Full wwPDB X-ray Structure Validation Report (i)

Jan 31, 2016 – 09:09 PM GMT

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
http://wwpdb.org/validation/2016/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The following versions of software and data (see references (1)) were used in the production of this report:

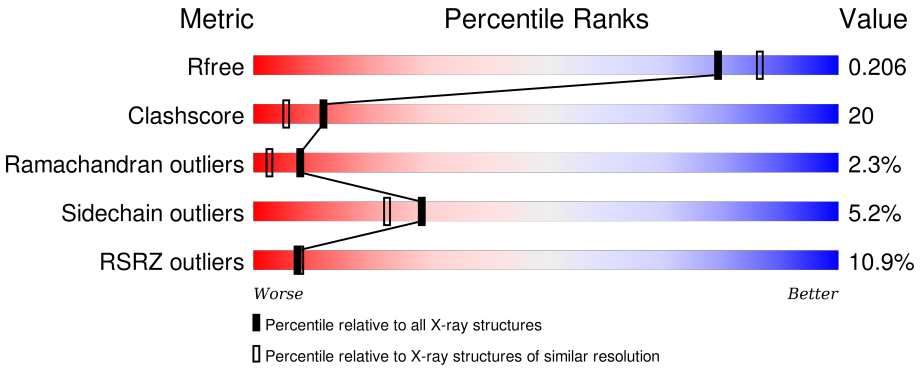
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	trunk26865

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 2.00 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}	91344	6249 (2.00-2.00)
Clashscore	102246	7340 (2.00-2.00)
Ramachandran outliers	100387	7248 (2.00-2.00)
Sidechain outliers	100360	7247 (2.00-2.00)
RSRZ outliers	91569	6262 (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. 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	248	% 80% 16%
1	B	248	15% 56% 37%
1	C	248	13% 61% 30%
1	D	248	14% 71% 21%

2 Entry composition

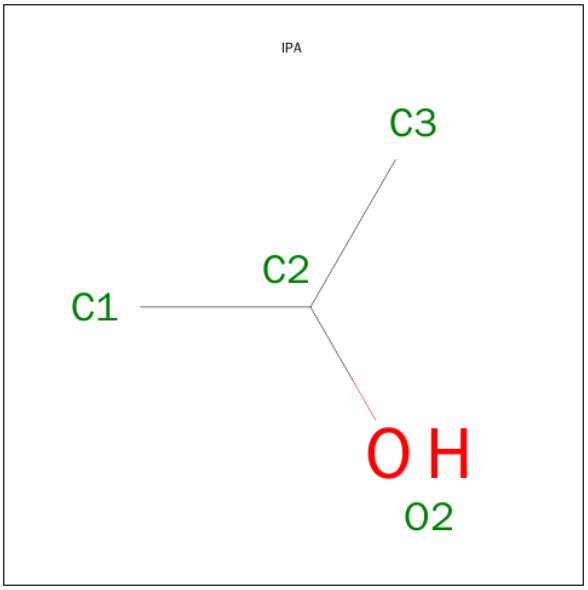
There are 3 unique types of molecules in this entry. The entry contains 8486 atoms, of which 0 are hydrogens and 0 are deuteriums.

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: C_3H_8O).



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.

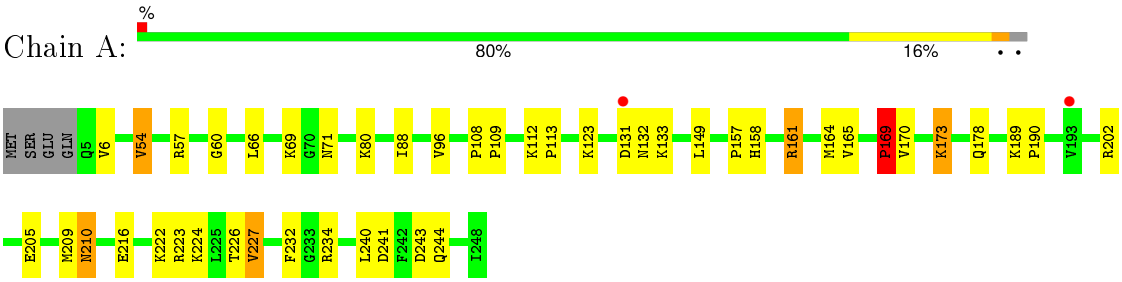
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	237	Total O 237 237	0	0
3	B	199	Total O 199 199	0	0
3	C	181	Total O 181 181	0	0
3	D	241	Total O 241 241	0	0

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 errors 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.

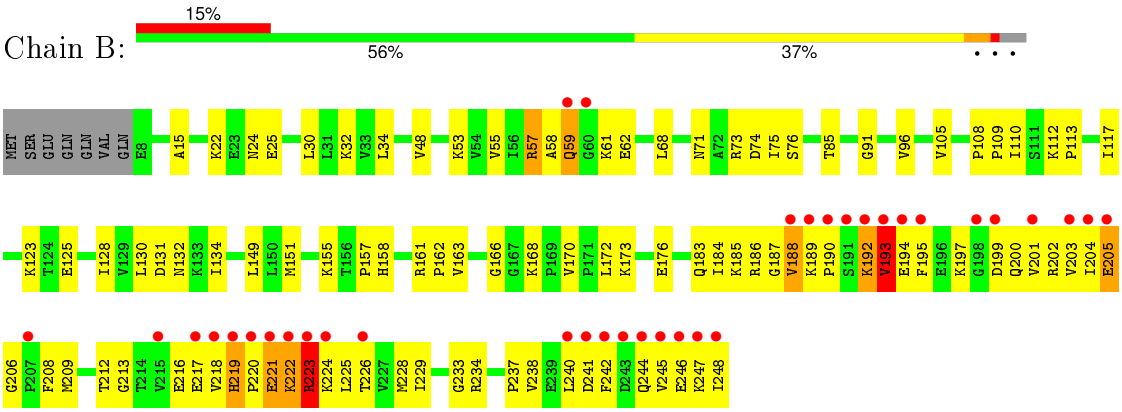
- Molecule 1: Transcription antitermination protein nusG

Chain A:



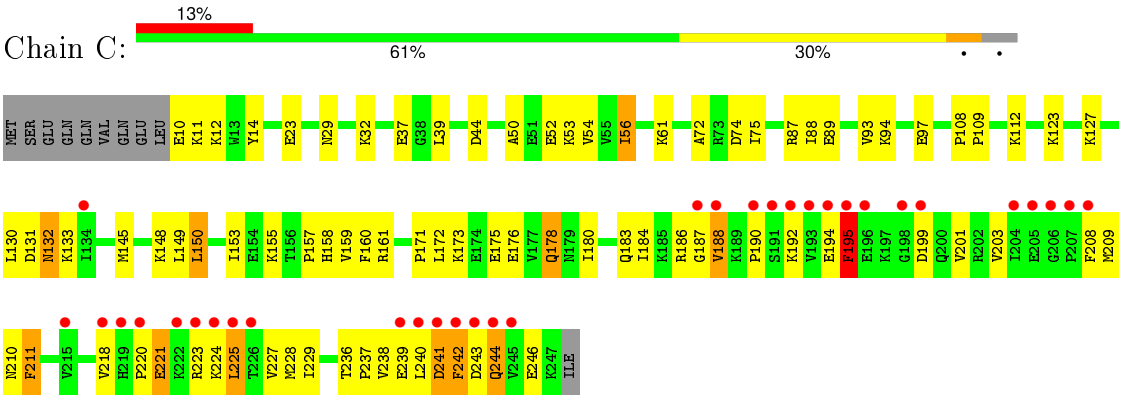
- Molecule 1: Transcription antitermination protein nusG

Chain B:



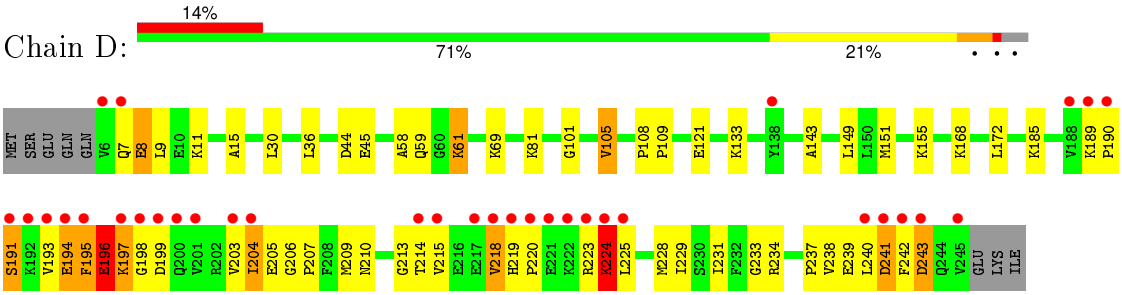
- Molecule 1: Transcription antitermination protein nusG

Chain C:



- Molecule 1: Transcription antitermination protein nusG

Chain D:


14%
71%
21%
MET SER GLU GLN GLN V6 Q7 E8 L9 E10 K11 A15 L30 L36 D44 E45 A58 Q59 G60 K61 K69 K81 G101 V105 P108 P109 E121 K133 Y138 A143 L149 L150 M151 K155 K168 L172 K185 V188 K189 P190
S191 K192 V193 E194 F195 E196 K197 G198 D199 Q200 V201 R202 V203 I204 E205 G206 P207 F208 M209 N210 G213 T214 V215 E216 E217 V218 H219 P220 E221 K222 R223 K224 L225 M228 I229 S230 I231 F232 G233 R234 P237 V238 E239 L240 D241 F242 D243 Q244 V245 GLU LYS ILE

4 Data and refinement statistics (i)

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
$< I/\sigma(I) >$ [1]	0.87 (at 1.92Å)	Xtriage
Refinement program	CNS 1.0	Depositor
R, R_{free}	0.219 , 0.279 0.206 , 0.206	Depositor DCC
R_{free} test set	2877 reflections (5.14%)	DCC
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
Estimated twinning fraction	0.029 for h,-k,-l	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Outliers	0 of 79949 reflections	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.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

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(^{o})	Ideal(^{o})
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

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:C:127:LYS:NZ	1:C:127:LYS:HB3	1.86	0.90
1:A:57:ARG:HD3	3:A:443:HOH:O	1.70	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: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:C:132:ASN:HD22	1:C:132:ASN:H	1.32	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:B:188:VAL:O	1:B:190:PRO:HD3	1.92	0.69
1:A:165:VAL:HG23	1:A:170:VAL:HG21	1.73	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:C:132:ASN:HD22	1:C:132:ASN:N	1.91	0.67
1:A:80:LYS:HD2	1:A:123:LYS:HD3	1.76	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:224:LYS:HG2	1:C:241:ASP:CG	2.16	0.66
1:C:145:MET:SD	1:C:150:LEU:HD13	2.35	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:D:196:GLU:HB2	1:D:199:ASP:OD2	1.99	0.63
1:C:195:PHE:O	1:C:218:VAL:HG11	1.98	0.63
1:C:175:GLU:HG2	3:C:325:HOH:O	1.98	0.63
1:B:183:GLN:HE21	1:B:188:VAL:HG11	1.63	0.63
1:A:173:LYS:NZ	1:B:233:GLY:C	2.52	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:194:GLU:O	1:C:195:PHE:HB3	2.03	0.58
1:C:157:PRO:O	1:C:158:HIS:HB2	2.02	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:B:217:GLU:HG3	1:B:218:VAL:H	1.69	0.58
1:A:6:VAL:HG22	3:A:473:HOH:O	2.04	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:D:199:ASP:O	1:D:214:THR:HG23	2.04	0.56
1:C:12:LYS:HB2	1:C:14:TYR:OH	2.05	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:209:MET:O	1:C:210:ASN:HB2	2.08	0.54
1:C:10:GLU:HG2	3:C:298:HOH:O	2.07	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:71:ASN:O	1:B:73:ARG:HD3	2.09	0.53
1:B:216:GLU:HB2	1:B:226:THR:O	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:B:189:LYS:HE2	1:B:189:LYS:HA	1.90	0.52
1:A:54:VAL:HG21	1:A:88:ILE:HD11	1.92	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:C:225:LEU:O	1:C:225:LEU:HD12	2.11	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:201:VAL:HA	1:B:248:ILE:HG12	1.93	0.51
1:A:210:ASN:HD21	1:C:178:GLN:HG2	1.76	0.51
1:B:59:GLN:NE2	3:B:306:HOH:O	2.44	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:D:204:ILE:HD12	1:D:205:GLU:H	1.76	0.49
1:C:239:GLU:O	1:C:240:LEU:HD23	2.12	0.49
1:C:53:LYS:NZ	3:C:267:HOH:O	2.44	0.49
1:C:112:LYS:HD3	3:C:394:HOH:O	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:A:178:GLN:OE1	1:A:178:GLN:HA	2.12	0.49
1:C:195:PHE:CE1	1:C:242:PHE:CZ	3.01	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:39:LEU:HD21	1:C:148:LYS:HD3	1.95	0.49
1:A:96:VAL:HG21	3:A:476:HOH:O	2.12	0.49
1:A:164:MET:SD	1:A:169:PRO:HD3	2.52	0.49
1:D:191:SER:C	1:D:193:VAL:H	2.14	0.49
1:C:94:LYS:HG2	3:C:416:HOH:O	2.12	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:D:195:PHE:O	1:D:196:GLU:HB3	2.13	0.48
1:B:194:GLU:CG	1:B:194:GLU:O	2.61	0.48
1:D:242:PHE:O	1:D:243:ASP:CB	2.59	0.48
1:D:231:ILE:HB	1:D:234:ARG:HB2	1.95	0.48
1:B:192:LYS:N	1:B:192:LYS:HD3	2.28	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:C:12:LYS:HB2	1:C:14:TYR:CE2	2.48	0.47
1:D:168:LYS:HG2	3:D:986:HOH:O	2.13	0.47
1:C:97:GLU:HG2	3:C:355:HOH:O	2.14	0.47
1:B:161:ARG:HB2	1:B:162:PRO:HD2	1.96	0.47
1:B:134:ILE:HA	1:B:190:PRO:HG3	1.95	0.47
1:A:157:PRO:O	1:A:158:HIS:HB2	2.14	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:200:GLN:O	1:B:248:ILE:HG12	2.15	0.47
1:B:223:ARG:HA	1:B:242:PHE:CZ	2.49	0.47
1:D:69:LYS:NZ	3:D:934:HOH:O	2.47	0.47
1:B:59:GLN:HB2	1:B:123:LYS:HB3	1.96	0.47
1:A:161:ARG:HH11	1:A:161:ARG:HB3	1.80	0.47
1:B:61:LYS:HE2	3:B:440:HOH:O	2.15	0.47
1:B:201:VAL:HG12	1:B:247:LYS:HA	1.97	0.47
1:B:108:PRO:HA	1:B:109:PRO:HD3	1.76	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:D:225:LEU:O	1:D:239:GLU:HA	2.15	0.46
1:C:228:MET:HE1	1:C:237:PRO:HA	1.97	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:D:191:SER:C	1:D:193:VAL:N	2.69	0.46
1:C:236:THR:HA	1:C:237:PRO:HD3	1.73	0.46
1:B:183:GLN:NE2	1:B:188:VAL:HG11	2.31	0.46
1:B:134:ILE:HD13	1:B:188:VAL:HG13	1.98	0.46
1:B:58:ALA:O	1:B:59:GLN:C	2.54	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:B:222:LYS:O	1:B:224:LYS:HG3	2.15	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:C:224:LYS:CG	1:C:241:ASP:OD2	2.64	0.45
1:A:6:VAL:O	1:A:6:VAL:HG23	2.17	0.45
1:D:213:GLY:HA3	1:D:228:MET:O	2.17	0.45
1:B:112:LYS:O	1:B:113:PRO:C	2.55	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:186:ARG:HD2	3:B:385:HOH:O	2.16	0.45
1:B:117:ILE:O	1:B:125:GLU:HB2	2.17	0.45
1:C:160:PHE:O	1:C:161:ARG:HB3	2.16	0.45
1:B:185:LYS:HG3	3:B:394:HOH:O	2.16	0.45
1:D:224:LYS:CB	1:D:241:ASP:HA	2.31	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:134:ILE:HG12	1:B:190:PRO:HD3	1.99	0.45
1:B:217:GLU:CG	1:B:218:VAL:N	2.80	0.44
1:B:188:VAL:O	1:B:190:PRO:CD	2.64	0.44
1:D:59:GLN:O	1:D:61:LYS:HD3	2.17	0.44
1:D:168:LYS:NZ	3:D:1043:HOH:O	2.38	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:C:203:VAL:HG22	1:C:240:LEU:CD1	2.47	0.44
1:A:173:LYS:NZ	1:A:173:LYS:CB	2.74	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:C:223:ARG:NH1	1:C:223:ARG:HG2	2.29	0.43
1:B:48:VAL:HG11	1:B:130:LEU:HD13	2.00	0.43
1:B:57:ARG:HG3	1:B:125:GLU:HG3	2.00	0.43
1:C:74:ASP:C	1:C:75:ILE:HD12	2.39	0.43
1:B:15:ALA:HB2	1:B:172:LEU:HD11	2.01	0.43
1:D:11:LYS:HD3	1:D:143:ALA:HA	2.01	0.43
1:B:238:VAL:CG1	1:B:240:LEU:HG	2.45	0.43
1:B:22:LYS:HA	1:B:25:GLU:OE1	2.19	0.43
1:A:189:LYS:HE2	3:A:457:HOH:O	2.19	0.43
1:A:210:ASN:ND2	1:C:178:GLN:HG2	2.34	0.43
1:A:71:ASN:ND2	1:C:87:ARG:HH12	2.13	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: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:C:11:LYS:NZ	3:C:350:HOH:O	2.49	0.42
1:C:242:PHE:CD1	1:C:242:PHE:N	2.87	0.42
1:A:131:ASP:OD2	1:A:133:LYS:HG3	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:53:LYS:HD2	1:B:131:ASP:HB2	2.01	0.42
1:D:218:VAL:HG13	1:D:242:PHE:CZ	2.55	0.42
1:C:155:LYS:NZ	1:C:155:LYS:CB	2.83	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:190:PRO:HA	1:C:89:GLU:OE1	2.20	0.41
1:A:71:ASN:HD21	1:C:87:ARG:NH1	2.15	0.41
1:C:11:LYS:HD2	1:C:44:ASP:OD2	2.21	0.41
1:B:168:LYS:NZ	3:B:435:HOH:O	2.37	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:195:PHE:CE1	1:B:245:VAL:HG23	2.56	0.41
1:B:157:PRO:O	1:B:158:HIS:HB2	2.21	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: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:A:132:ASN:HA	3:A:359:HOH:O	2.21	0.41
1:C:123:LYS:HD3	1:C:123:LYS:HA	1.87	0.41
1:A:232:PHE:N	1:B:176:GLU:OE2	2.54	0.41
1:D:237:PRO:O	1:D:238:VAL:HG23	2.20	0.41
1:B:228:MET:HE3	1:B:237:PRO:HG3	2.02	0.41
1:A:112:LYS:O	1:A:113:PRO:C	2.59	0.41
1:C:223:ARG:C	1:C:224:LYS:HG3	2.42	0.40
1:C:155:LYS:NZ	1:C:155:LYS:HB2	2.36	0.40
1:B:166:GLY:HA2	3:B:396:HOH:O	2.20	0.40
1:D:58:ALA:O	1:D:61:LYS:HD3	2.20	0.40
1:A:223:ARG:HB3	3:A:484:HOH:O	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 (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	242/248 (98%)	233 (96%)	9 (4%)	0	100 100
1	B	239/248 (96%)	220 (92%)	12 (5%)	7 (3%)	6 2
1	C	236/248 (95%)	216 (92%)	16 (7%)	4 (2%)	11 4
1	D	238/248 (96%)	212 (89%)	15 (6%)	11 (5%)	3 1
All	All	955/992 (96%)	881 (92%)	52 (5%)	22 (2%)	8 3

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 (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	218/222 (98%)	209 (96%)	9 (4%)	37	32
1	B	215/222 (97%)	205 (95%)	10 (5%)	32	27
1	C	212/222 (96%)	198 (93%)	14 (7%)	21	14
1	D	214/222 (96%)	202 (94%)	12 (6%)	26	20
All	All	859/888 (97%)	814 (95%)	45 (5%)	29	23

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	859	-	3,3,3	0.48	0	3,3,3	0.84	0
2	IPA	D	860	-	3,3,3	0.64	0	3,3,3	0.77	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the chemical component dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	IPA	D	859	-	-	0/0/0/0	0/0/0/0
2	IPA	D	860	-	-	0/0/0/0	0/0/0/0

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, 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	244/248 (98%)	0.03	2 (0%) 87 88	21, 38, 65, 82	0
1	B	241/248 (97%)	0.74	36 (14%) 3 3	18, 38, 93, 99	2 (0%)
1	C	238/248 (95%)	0.65	33 (13%) 4 4	22, 42, 89, 97	2 (0%)
1	D	240/248 (96%)	0.60	34 (14%) 4 4	19, 33, 91, 100	9 (3%)
All	All	963/992 (97%)	0.50	105 (10%) 7 8	18, 38, 89, 100	13 (1%)

All (105) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	245	VAL	9.3
1	B	193	VAL	9.3
1	D	195	PHE	9.2
1	B	220	PRO	9.1
1	D	190	PRO	9.0
1	C	195	PHE	8.6
1	B	190	PRO	8.4
1	B	219	HIS	8.3
1	B	248	ILE	7.8
1	D	219	HIS	7.8
1	B	203	VAL	7.7
1	B	195	PHE	7.5
1	B	221	GLU	7.5
1	C	192	LYS	7.5
1	D	198	GLY	7.4
1	C	220	PRO	7.3
1	C	193	VAL	7.1
1	C	215	VAL	6.9
1	B	199	ASP	6.5
1	B	192	LYS	6.4
1	D	225	LEU	6.4

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Mol	Chain	Res	Type	RSRZ
1	D	222	LYS	6.3
1	B	191	SER	6.3
1	C	190	PRO	6.1
1	D	6	VAL	6.1
1	D	191	SER	6.0
1	D	223	ARG	6.0
1	D	193	VAL	5.9
1	B	246	GLU	5.6
1	B	60	GLY	5.5
1	B	218	VAL	5.5
1	D	220	PRO	5.4
1	D	221	GLU	5.2
1	D	192	LYS	5.0
1	B	198	GLY	4.9
1	C	222	LYS	4.9
1	D	188	VAL	4.9
1	D	194	GLU	4.9
1	B	188	VAL	4.8
1	D	204	ILE	4.7
1	D	200	GLN	4.7
1	C	191	SER	4.6
1	C	206	GLY	4.5
1	C	241	ASP	4.5
1	B	215	VAL	4.3
1	C	225	LEU	4.2
1	D	215	VAL	4.2
1	C	245	VAL	4.1
1	C	208	PHE	4.0
1	D	224	LYS	4.0
1	B	226	THR	3.9
1	D	203	VAL	3.9
1	C	188	VAL	3.8
1	B	217	GLU	3.8
1	C	199	ASP	3.7
1	B	247	LYS	3.6
1	B	207	PRO	3.6
1	B	242	PHE	3.5
1	D	242	PHE	3.5
1	D	214	THR	3.4
1	D	217	GLU	3.4
1	C	240	LEU	3.3
1	B	222	LYS	3.3

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Mol	Chain	Res	Type	RSRZ
1	D	7	GLN	3.3
1	B	189	LYS	3.3
1	D	240	LEU	3.3
1	C	204	ILE	3.2
1	D	199	ASP	3.1
1	B	205	GLU	3.1
1	B	243	ASP	3.1
1	C	194	GLU	3.1
1	B	224	LYS	3.1
1	C	239	GLU	2.9
1	C	205	GLU	2.9
1	B	194	GLU	2.8
1	C	218	VAL	2.8
1	B	240	LEU	2.8
1	D	243	ASP	2.7
1	D	201	VAL	2.7
1	C	223	ARG	2.7
1	B	245	VAL	2.7
1	C	243	ASP	2.6
1	C	198	GLY	2.6
1	D	138	TYR	2.6
1	C	219	HIS	2.6
1	C	244	GLN	2.5
1	D	218	VAL	2.5
1	B	241	ASP	2.5
1	C	134	ILE	2.5
1	A	131	ASP	2.4
1	B	223	ARG	2.4
1	C	242	PHE	2.4
1	D	241	ASP	2.4
1	C	196	GLU	2.3
1	C	226	THR	2.3
1	B	204	ILE	2.3
1	B	59	GLN	2.3
1	C	207	PRO	2.3
1	A	193	VAL	2.2
1	C	187	GLY	2.1
1	B	244	GLN	2.1
1	D	189	LYS	2.1
1	B	201	VAL	2.1
1	D	197	LYS	2.0
1	C	224	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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95^{th} 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	LLDF	B-factors(Å^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	0.22	-	51,52,52,55	0

6.5 Other polymers (i)

There are no such residues in this entry.