Full wwPDB X-ray Structure Validation Report (i)

Feb 1, 2016 – 09:06 AM GMT

PDB ID	:	3H5V
Title	:	Crystal structure of the GluR2-ATD
Authors	:	Jin, R.; Singh, S.K.; Gu, S.; Furukawa, H.; Sobolevsky, A.; Zhou, J.; Jin, Y.; Gouaux, E.
Deposited on	:	2009-04-22
Resolution	:	2.33 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:

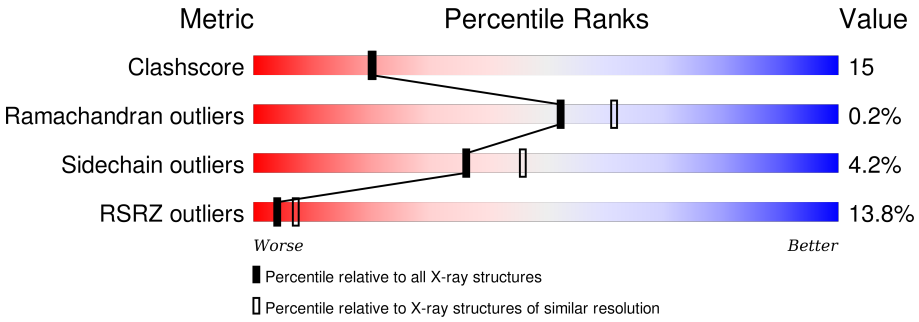
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	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 2.33 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))
Clashscore	102246	1509 (2.36-2.32)
Ramachandran outliers	100387	1490 (2.36-2.32)
Sidechain outliers	100360	1491 (2.36-2.32)
RSRZ outliers	91569	1412 (2.36-2.32)

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	394	4% 75% 19% • 5%
1	B	394	8% 69% 26% • 5%
1	C	394	27% 57% 35% • 5%

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 9392 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 Glutamate receptor 2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	376	Total	C	N	O	S	43	0	0
			2996	1907	512	568	9			
1	B	376	Total	C	N	O	S	34	0	0
			2996	1907	512	568	9			
1	C	373	Total	C	N	O	S	35	0	0
			2976	1897	508	562	9			

There are 30 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-4	ILE	-	EXPRESSION TAG	UNP P19491
A	-3	GLU	-	EXPRESSION TAG	UNP P19491
A	-2	GLU	-	EXPRESSION TAG	UNP P19491
A	-1	ARG	-	EXPRESSION TAG	UNP P19491
A	384	LEU	-	EXPRESSION TAG	UNP P19491
A	385	GLU	-	EXPRESSION TAG	UNP P19491
A	386	LEU	-	EXPRESSION TAG	UNP P19491
A	387	VAL	-	EXPRESSION TAG	UNP P19491
A	388	PRO	-	EXPRESSION TAG	UNP P19491
A	389	ARG	-	EXPRESSION TAG	UNP P19491
B	-4	ILE	-	EXPRESSION TAG	UNP P19491
B	-3	GLU	-	EXPRESSION TAG	UNP P19491
B	-2	GLU	-	EXPRESSION TAG	UNP P19491
B	-1	ARG	-	EXPRESSION TAG	UNP P19491
B	384	LEU	-	EXPRESSION TAG	UNP P19491
B	385	GLU	-	EXPRESSION TAG	UNP P19491
B	386	LEU	-	EXPRESSION TAG	UNP P19491
B	387	VAL	-	EXPRESSION TAG	UNP P19491
B	388	PRO	-	EXPRESSION TAG	UNP P19491
B	389	ARG	-	EXPRESSION TAG	UNP P19491
C	-4	ILE	-	EXPRESSION TAG	UNP P19491
C	-3	GLU	-	EXPRESSION TAG	UNP P19491
C	-2	GLU	-	EXPRESSION TAG	UNP P19491

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
C	-1	ARG	-	EXPRESSION TAG	UNP P19491
C	384	LEU	-	EXPRESSION TAG	UNP P19491
C	385	GLU	-	EXPRESSION TAG	UNP P19491
C	386	LEU	-	EXPRESSION TAG	UNP P19491
C	387	VAL	-	EXPRESSION TAG	UNP P19491
C	388	PRO	-	EXPRESSION TAG	UNP P19491
C	389	ARG	-	EXPRESSION TAG	UNP P19491

- Molecule 2 is a polymer of unknown type called SUGAR (2-MER).

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	2	Total	C	N	O	0	0
			28	16	2	10		
2	B	2	Total	C	N	O	0	0
			28	16	2	10		

- Molecule 3 is water.

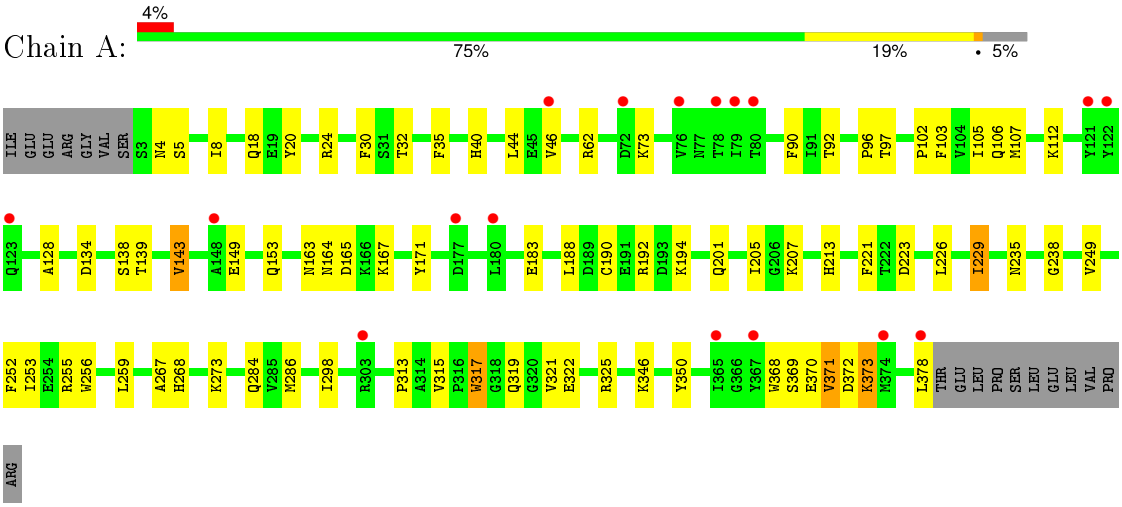
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	229	Total	O	0	0
			229	229		
3	B	118	Total	O	0	0
			118	118		
3	C	21	Total	O	0	0
			21	21		

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.

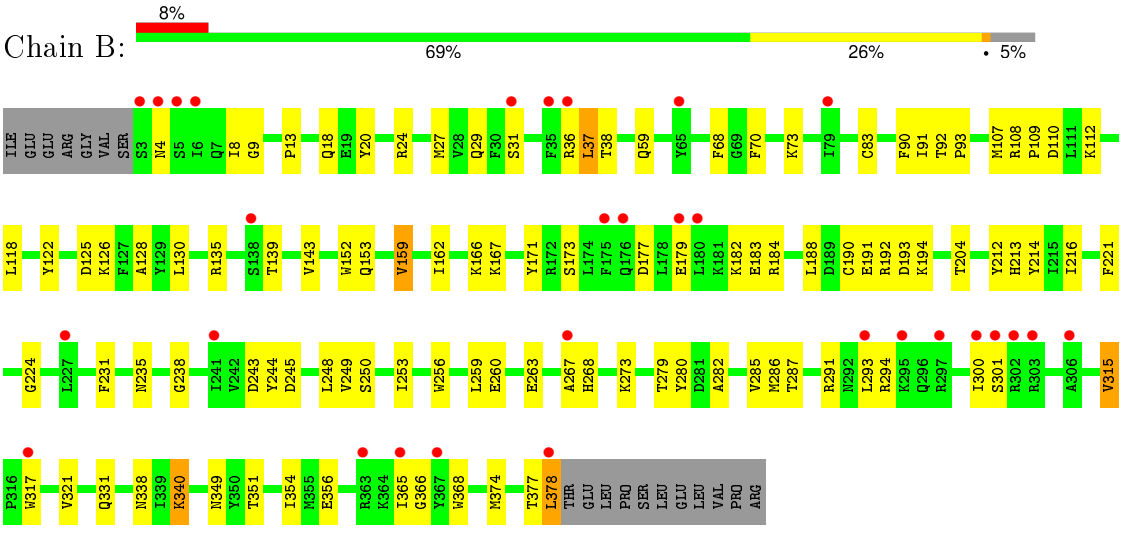
- Molecule 1: Glutamate receptor 2

Chain A:



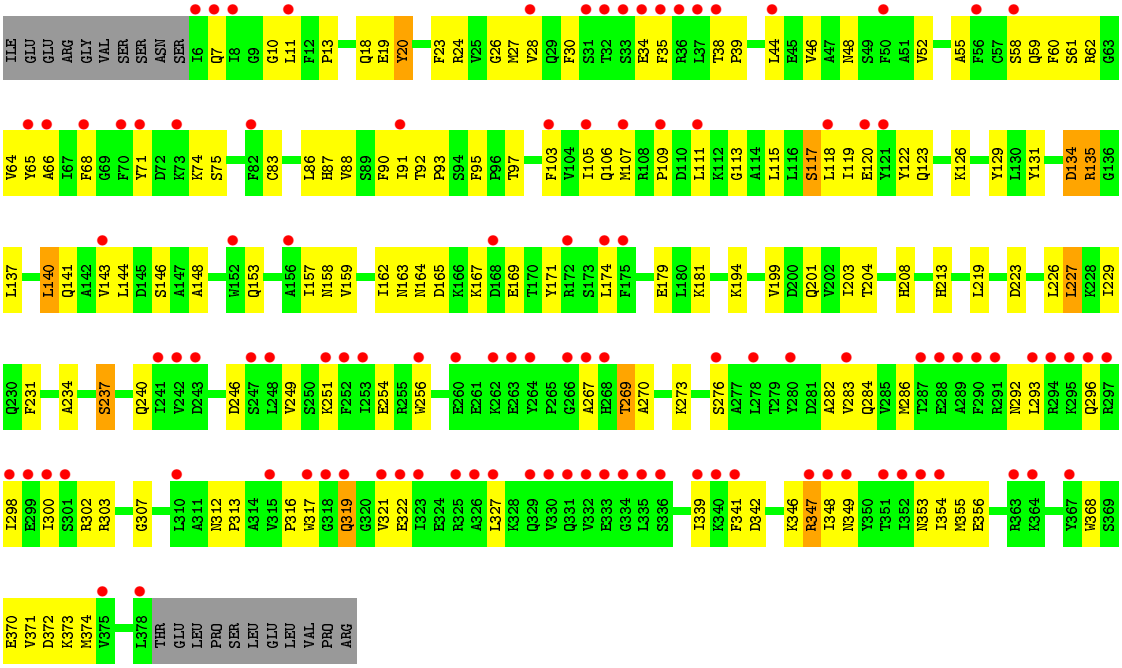
- Molecule 1: Glutamate receptor 2

Chain B:



- Molecule 1: Glutamate receptor 2

Chain C:


ILE GLU GLU ARG GLY VAL SER SER ASN SER I6 Q7 I8 G9 G10 L11 F12 P13 Q18 E19 Y20 F23 R24 V25 G26 M27 V28 Q29 F30 S31 T32 S33 E34 F35 R36 L37 T38 P39 L44 E45 V46 A47 N48 S49 F50 A51 V52 A55 F56 C57 S58 Q59 F60 S61 R62 G63
V64 V65 A66 I67 F68 G69 F70 Y71 D72 K73 K74 S75 F82 C83 L86 H87 V88 S89 F90 I91 T92 P93 S94 F95 P96 T97 F103 V104 I105 Q106 M107 R108 P109 D110 L111 K112 G113 A114 L115 L116 S117 L118 I119 E120 Y121 Y122 Q123 K126 Y129 L130 Y131 D134 R135 G136
L137 L140 Q141 A142 V143 L144 D145 S146 A147 A148 W152 Q153 A156 I157 N158 V159 I162 N163 N164 D165 K166 K167 D168 E169 T170 Y171 R172 S173 L174 F175 E179 L180 K181 K194 V199 D200 Q201 V202 I203 T204 H208 H213 L219 D223 L226 L227 K228 I229
Q230 F231 A234 S237 Q240 I241 V242 D243 D246 S247 I248 V249 S250 K251 F252 I253 E254 R255 W256 E260 E261 K262 E263 Y264 P265 G266 A267 H268 T269 A270 K273 S276 A277 L278 T279 Y280 D281 A282 V283 Q284 V285 M286 T287 E288 A289 F290 R291 N292 L293 R294 K295 Q296 R297
I298 E299 I300 S301 R302 R303 G307 L310 A311 N312 P313 A314 V315 P316 W317 G318 Q319 G320 V321 E322 I323 E324 R325 A326 L327 K328 Q329 V330 Q331 V332 E333 G334 L335 S336 I339 K340 F341 D342 K346 R347 I348 N349 Y350 T351 I352 N353 I354 M355 E356 R363 K364 Y367 W368 S369
E370 V371 D372 K373 M374 V375 L378 THR GLU LEU PRO SER LEU GLU LEU VAL PRO ARG

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, α, β, γ	64.00Å 362.99Å 61.43Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	19.91 – 2.33 46.90 – 2.28	Depositor EDS
% Data completeness (in resolution range)	99.9 (19.91-2.33) 92.4 (46.90-2.28)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.91 (at 2.29Å)	Xtriage
Refinement program	PHENIX (phenix.refine)	Depositor
R, R_{free}	0.186 , 0.235 0.218 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	DCC
Wilson B-factor (Å^2)	48.1	Xtriage
Anisotropy	0.211	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.30 , 52.9	EDS
Estimated twinning fraction	0.027 for l,-k,h	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Outliers	0 of 65797 reflections	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	9392	wwPDB-VP
Average B, all atoms (Å^2)	85.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.37% 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: NAG

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	0.52	0/3058	0.61	0/4136
1	B	0.43	0/3058	0.56	0/4136
1	C	0.30	0/3038	0.47	0/4109
All	All	0.43	0/9154	0.55	0/12381

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2996	0	2952	62	0
1	B	2996	0	2952	78	0
1	C	2976	0	2937	123	0
2	A	28	0	25	0	0
2	B	28	0	25	0	0
3	A	229	0	0	5	0
3	B	118	0	0	8	0
3	C	21	0	0	4	0
All	All	9392	0	8891	259	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 15.

All (259) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:373:LYS:HD3	1:A:373:LYS:N	1.81	0.96
1:C:246:ASP:HB2	1:C:249:VAL:HG22	1.57	0.84
1:A:97:THR:H	1:A:106:GLN:NE2	1.77	0.82
1:B:4:ASN:HB3	1:B:294:ARG:HH22	1.46	0.81
1:A:259:LEU:O	1:A:268:HIS:HD2	1.68	0.77
1:A:378:LEU:HD23	1:A:378:LEU:H	1.50	0.77
1:B:366:GLY:HA2	1:B:377:THR:OG1	1.84	0.76
1:B:128:ALA:HB2	1:B:183:GLU:HG2	1.69	0.74
1:B:315:VAL:HG22	1:B:315:VAL:O	1.88	0.73
1:C:7:GLN:HA	1:C:38:THR:O	1.90	0.71
1:C:368:TRP:HA	1:C:373:LYS:O	1.90	0.71
1:B:18:GLN:HE22	1:B:273:LYS:H	1.39	0.70
1:C:339:ILE:HG12	1:C:347:ARG:HH12	1.56	0.70
1:A:97:THR:H	1:A:106:GLN:HE21	1.39	0.70
1:B:293:LEU:HD13	1:B:300:ILE:HG21	1.73	0.69
1:A:373:LYS:H	1:A:373:LYS:HD3	1.55	0.69
1:C:131:TYR:CZ	1:C:158:ASN:HB2	2.29	0.68
1:B:213:HIS:CG	1:B:235:ASN:HB2	2.30	0.67
1:C:237:SER:HB3	1:C:356:GLU:HG2	1.77	0.66
1:C:44:LEU:C	1:C:44:LEU:HD12	2.16	0.66
1:A:252:PHE:HD2	1:A:253:ILE:HD12	1.61	0.66
1:C:97:THR:H	1:C:106:GLN:HE21	1.43	0.66
1:C:269:THR:HG22	1:C:270:ALA:H	1.60	0.66
1:C:126:LYS:NZ	1:C:181:LYS:HB3	2.11	0.65
1:C:66:ALA:HB1	1:C:88:VAL:HG13	1.78	0.65
1:A:106:GLN:HE22	1:A:346:LYS:NZ	1.95	0.64
1:C:129:TYR:CE1	1:C:131:TYR:HB3	2.32	0.64
1:A:18:GLN:HE22	1:A:273:LYS:H	1.44	0.63
1:C:87:HIS:HD2	1:C:321:VAL:HG22	1.62	0.63
1:B:188:LEU:HD12	1:B:216:ILE:HD13	1.80	0.63
1:C:83:CYS:SG	1:C:90:PHE:HB2	2.38	0.63
1:A:112:LYS:HE2	1:A:138:SER:OG	1.98	0.62
1:B:107:MET:CE	1:B:282:ALA:HA	2.29	0.62
1:C:97:THR:HG23	1:C:106:GLN:NE2	2.13	0.62
1:A:105:ILE:HG22	1:A:107:MET:CE	2.29	0.62
1:B:159:VAL:HG13	1:B:194:LYS:HE3	1.80	0.62
1:A:213:HIS:CG	1:A:235:ASN:HB2	2.34	0.62
1:C:13:PRO:HA	1:C:44:LEU:O	2.00	0.61

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:191:GLU:HG2	1:B:193:ASP:H	1.64	0.61
1:A:298:ILE:HG21	1:A:322:GLU:HG2	1.81	0.61
1:B:107:MET:HE3	1:B:282:ALA:HA	1.81	0.61
1:C:105:ILE:HG22	1:C:341:PHE:CE2	2.37	0.60
1:C:90:PHE:O	1:C:105:ILE:HG12	2.00	0.60
1:B:260:GLU:OE2	1:B:263:GLU:HB2	2.01	0.60
1:B:9:GLY:HA3	3:B:471:HOH:O	2.01	0.60
1:C:317:TRP:CE3	1:C:319:GLN:HG2	2.36	0.60
1:C:157:ILE:HA	3:C:393:HOH:O	2.03	0.59
1:C:339:ILE:CG1	1:C:347:ARG:HH12	2.16	0.59
1:B:130:LEU:O	1:B:188:LEU:O	2.20	0.59
1:C:20:TYR:O	1:C:23:PHE:HB3	2.02	0.59
1:C:44:LEU:O	1:C:44:LEU:HD12	2.03	0.59
1:B:331:GLN:CD	1:B:340:LYS:HG3	2.23	0.59
1:B:321:VAL:HG23	3:B:396:HOH:O	2.03	0.58
1:B:20:TYR:CE2	1:B:24:ARG:HD2	2.38	0.58
1:C:91:ILE:HD12	1:C:91:ILE:N	2.18	0.58
1:A:171:TYR:CG	1:A:201:GLN:HG2	2.38	0.58
1:B:68:PHE:CZ	1:B:279:THR:HG23	2.38	0.58
1:C:317:TRP:HE3	1:C:319:GLN:OE1	1.86	0.58
1:C:162:ILE:O	1:C:162:ILE:HG13	2.03	0.58
1:A:226:LEU:O	1:A:229:ILE:HD12	2.04	0.58
1:B:378:LEU:C	1:B:378:LEU:CD1	2.73	0.57
1:C:55:ALA:O	1:C:59:GLN:HG2	2.04	0.57
1:C:97:THR:H	1:C:106:GLN:NE2	2.02	0.57
1:C:59:GLN:HB3	1:C:64:VAL:HG11	1.87	0.57
1:A:97:THR:N	1:A:106:GLN:NE2	2.51	0.57
1:C:97:THR:HG23	1:C:106:GLN:HE21	1.70	0.57
1:A:97:THR:N	1:A:106:GLN:HE21	2.02	0.57
1:A:106:GLN:HE22	1:A:346:LYS:HZ3	1.53	0.57
1:C:317:TRP:HB2	1:C:319:GLN:OE1	2.03	0.57
1:A:317:TRP:CE3	1:A:319:GLN:HG2	2.40	0.57
1:A:153:GLN:HE21	1:B:153:GLN:NE2	2.03	0.57
1:B:27:MET:HE1	1:B:37:LEU:O	2.05	0.56
1:A:153:GLN:HE21	1:B:153:GLN:HE21	1.53	0.56
1:B:204:THR:HG22	1:C:231:PHE:HB2	1.87	0.56
1:C:223:ASP:OD2	1:C:273:LYS:HA	2.05	0.56
1:C:179:GLU:HA	3:C:401:HOH:O	2.05	0.56
1:C:109:PRO:HG3	1:C:347:ARG:HD2	1.87	0.56
1:A:249:VAL:O	1:A:253:ILE:HD13	2.06	0.56
1:C:118:LEU:HD12	1:C:374:MET:HE1	1.88	0.55

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:244:TYR:HA	1:B:249:VAL:HG11	1.87	0.55
1:B:179:GLU:HA	3:B:504:HOH:O	2.06	0.55
1:C:11:LEU:HD23	1:C:44:LEU:HD21	1.88	0.55
1:A:205:ILE:HD11	1:A:207:LYS:HD2	1.89	0.55
1:C:129:TYR:HE1	1:C:131:TYR:HB3	1.72	0.55
1:B:287:THR:HG22	1:B:291:ARG:HH12	1.71	0.55
1:C:65:TYR:N	1:C:66:ALA:HA	2.21	0.54
1:C:13:PRO:HB3	1:C:46:VAL:HG13	1.89	0.54
1:A:350:TYR:CE2	1:A:370:GLU:HG3	2.42	0.54
1:C:339:ILE:HA	1:C:347:ARG:NH1	2.23	0.54
1:B:190:CYS:HB3	1:B:194:LYS:HB3	1.89	0.54
1:A:138:SER:HB2	3:A:528:HOH:O	2.08	0.54
1:B:36:ARG:HD2	1:B:38:THR:HG22	1.88	0.54
1:C:87:HIS:CD2	1:C:321:VAL:HG22	2.42	0.54
1:C:106:GLN:OE1	1:C:346:LYS:HD3	2.08	0.53
1:A:255:ARG:HD2	1:A:255:ARG:O	2.08	0.53
1:C:348:ILE:HD12	1:C:349:ASN:HB2	1.88	0.53
1:A:221:PHE:CD1	1:A:238:GLY:HA3	2.43	0.53
1:A:190:CYS:HB3	1:A:194:LYS:HB3	1.91	0.53
1:C:146:SER:C	1:C:148:ALA:N	2.62	0.53
1:B:27:MET:O	1:B:31:SER:HB3	2.08	0.53
1:C:240:GLN:O	1:C:353:ASN:HB2	2.09	0.53
1:C:115:LEU:O	1:C:119:ILE:HG13	2.09	0.52
1:C:162:ILE:HD11	1:C:194:LYS:HZ1	1.75	0.52
1:B:259:LEU:O	1:B:268:HIS:HD2	1.92	0.52
1:C:122:TYR:CE2	1:C:213:HIS:HE1	2.27	0.52
1:A:40:HIS:HE1	3:A:565:HOH:O	1.92	0.52
1:C:18:GLN:HE22	1:C:273:LYS:H	1.59	0.51
1:A:317:TRP:CE3	1:A:319:GLN:CG	2.93	0.51
1:C:10:GLY:HA2	1:C:68:PHE:O	2.11	0.51
1:C:134:ASP:OD1	1:C:134:ASP:N	2.43	0.51
1:C:109:PRO:HG3	1:C:347:ARG:CD	2.40	0.51
1:A:371:VAL:O	1:A:371:VAL:HG23	2.11	0.51
1:C:131:TYR:CE1	1:C:140:LEU:HD13	2.46	0.51
1:A:112:LYS:CE	1:A:138:SER:OG	2.59	0.51
1:B:159:VAL:O	1:B:194:LYS:HE3	2.11	0.51
1:B:184:ARG:HD3	1:B:212:TYR:CE2	2.46	0.51
1:C:174:LEU:HD12	1:C:174:LEU:O	2.11	0.51
1:C:48:ASN:O	1:C:52:VAL:HG23	2.11	0.50
1:B:221:PHE:CD1	1:B:238:GLY:HA3	2.46	0.50
1:C:44:LEU:HD23	1:C:55:ALA:CB	2.41	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:370:GLU:CD	1:C:370:GLU:H	2.14	0.50
1:A:44:LEU:HD12	1:A:44:LEU:C	2.31	0.50
1:A:96:PRO:HA	1:A:106:GLN:HE21	1.76	0.50
1:A:298:ILE:HG21	1:A:322:GLU:CG	2.41	0.49
1:C:91:ILE:HD13	1:C:286:MET:CE	2.42	0.49
1:C:87:HIS:ND1	1:C:316:PRO:HB3	2.27	0.49
1:A:205:ILE:HG13	1:A:207:LYS:HG3	1.94	0.49
1:C:30:PHE:CE1	1:C:284:GLN:HG3	2.47	0.49
1:C:109:PRO:HG3	1:C:347:ARG:NE	2.27	0.49
1:B:59:GLN:CD	3:B:471:HOH:O	2.50	0.49
1:C:111:LEU:HD13	1:C:219:LEU:CD2	2.43	0.49
1:C:106:GLN:HE22	1:C:346:LYS:NZ	2.11	0.49
1:B:354:ILE:N	1:B:354:ILE:HD12	2.28	0.49
1:A:325:ARG:HG3	1:A:325:ARG:HH11	1.77	0.49
1:C:140:LEU:O	1:C:140:LEU:HG	2.13	0.49
1:A:40:HIS:CE1	3:A:565:HOH:O	2.66	0.48
1:A:149:GLU:O	1:A:149:GLU:HG2	2.12	0.48
1:C:292:ASN:O	1:C:296:GLN:HG3	2.14	0.48
1:C:26:GLY:C	1:C:283:VAL:HG11	2.33	0.48
1:B:191:GLU:HG2	1:B:192:ARG:N	2.27	0.48
1:B:8:ILE:HD13	1:B:286:MET:CE	2.43	0.48
1:C:317:TRP:CZ3	1:C:319:GLN:HG2	2.49	0.48
1:C:137:LEU:O	1:C:141:GLN:HG3	2.13	0.48
1:C:163:ASN:C	1:C:165:ASP:H	2.17	0.48
1:B:29:GLN:HG2	1:B:280:TYR:OH	2.14	0.47
1:C:157:ILE:HG12	3:C:393:HOH:O	2.14	0.47
1:B:8:ILE:HD13	1:B:286:MET:HE2	1.96	0.47
1:C:95:PHE:CD2	1:C:135:ARG:HA	2.50	0.47
1:A:62:ARG:NH1	1:A:62:ARG:HG2	2.29	0.47
1:C:251:LYS:HD2	1:C:254:GLU:OE1	2.14	0.47
1:C:131:TYR:OH	1:C:158:ASN:HB2	2.15	0.46
1:B:91:ILE:CG2	1:B:107:MET:HE2	2.45	0.46
1:B:182:LYS:HA	3:B:504:HOH:O	2.15	0.46
1:C:118:LEU:HD12	1:C:374:MET:CE	2.45	0.46
1:B:354:ILE:HD11	1:B:368:TRP:HB2	1.97	0.46
1:A:171:TYR:CD2	1:A:201:GLN:HG2	2.51	0.46
1:C:113:GLY:HA3	1:C:368:TRP:CZ2	2.50	0.46
1:C:120:GLU:O	1:C:123:GLN:N	2.42	0.46
1:B:260:GLU:HG3	1:B:263:GLU:HB3	1.96	0.46
1:B:248:LEU:HD23	1:B:248:LEU:O	2.16	0.46
1:C:229:ILE:O	1:C:229:ILE:HG12	2.15	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:338:ASN:ND2	1:B:349:ASN:HD22	2.13	0.46
1:C:293:LEU:HD21	1:C:300:ILE:HG21	1.98	0.45
1:B:73:LYS:NZ	3:B:506:HOH:O	2.47	0.45
1:C:58:SER:O	1:C:62:ARG:HB2	2.17	0.45
1:A:315:VAL:HG12	3:A:500:HOH:O	2.15	0.45
1:B:20:TYR:CZ	1:B:24:ARG:HD2	2.51	0.45
1:C:162:ILE:HD13	1:C:171:TYR:OH	2.17	0.45
1:B:224:GLY:HA3	3:B:466:HOH:O	2.17	0.45
1:A:8:ILE:HG21	1:A:286:MET:CE	2.47	0.45
1:B:256:TRP:CH2	1:B:267:ALA:HB2	2.52	0.45
1:C:90:PHE:HE2	1:C:92:THR:HB	1.82	0.45
1:B:159:VAL:HG22	1:B:171:TYR:HE2	1.82	0.45
1:C:74:LYS:HE3	1:C:74:LYS:HB2	1.64	0.44
1:B:13:PRO:HD3	1:B:70:PHE:CD1	2.52	0.44
1:C:60:PHE:CE1	1:C:86:LEU:HD13	2.52	0.44
1:C:7:GLN:HG2	1:C:38:THR:CG2	2.47	0.44
1:C:46:VAL:O	1:C:75:SER:HB3	2.18	0.44
1:C:61:SER:HB3	1:C:307:GLY:O	2.18	0.44
1:A:4:ASN:HB2	1:A:35:PHE:HA	1.99	0.44
1:A:259:LEU:O	1:A:268:HIS:CD2	2.59	0.44
1:C:44:LEU:CD1	1:C:44:LEU:C	2.83	0.44
1:A:128:ALA:HB2	1:A:183:GLU:HG2	1.99	0.44
1:C:113:GLY:O	1:C:117:SER:HB2	2.17	0.44
1:C:339:ILE:HG12	1:C:347:ARG:NH1	2.30	0.44
1:B:354:ILE:HG22	1:B:365:ILE:HG22	2.00	0.44
1:B:92:THR:HA	1:B:93:PRO:HD3	1.82	0.44
1:B:166:LYS:O	1:B:167:LYS:HB3	2.18	0.44
1:B:231:PHE:HB2	1:C:204:THR:HG22	2.00	0.43
1:C:208:HIS:C	1:C:234:ALA:HB2	2.38	0.43
1:B:248:LEU:HD23	1:B:248:LEU:C	2.39	0.43
1:A:139:THR:O	1:A:143:VAL:HG13	2.18	0.43
1:C:91:ILE:HG13	1:C:105:ILE:HG13	2.00	0.43
1:B:177:ASP:C	1:B:179:GLU:N	2.72	0.43
1:C:65:TYR:CZ	1:C:302:ARG:NH1	2.87	0.43
1:A:8:ILE:HG21	1:A:286:MET:HE2	1.99	0.43
1:C:126:LYS:HG3	1:C:153:GLN:HB3	2.01	0.43
1:C:163:ASN:O	1:C:164:ASN:HB3	2.18	0.43
1:C:371:VAL:HG23	1:C:372:ASP:H	1.84	0.43
1:B:36:ARG:HD2	1:B:38:THR:CG2	2.49	0.43
1:A:163:ASN:C	1:A:165:ASP:H	2.22	0.43
1:C:65:TYR:CE2	1:C:302:ARG:NH1	2.86	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:378:LEU:HD13	1:B:378:LEU:C	2.40	0.43
1:B:244:TYR:HA	1:B:249:VAL:CG1	2.49	0.43
1:C:24:ARG:O	1:C:28:VAL:HG23	2.19	0.43
1:A:256:TRP:O	1:A:267:ALA:O	2.37	0.43
1:B:159:VAL:HG13	1:B:159:VAL:O	2.17	0.42
1:B:213:HIS:HD2	1:B:214:TYR:N	2.17	0.42
1:C:105:ILE:HG13	1:C:327:LEU:HD13	2.00	0.42
1:C:92:THR:HA	1:C:93:PRO:HD3	1.85	0.42
1:C:27:MET:HE1	1:C:39:PRO:HD3	2.01	0.42
1:C:339:ILE:HG23	1:C:347:ARG:NH1	2.34	0.42
1:C:167:LYS:C	1:C:169:GLU:H	2.22	0.42
1:A:255:ARG:HD3	1:A:255:ARG:HA	1.76	0.42
1:C:353:ASN:HB3	1:C:355:MET:HE2	2.01	0.42
1:C:342:ASP:OD1	1:C:342:ASP:C	2.58	0.42
1:B:356:GLU:CD	1:B:365:ILE:HD12	2.40	0.42
1:A:163:ASN:O	1:A:167:LYS:HB2	2.20	0.42
1:C:201:GLN:OE1	1:C:201:GLN:HA	2.19	0.42
1:A:20:TYR:CE2	1:A:24:ARG:HD2	2.54	0.42
1:B:125:ASP:OD1	1:B:126:LYS:N	2.53	0.42
1:B:118:LEU:HD11	1:B:122:TYR:CE1	2.55	0.42
1:A:368:TRP:CZ2	1:A:373:LYS:HD2	2.54	0.42
1:B:110:ASP:OD1	1:B:112:LYS:HG3	2.20	0.41
1:C:342:ASP:HB3	1:C:348:ILE:HG21	2.01	0.41
1:C:107:MET:CE	1:C:282:ALA:HA	2.49	0.41
1:B:4:ASN:HD22	1:B:4:ASN:H	1.68	0.41
1:B:349:ASN:ND2	3:B:487:HOH:O	2.49	0.41
1:B:243:ASP:OD1	1:B:245:ASP:HB2	2.20	0.41
1:B:108:ARG:HA	1:B:109:PRO:HD2	1.96	0.41
1:C:109:PRO:HG3	1:C:347:ARG:HE	1.85	0.41
1:A:102:PRO:HB2	1:A:103:PHE:CD2	2.56	0.41
1:C:312:ASN:HA	1:C:313:PRO:HA	1.92	0.41
1:A:30:PHE:CZ	1:A:284:GLN:HB2	2.55	0.41
1:C:256:TRP:CZ2	1:C:267:ALA:HA	2.56	0.41
1:A:164:ASN:N	1:A:164:ASN:HD22	2.18	0.41
1:C:373:LYS:HE2	1:C:373:LYS:HB3	1.90	0.41
1:C:87:HIS:CD2	1:C:103:PHE:CZ	3.09	0.41
1:C:90:PHE:CE2	1:C:92:THR:HB	2.56	0.41
1:B:107:MET:HE3	1:B:285:VAL:HB	2.02	0.41
1:A:62:ARG:HH11	1:A:62:ARG:HG2	1.85	0.41
1:A:313:PRO:HD2	3:A:520:HOH:O	2.20	0.41
1:C:354:ILE:N	1:C:354:ILE:HD12	2.36	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:90:PHE:CE2	1:A:92:THR:HB	2.56	0.41
1:C:227:LEU:HD23	1:C:227:LEU:HA	1.84	0.41
1:A:192:ARG:HH22	1:A:223:ASP:HB3	1.86	0.41
1:C:199:VAL:O	1:C:203:ILE:HG13	2.20	0.41
1:A:369:SER:HB3	1:A:372:ASP:HB2	2.03	0.41
1:B:118:LEU:HA	1:B:374:MET:CE	2.51	0.40
1:C:19:GLU:HG3	1:C:276:SER:HA	2.03	0.40
1:C:146:SER:C	1:C:148:ALA:H	2.24	0.40
1:C:298:ILE:HG21	1:C:322:GLU:HG2	2.04	0.40
1:B:8:ILE:CD1	1:B:286:MET:HE1	2.51	0.40
1:B:125:ASP:O	1:B:152:TRP:HA	2.22	0.40
1:C:169:GLU:HG3	3:C:408:HOH:O	2.20	0.40
1:C:140:LEU:O	1:C:144:LEU:HG	2.22	0.40
1:B:130:LEU:N	1:B:130:LEU:HD23	2.36	0.40
1:B:253:ILE:HA	1:B:253:ILE:HD13	1.74	0.40
1:B:83:CYS:SG	1:B:90:PHE:HB2	2.61	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	374/394 (95%)	362 (97%)	12 (3%)	0	100	100
1	B	374/394 (95%)	355 (95%)	19 (5%)	0	100	100
1	C	371/394 (94%)	332 (90%)	37 (10%)	2 (0%)	34	37
All	All	1119/1182 (95%)	1049 (94%)	68 (6%)	2 (0%)	52	61

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	34	GLU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	C	303	ARG

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	325/342 (95%)	313 (96%)	12 (4%)	41	53
1	B	325/342 (95%)	311 (96%)	14 (4%)	35	45
1	C	322/342 (94%)	307 (95%)	15 (5%)	32	40
All	All	972/1026 (95%)	931 (96%)	41 (4%)	36	46

All (41) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	5	SER
1	A	32	THR
1	A	46	VAL
1	A	73	LYS
1	A	134	ASP
1	A	143	VAL
1	A	188	LEU
1	A	229	ILE
1	A	317	TRP
1	A	321	VAL
1	A	371	VAL
1	A	373	LYS
1	B	37	LEU
1	B	135	ARG
1	B	139	THR
1	B	143	VAL
1	B	159	VAL
1	B	162	ILE
1	B	173	SER
1	B	250	SER
1	B	301	SER

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	315	VAL
1	B	317	TRP
1	B	340	LYS
1	B	351	THR
1	B	378	LEU
1	C	20	TYR
1	C	35	PHE
1	C	71	TYR
1	C	117	SER
1	C	134	ASP
1	C	135	ARG
1	C	140	LEU
1	C	143	VAL
1	C	159	VAL
1	C	226	LEU
1	C	227	LEU
1	C	237	SER
1	C	269	THR
1	C	319	GLN
1	C	347	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (26) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	18	GLN
1	A	54	ASN
1	A	106	GLN
1	A	164	ASN
1	A	268	HIS
1	A	284	GLN
1	A	292	ASN
1	A	296	GLN
1	B	4	ASN
1	B	7	GLN
1	B	18	GLN
1	B	59	GLN
1	B	153	GLN
1	B	268	HIS
1	B	292	ASN
1	B	338	ASN
1	B	343	GLN
1	C	18	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	C	87	HIS
1	C	106	GLN
1	C	163	ASN
1	C	268	HIS
1	C	292	ASN
1	C	296	GLN
1	C	331	GLN
1	C	349	ASN

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

4 carbohydrates 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	NAG	A	400	1,2	14,14,15	0.51	0	15,19,21	0.85	0
2	NAG	A	401	2	14,14,15	0.49	0	15,19,21	2.37	3 (20%)
2	NAG	B	402	1,2	14,14,15	0.47	0	15,19,21	1.92	3 (20%)
2	NAG	B	403	2	14,14,15	0.41	0	15,19,21	1.42	1 (6%)

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	NAG	A	400	1,2	-	0/6/23/26	0/1/1/1
2	NAG	A	401	2	-	0/6/23/26	0/1/1/1
2	NAG	B	402	1,2	-	0/6/23/26	0/1/1/1
2	NAG	B	403	2	-	0/6/23/26	0/1/1/1

There are no bond length outliers.

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	402	NAG	C4-C3-C2	-3.18	106.28	111.23
2	B	402	NAG	C2-N2-C7	-3.12	119.03	123.04
2	A	401	NAG	C4-C3-C2	-2.73	106.98	111.23
2	A	401	NAG	C2-N2-C7	-2.33	120.04	123.04
2	B	403	NAG	C1-O5-C5	4.49	117.95	112.25
2	B	402	NAG	C1-O5-C5	5.30	118.98	112.25
2	A	401	NAG	C1-O5-C5	8.00	122.41	112.25

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

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, 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	376/394 (95%)	0.34	17 (4%) 37 50	29, 50, 91, 155	11 (2%)
1	B	376/394 (95%)	0.69	30 (7%) 15 23	32, 67, 117, 178	10 (2%)
1	C	373/394 (94%)	1.63	108 (28%) 1 1	69, 121, 182, 220	10 (2%)
All	All	1125/1182 (95%)	0.88	155 (13%) 4 7	29, 74, 164, 220	31 (2%)

All (155) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	332	VAL	11.3
1	C	31	SER	10.5
1	C	335	LEU	8.5
1	C	66	ALA	7.9
1	C	293	LEU	7.7
1	B	3	SER	7.1
1	C	248	LEU	7.1
1	B	303	ARG	7.0
1	C	290	PHE	6.8
1	C	32	THR	6.7
1	C	36	ARG	6.6
1	C	247	SER	6.3
1	C	326	ALA	6.1
1	C	65	TYR	6.0
1	C	294	ARG	5.8
1	C	28	VAL	5.7
1	C	35	PHE	5.7
1	B	5	SER	5.5
1	C	327	LEU	5.5
1	C	375	VAL	5.2
1	C	325	ARG	5.2
1	C	34	GLU	5.1
1	B	180	LEU	5.1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	B	36	ARG	5.0
1	C	6	ILE	4.9
1	C	91	ILE	4.9
1	B	300	ILE	4.8
1	C	253	ILE	4.8
1	C	105	ILE	4.6
1	C	339	ILE	4.4
1	C	319	GLN	4.4
1	C	289	ALA	4.3
1	C	264	TYR	4.3
1	C	268	HIS	4.1
1	C	287	THR	4.1
1	C	323	ILE	4.0
1	C	8	ILE	4.0
1	A	148	ALA	3.9
1	C	341	PHE	3.9
1	A	374	MET	3.8
1	C	378	LEU	3.7
1	B	267	ALA	3.7
1	C	322	GLU	3.6
1	B	35	PHE	3.5
1	B	378	LEU	3.4
1	B	179	GLU	3.4
1	C	321	VAL	3.3
1	C	172	ARG	3.3
1	C	262	LYS	3.3
1	C	297	ARG	3.3
1	C	103	PHE	3.3
1	C	329	GLN	3.3
1	C	291	ARG	3.3
1	C	267	ALA	3.3
1	C	33	SER	3.2
1	B	65	TYR	3.2
1	C	296	GLN	3.1
1	C	331	GLN	3.1
1	A	378	LEU	3.1
1	B	6	ILE	3.1
1	C	288	GLU	3.1
1	C	107	MET	3.1
1	C	260	GLU	3.1
1	C	56	PHE	3.1
1	A	367	TYR	3.0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	C	38	THR	3.0
1	C	121	TYR	3.0
1	C	280	TYR	3.0
1	C	7	GLN	3.0
1	B	317	TRP	3.0
1	C	330	VAL	3.0
1	B	302	ARG	3.0
1	C	68	PHE	3.0
1	B	365	ILE	3.0
1	C	352	ILE	3.0
1	B	4	ASN	2.9
1	B	297	ARG	2.9
1	C	354	ILE	2.9
1	C	174	LEU	2.9
1	C	73	LYS	2.9
1	A	121	TYR	2.9
1	C	82	PHE	2.9
1	C	315	VAL	2.9
1	A	76	VAL	2.8
1	B	175	PHE	2.8
1	C	11	LEU	2.8
1	B	176	GLN	2.8
1	B	31	SER	2.8
1	C	37	LEU	2.8
1	C	317	TRP	2.8
1	C	301	SER	2.7
1	B	306	ALA	2.7
1	C	118	LEU	2.7
1	C	263	GLU	2.7
1	C	353	ASN	2.7
1	C	251	LYS	2.7
1	C	299	GLU	2.7
1	C	241	ILE	2.6
1	B	241	ILE	2.6
1	A	365	ILE	2.6
1	C	168	ASP	2.6
1	C	252	PHE	2.6
1	C	243	ASP	2.6
1	A	303	ARG	2.5
1	C	70	PHE	2.5
1	C	278	LEU	2.5
1	C	300	ILE	2.5

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	C	334	GLY	2.4
1	A	80	THR	2.4
1	C	58	SER	2.4
1	C	347	ARG	2.4
1	C	363	ARG	2.4
1	A	177	ASP	2.4
1	A	79	ILE	2.4
1	C	295	LYS	2.3
1	C	283	VAL	2.3
1	B	79	ILE	2.3
1	C	143	VAL	2.3
1	C	367	TYR	2.3
1	C	340	LYS	2.3
1	C	364	LYS	2.3
1	C	256	TRP	2.3
1	C	266	GLY	2.2
1	C	50	PHE	2.2
1	B	227	LEU	2.2
1	A	72	ASP	2.2
1	C	298	ILE	2.2
1	C	333	GLU	2.2
1	B	301	SER	2.2
1	C	120	GLU	2.2
1	C	242	VAL	2.1
1	A	122	TYR	2.1
1	A	180	LEU	2.1
1	C	310	LEU	2.1
1	B	363	ARG	2.1
1	C	348	ILE	2.1
1	C	71	TYR	2.1
1	C	175	PHE	2.1
1	C	351	THR	2.1
1	C	109	PRO	2.1
1	B	295	LYS	2.1
1	C	336	SER	2.1
1	C	44	LEU	2.1
1	C	349	ASN	2.1
1	B	138	SER	2.1
1	A	46	VAL	2.1
1	C	318	GLY	2.0
1	B	367	TYR	2.0
1	C	156	ALA	2.0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	123	GLN	2.0
1	C	152	TRP	2.0
1	C	276	SER	2.0
1	A	78	THR	2.0
1	B	293	LEU	2.0
1	C	111	LEU	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)

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	NAG	B	402	14/15	0.87	0.23	1.35	76,88,120,135	0
2	NAG	A	400	14/15	0.90	0.15	0.68	42,79,95,113	0
2	NAG	B	403	14/15	0.60	0.50	-	152,163,166,166	0
2	NAG	A	401	14/15	0.77	0.20	-	129,137,146,148	0

6.4 Ligands (i)

There are no ligands in this entry.

6.5 Other polymers (i)

There are no such residues in this entry.