG:HH21	1.83	0.44
1:A:173:LYS:NZ	1:A:173:LYS:CB	2.74	0.44
1:C:203:VAL:HG22	1:C:240:LEU:CD1	2.47	0.44
1:C:176:GLU:HG2	1:D:233:GLY:HA3	1.99	0.44
1:C:54:VAL:HG12	1:C:56:ILE:CD1	2.48	0.44
1:B:195:PHE:H	1:B:247:LYS:HD2	1.83	0.43
1:C:52:GLU:HG2	1:C:130:LEU:HD21	1.99	0.43
1:C:88:ILE:HG12	1:C:93:VAL:HG22	2.00	0.43
1:B:55:VAL:HG13	1:B:62:GLU:HG3	2.01	0.43
1:B:48:VAL:HG11	1:B:130:LEU:HD13	2.00	0.43
1:C:223:ARG:NH1	1:C:223:ARG:HG2	2.29	0.43
1:B:57:ARG:HG3	1:B:125:GLU:HG3	2.00	0.43
1:B:15:ALA:HB2	1:B:172:LEU:HD11	2.01	0.43
1:C:74:ASP:C	1:C:75:ILE:HD12	2.39	0.43
1:D:11:LYS:HD3	1:D:143:ALA:HA	2.01	0.43
1:A:189:LYS:HE2	3:A:457:HOH:O	2.19	0.43
1:B:22:LYS:HA	1:B:25:GLU:OE1	2.19	0.43
1:B:238:VAL:CG1	1:B:240:LEU:HG	2.45	0.43
1:A:71:ASN:ND2	1:C:87:ARG:HH12	2.13	0.43
1:A:210:ASN:ND2	1:C:178:GLN:HG2	2.34	0.43
1:A:205:GLU:HA	1:A:209:MET:CE	2.48	0.42
1:A:224:LYS:NZ	1:A:241:ASP:OD2	2.46	0.42
1:C:153:ILE:HG23	1:C:159:VAL:HG11	2.01	0.42
1:B:204:ILE:HG13	1:B:205:GLU:H	1.84	0.42
1:C:11:LYS:NZ	3:C:350:HOH:O	2.49	0.42
1:D:101:GLY:HA3	1:D:121:GLU:HG3	2.00	0.42
1:D:8:GLU:HG3	1:D:8:GLU:O	2.18	0.42
1:A:131:ASP:OD2	1:A:133:LYS:HG3	2.19	0.42
1:B:53:LYS:HD2	1:B:131:ASP:HB2	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:242:PHE:CD1	1:C:242:PHE:N	2.87	0.42
1:C:155:LYS:NZ	1:C:155:LYS:CB	2.83	0.42
1:D:218:VAL:HG13	1:D:242:PHE:CZ	2.55	0.42
1:B:110:ILE:HD12	1:B:128:ILE:HG12	2.01	0.42
1:D:197:LYS:HZ2	1:D:197:LYS:C	2.24	0.42
1:C:172:LEU:HA	1:D:234:ARG:HG2	2.02	0.41
1:A:71:ASN:HD21	1:C:87:ARG:NH1	2.15	0.41
1:A:190:PRO:HA	1:C:89:GLU:OE1	2.20	0.41
1:B:168:LYS:NZ	3:B:435:HOH:O	2.37	0.41
1:C:11:LYS:HD2	1:C:44:ASP:OD2	2.21	0.41
1:D:224:LYS:HB2	1:D:225:LEU:H	1.42	0.41
1:A:205:GLU:OE1	1:A:244:GLN:HG2	2.21	0.41
1:B:202:ARG:HG3	1:B:212:THR:CG2	2.50	0.41
1:B:30:LEU:O	1:B:34:LEU:HG	2.21	0.41
1:B:157:PRO:O	1:B:158:HIS:HB2	2.21	0.41
1:B:195:PHE:CE1	1:B:245:VAL:HG23	2.56	0.41
1:C:108:PRO:HA	1:C:109:PRO:HD3	1.91	0.41
1:D:108:PRO:HA	1:D:109:PRO:HD3	1.83	0.41
1:C:123:LYS:HD3	1:C:123:LYS:HA	1.87	0.41
1:A:132:ASN:HA	3:A:359:HOH:O	2.21	0.41
1:A:232:PHE:N	1:B:176:GLU:OE2	2.54	0.41
1:C:208:PHE:CE2	1:C:238:VAL:HG21	2.56	0.41
1:D:101:GLY:CA	1:D:121:GLU:HG3	2.51	0.41
1:D:237:PRO:O	1:D:238:VAL:HG23	2.20	0.41
1:A:112:LYS:O	1:A:113:PRO:C	2.59	0.41
1:B:228:MET:HE3	1:B:237:PRO:HG3	2.02	0.41
1:C:155:LYS:NZ	1:C:155:LYS:HB2	2.36	0.40
1:C:223:ARG:C	1:C:224:LYS:HG3	2.42	0.40
1:B:166:GLY:HA2	3:B:396:HOH:O	2.20	0.40
1:A:223:ARG:HB3	3:A:484:HOH:O	2.20	0.40
1:D:58:ALA:O	1:D:61:LYS:HD3	2.20	0.40
1:A:108:PRO:HA	1:A:109:PRO:HD3	1.85	0.40
1:B:85:THR:CG2	3:B:276:HOH:O	2.68	0.40
1:C:208:PHE:HD2	1:C:229:ILE:CD1	2.35	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	242/248 (98%)	233 (96%)	9 (4%)	0	100	100
1	B	239/248 (96%)	220 (92%)	12 (5%)	7 (3%)	4	1
1	C	236/248 (95%)	216 (92%)	16 (7%)	4 (2%)	9	4
1	D	238/248 (96%)	212 (89%)	15 (6%)	11 (5%)	2	0
All	All	955/992 (96%)	881 (92%)	52 (5%)	22 (2%)	6	2

All (22) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	188	VAL
1	B	223	ARG
1	D	194	GLU
1	D	195	PHE
1	D	220	PRO
1	D	224	LYS
1	D	243	ASP
1	B	59	GLN
1	B	221	GLU
1	C	187	GLY
1	C	195	PHE
1	D	204	ILE
1	C	192	LYS
1	D	191	SER
1	D	197	LYS
1	B	193	VAL
1	B	222	LYS
1	C	188	VAL
1	B	219	HIS
1	D	196	GLU
1	D	218	VAL
1	D	189	LYS

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	218/222 (98%)	209 (96%)	9 (4%)	30	28
1	B	215/222 (97%)	205 (95%)	10 (5%)	26	22
1	C	212/222 (96%)	198 (93%)	14 (7%)	16	12
1	D	214/222 (96%)	202 (94%)	12 (6%)	21	17
All	All	859/888 (97%)	814 (95%)	45 (5%)	23	19

All (45) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	54	VAL
1	A	66	LEU
1	A	149	LEU
1	A	161	ARG
1	A	169	PRO
1	A	173	LYS
1	A	210	ASN
1	A	227	VAL
1	A	243	ASP
1	B	57	ARG
1	B	105	VAL
1	B	149	LEU
1	B	192	LYS
1	B	193	VAL
1	B	199	ASP
1	B	205	GLU
1	B	223	ARG
1	B	241	ASP
1	B	246	GLU
1	C	37	GLU
1	C	56	ILE
1	C	132	ASN
1	C	149	LEU
1	C	150	LEU

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Mol	Chain	Res	Type
1	C	178	GLN
1	C	195	PHE
1	C	211	PHE
1	C	221	GLU
1	C	225	LEU
1	C	241	ASP
1	C	242	PHE
1	C	243	ASP
1	C	244	GLN
1	D	7	GLN
1	D	8	GLU
1	D	30	LEU
1	D	36	LEU
1	D	61	LYS
1	D	105	VAL
1	D	149	LEU
1	D	151	MET
1	D	196	GLU
1	D	224	LYS
1	D	240	LEU
1	D	241	ASP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (13) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	7	GLN
1	A	71	ASN
1	A	132	ASN
1	A	210	ASN
1	B	183	GLN
1	C	29	ASN
1	C	106	ASN
1	C	132	ASN
1	C	178	GLN
1	C	244	GLN
1	D	24	ASN
1	D	90	ASN
1	D	219	HIS

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry ⓘ

2 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
2	IPA	D	860	-	3,3,3	0.64	0	3,3,3	0.82	0
2	IPA	D	859	-	3,3,3	0.48	0	3,3,3	0.89	0

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	D	860	IPA	1	0

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, 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	244/248 (98%)	-0.01	3 (1%) 79 78	21, 38, 65, 82	0
1	B	241/248 (97%)	0.66	35 (14%) 2 2	18, 38, 93, 99	2 (0%)
1	C	238/248 (95%)	0.58	32 (13%) 3 2	22, 42, 89, 97	2 (0%)
1	D	240/248 (96%)	0.51	33 (13%) 2 2	19, 33, 91, 100	9 (3%)
All	All	963/992 (97%)	0.43	103 (10%) 6 5	18, 38, 89, 100	13 (1%)

All (103) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	245	VAL	8.6
1	B	220	PRO	8.6
1	D	195	PHE	8.5
1	D	190	PRO	8.4
1	B	190	PRO	8.3
1	B	219	HIS	8.1
1	B	193	VAL	8.1
1	C	195	PHE	7.7
1	B	195	PHE	7.4
1	C	192	LYS	7.2
1	B	248	ILE	7.2
1	B	203	VAL	7.1
1	C	220	PRO	7.0
1	D	219	HIS	6.9
1	B	221	GLU	6.9
1	C	215	VAL	6.8
1	D	198	GLY	6.8
1	C	193	VAL	6.7
1	B	199	ASP	6.6
1	D	222	LYS	6.5
1	B	192	LYS	6.3

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Mol	Chain	Res	Type	RSRZ
1	D	225	LEU	6.2
1	D	191	SER	5.9
1	B	191	SER	5.8
1	D	193	VAL	5.8
1	D	223	ARG	5.7
1	C	190	PRO	5.5
1	D	6	VAL	5.4
1	B	246	GLU	5.1
1	D	221	GLU	5.1
1	B	188	VAL	5.0
1	D	220	PRO	5.0
1	B	218	VAL	4.9
1	B	60	GLY	4.9
1	C	206	GLY	4.7
1	D	192	LYS	4.6
1	D	200	GLN	4.5
1	C	222	LYS	4.4
1	B	198	GLY	4.3
1	D	188	VAL	4.3
1	D	194	GLU	4.3
1	D	204	ILE	4.3
1	B	215	VAL	4.2
1	C	191	SER	4.1
1	C	241	ASP	4.1
1	C	245	VAL	4.1
1	C	225	LEU	4.0
1	D	215	VAL	3.9
1	C	208	PHE	3.9
1	D	224	LYS	3.8
1	B	217	GLU	3.7
1	B	247	LYS	3.6
1	C	188	VAL	3.6
1	B	226	THR	3.5
1	D	242	PHE	3.4
1	D	203	VAL	3.4
1	C	199	ASP	3.3
1	B	222	LYS	3.3
1	D	217	GLU	3.3
1	D	240	LEU	3.3
1	B	189	LYS	3.2
1	C	240	LEU	3.2
1	B	207	PRO	3.2

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Mol	Chain	Res	Type	RSRZ
1	D	7	GLN	3.2
1	D	214	THR	3.2
1	B	205	GLU	3.1
1	C	204	ILE	3.0
1	B	243	ASP	3.0
1	D	199	ASP	3.0
1	B	242	PHE	2.9
1	C	194	GLU	2.9
1	C	239	GLU	2.9
1	B	224	LYS	2.9
1	C	218	VAL	2.8
1	C	205	GLU	2.7
1	D	243	ASP	2.7
1	B	240	LEU	2.6
1	C	243	ASP	2.6
1	B	194	GLU	2.6
1	B	245	VAL	2.6
1	C	242	PHE	2.6
1	C	223	ARG	2.5
1	D	241	ASP	2.5
1	D	138	TYR	2.5
1	C	219	HIS	2.5
1	C	244	GLN	2.5
1	A	193	VAL	2.5
1	C	198	GLY	2.4
1	B	223	ARG	2.4
1	B	241	ASP	2.3
1	C	207	PRO	2.3
1	A	131	ASP	2.3
1	B	59	GLN	2.2
1	D	201	VAL	2.2
1	D	218	VAL	2.2
1	C	226	THR	2.2
1	B	244	GLN	2.1
1	B	204	ILE	2.1
1	C	196	GLU	2.0
1	C	197	LYS	2.0
1	C	134	ILE	2.0
1	A	60	GLY	2.0
1	D	197	LYS	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 carbohydrates in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
2	IPA	D	860	4/4	0.69	0.20	41,45,48,56	0
2	IPA	D	859	4/4	0.91	0.23	51,52,52,55	0

6.5 Other polymers [i](#)

There are no such residues in this entry.