Full wwPDB X-ray Structure Validation Report

Apr 26, 2016 – 08:23 PM EDT

PDB ID	:	5I73
Title	:	X-ray structure of the ts3 human serotonin transporter complexed with s-citalopram at the central and allosteric sites
Authors	:	Coleman, J.A.; Green, E.M.; Gouaux, E.
Deposited on	:	2016-02-16
Resolution	:	3.24 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:

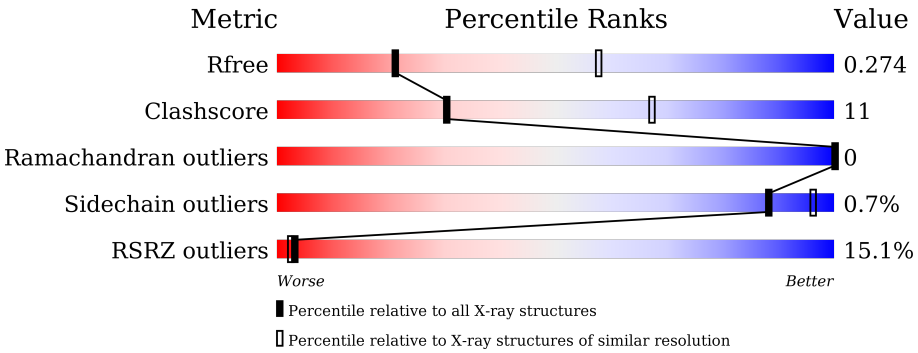
MolProbity	:	4.02b-467
Mogul	:	1.7.1 (RC1), CSD as537be (2016)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20027457
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	rb-20027457

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 3.24 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	1092 (3.28-3.20)
Clashscore	102246	1227 (3.28-3.20)
Ramachandran outliers	100387	1204 (3.28-3.20)
Sidechain outliers	100360	1203 (3.28-3.20)
RSRZ outliers	91569	1097 (3.28-3.20)

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	549	9% 75% 23%
2	B	221	19% 82% 16%
3	C	214	27% 81% 19%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
4	68P	A	701	-	-	-	X
4	68P	A	705	-	-	-	X
5	NAG	A	706	-	-	-	X
6	CLR	A	703	-	-	-	X
7	C14	A	704	-	-	-	X

2 Entry composition

There are 10 unique types of molecules in this entry. The entry contains 7633 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 Sodium-dependent serotonin transporter.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	540	Total	C	N	O	S	0	0	0
			4198	2804	650	720	24			

There are 10 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	74	GLY	-	cloning artifact	UNP P31645
A	75	SER	-	cloning artifact	UNP P31645
A	291	ALA	ILE	engineered mutation	UNP P31645
A	439	SER	THR	engineered mutation	UNP P31645
A	554	ALA	CYS	engineered mutation	UNP P31645
A	580	ALA	CYS	engineered mutation	UNP P31645
A	619	LEU	-	cloning artifact	UNP P31645
A	620	VAL	-	cloning artifact	UNP P31645
A	621	PRO	-	cloning artifact	UNP P31645
A	622	ARG	-	cloning artifact	UNP P31645

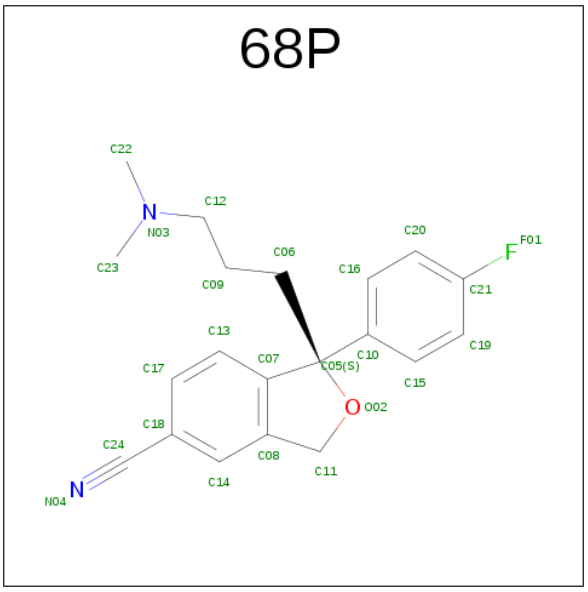
- Molecule 2 is a protein called 8B6 antibody, heavy chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	218	Total	C	N	O	S	0	0	0
			1643	1038	266	331	8			

- Molecule 3 is a protein called 8B6 antibody, light chain.

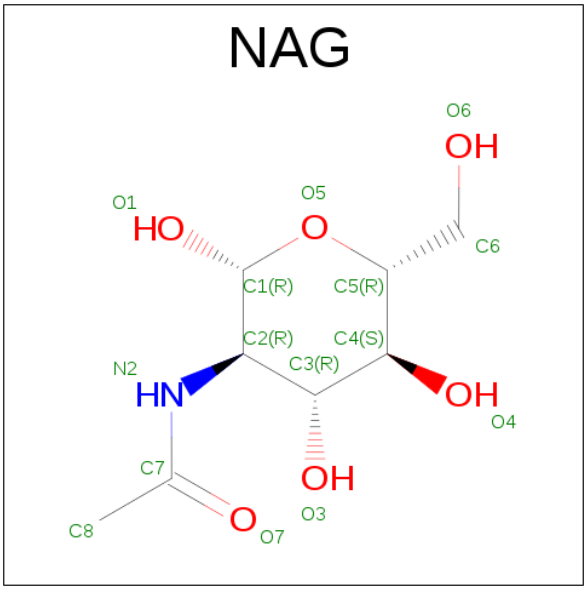
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	214	Total	C	N	O	S	0	0	0
			1662	1037	280	337	8			

- Molecule 4 is (1S)-1-[3-(dimethylamino)propyl]-1-(4-fluorophenyl)-1,3-dihydro-2-benzofuran-5-carbonitrile (three-letter code: 68P) (formula: $C_{20}H_{21}FN_2O$).



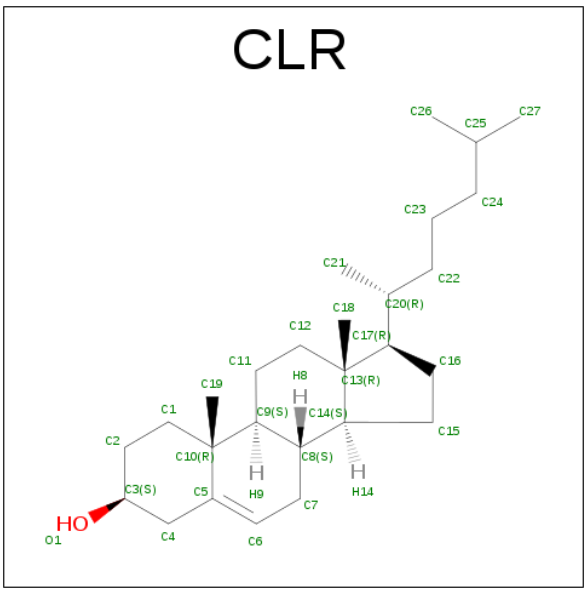
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	A	1	Total	C	F	N	O	0	0
			24	20	1	2	1		
4	A	1	Total	C	F	N	O	0	0
			24	20	1	2	1		

- Molecule 5 is N-ACETYL-D-GLUCOSAMINE (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).



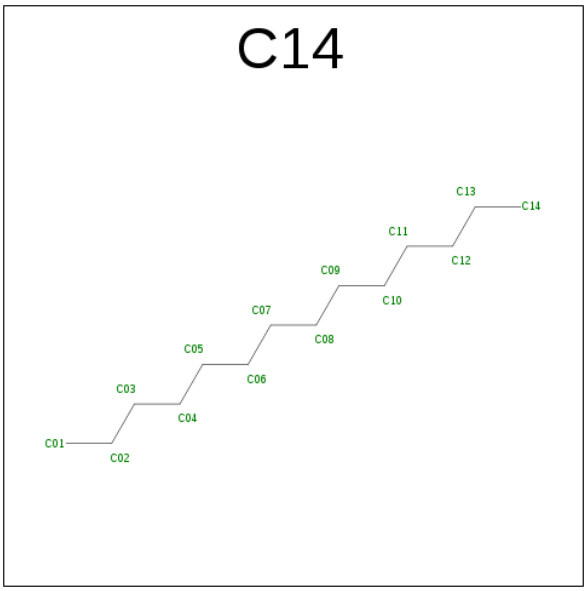
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
5	A	1	Total	C	N	O		0	0
			14	8	1	5			
5	A	1	Total	C	N	O		0	0
			14	8	1	5			

- Molecule 6 is CHOLESTEROL (three-letter code: CLR) (formula: $C_{27}H_{46}O$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	1	Total C O 28 27 1	0	0

- Molecule 7 is TETRADECANE (three-letter code: C14) (formula: $C_{14}H_{30}$).

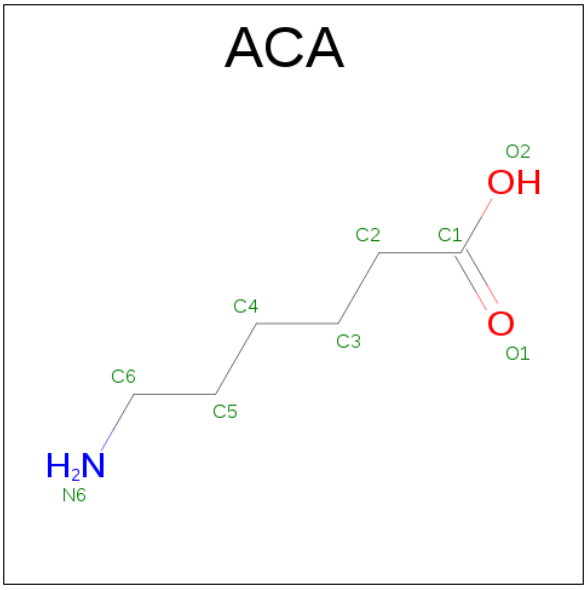


Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	A	1	Total C 14 14	0	0

- Molecule 8 is SODIUM ION (three-letter code: NA) (formula: Na).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
8	A	2	Total Na 2 2	0	0

- Molecule 9 is 6-AMINOHEXANOIC ACID (three-letter code: ACA) (formula: $C_6H_{13}NO_2$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
9	A	1	Total C N O 9 6 1 2	0	0

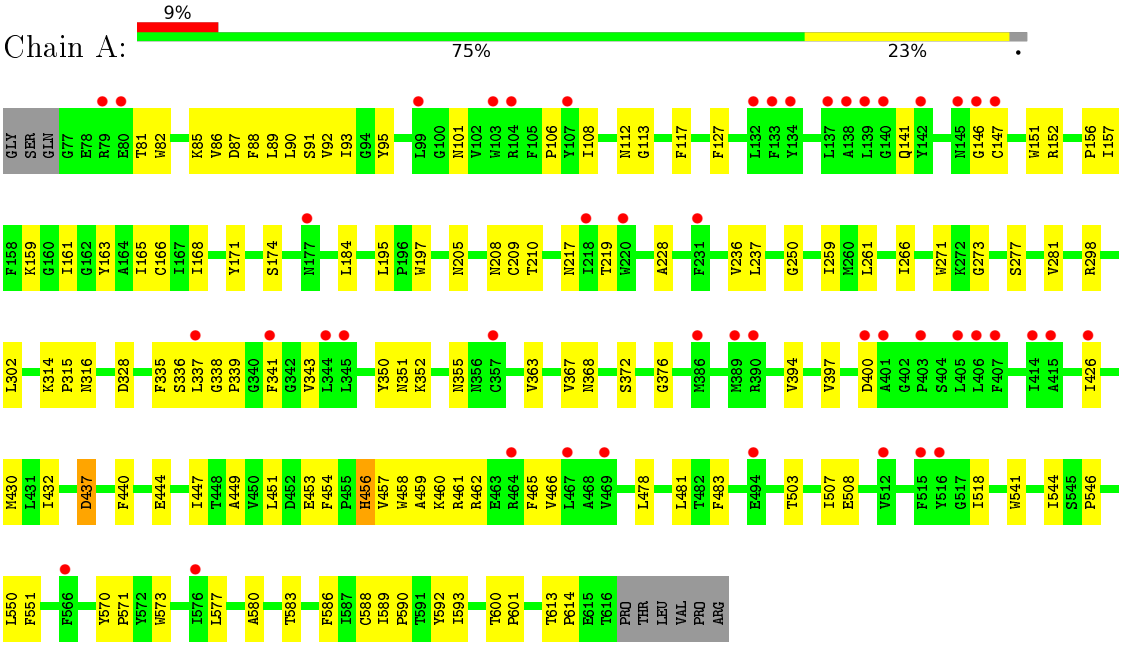
- Molecule 10 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
10	A	1	Total O 1 1	0	0

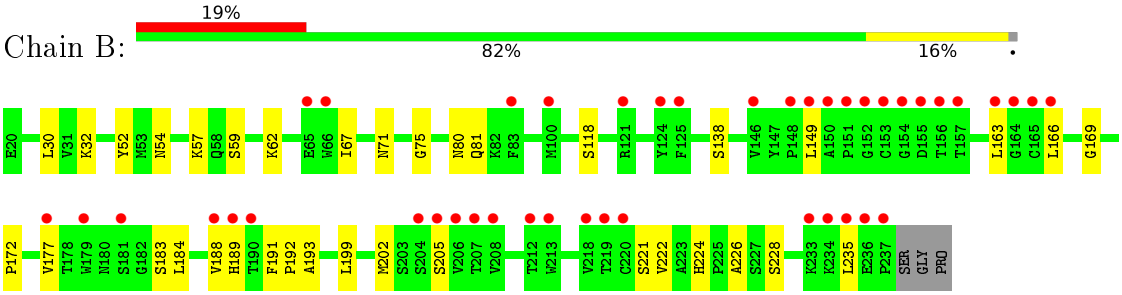
3 Residue-property plots (i)

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.

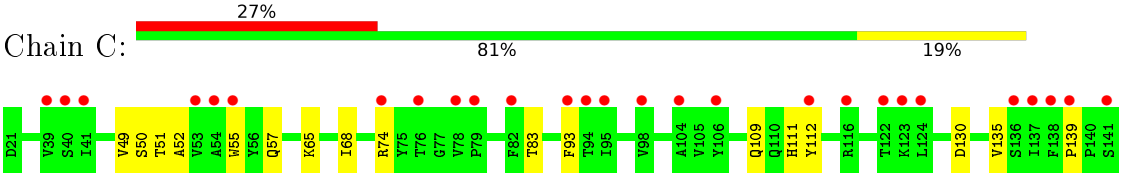
- Molecule 1: Sodium-dependent serotonin transporter

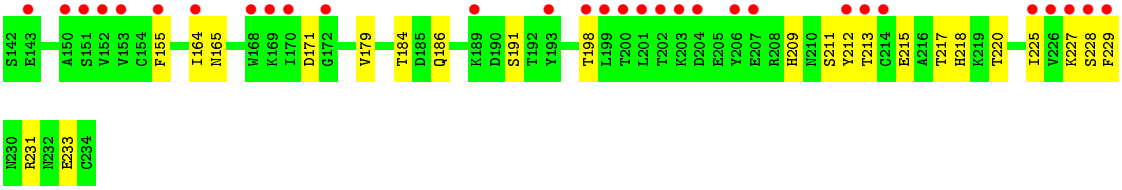


- Molecule 2: 8B6 antibody, heavy chain



- Molecule 3: 8B6 antibody, light chain




S142
E143
A150
S151
V152
V153
C154
F155
I164
N165
W168
K169
I170
D171
Q172
V179
T184
D185
Q186
K189
D190
S191
T192
Y193
T198
L199
T200
L201
T202
K203
D204
E205
Y206
E207
R208
H209
N210
S211
Y212
T213
C214
E215
A216
T217
H218
K219
T220
I225
V226
K227
S228
F229
N230
R231
N232
E233
C234

4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α, β, γ	129.85Å 163.21Å 140.47Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	50.18 – 3.24 82.33 – 3.24	Depositor EDS
% Data completeness (in resolution range)	98.3 (50.18-3.24) 98.3 (82.33-3.24)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.27 (at 3.26Å)	Xtriage
Refinement program	PHENIX (DEV_2000: ???)	Depositor
R, R_{free}	0.233 , 0.275 0.231 , 0.274	Depositor DCC
R_{free} test set	2253 reflections (5.01%)	DCC
Wilson B-factor (Å^2)	125.9	Xtriage
Anisotropy	0.095	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.27 , 112.8	EDS
L-test for twinning[2]	$< \|L\| > = 0.41$, $< L^2 > = 0.24$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.87	EDS
Total number of atoms	7633	wwPDB-VP
Average B, all atoms (Å^2)	175.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.61% 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: ACA, NAG, NA, 68P, CLR, C14

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	0.29	0/4331	0.44	0/5922
2	B	0.22	0/1688	0.41	0/2309
3	C	0.23	0/1700	0.40	0/2307
All	All	0.26	0/7719	0.42	0/10538

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	456	HIS	Peptide

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	4198	0	4094	114	0
2	B	1643	0	1589	22	0
3	C	1662	0	1585	27	0
4	A	48	0	0	1	0
5	A	28	0	26	1	0
6	A	28	0	46	5	0
7	A	14	0	30	4	0
8	A	2	0	0	0	0
9	A	9	0	12	0	0
10	A	1	0	0	0	0
All	All	7633	0	7382	165	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 11.

All (165) 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)
2:B:188:VAL:HG23	2:B:205:SER:O	1.50	1.12
1:A:86:VAL:CG1	1:A:90:LEU:HD13	1.92	0.98
1:A:277:SER:O	1:A:281:VAL:HG23	1.64	0.98
1:A:338:GLY:N	1:A:339:PRO:HD2	1.78	0.95
1:A:589:ILE:CG2	1:A:590:PRO:HD3	1.98	0.93
1:A:589:ILE:HG23	1:A:590:PRO:HD3	1.52	0.92
1:A:86:VAL:HG12	1:A:90:LEU:HD13	1.53	0.89
1:A:86:VAL:HG13	1:A:90:LEU:CD1	2.02	0.89
1:A:458:TRP:O	1:A:459:ALA:HB3	1.72	0.88
1:A:338:GLY:N	1:A:339:PRO:CD	2.39	0.86
1:A:161:ILE:HG13	1:A:589:ILE:HD12	1.57	0.85
1:A:454:PHE:HB3	1:A:457:VAL:HG11	1.59	0.85
1:A:444:GLU:OE1	1:A:462:ARG:NH2	2.10	0.84
1:A:277:SER:O	1:A:281:VAL:CG2	2.25	0.84
1:A:454:PHE:HB3	1:A:457:VAL:CG1	2.08	0.83
1:A:147:CYS:H	1:A:449:ALA:HB2	1.45	0.80
1:A:86:VAL:HG13	1:A:90:LEU:HD13	1.62	0.79
1:A:86:VAL:CG1	1:A:90:LEU:CD1	2.61	0.77
1:A:583:THR:HG21	7:A:704:C14:H081	1.68	0.76
1:A:205:ASN:ND2	1:A:209:CYS:SG	2.59	0.75
1:A:454:PHE:O	1:A:457:VAL:CG1	2.36	0.73
1:A:88:PHE:HE2	1:A:350:TYR:HB2	1.53	0.73
1:A:454:PHE:O	1:A:458:TRP:HB2	1.89	0.73
1:A:458:TRP:O	1:A:459:ALA:CB	2.36	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:52:ALA:HB1	3:C:111:HIS:CE1	2.23	0.72
1:A:113:GLY:HA2	1:A:316:ASN:HB3	1.71	0.71
1:A:141:GLN:NE2	1:A:351:ASN:OD1	2.24	0.71
1:A:394:VAL:O	1:A:397:VAL:HG12	1.92	0.70
1:A:157:ILE:HB	1:A:593:ILE:HG12	1.71	0.70
1:A:208:ASN:O	1:A:210:THR:HG23	1.91	0.69
1:A:91:SER:HA	1:A:281:VAL:HG11	1.73	0.69
1:A:589:ILE:HG23	1:A:590:PRO:CD	2.22	0.69
1:A:108:ILE:HD11	1:A:328:ASP:HB3	1.74	0.69
1:A:447:ILE:HD13	1:A:466:VAL:HG22	1.76	0.68
2:B:188:VAL:CG2	2:B:205:SER:O	2.37	0.67
1:A:88:PHE:CE2	1:A:350:TYR:HB2	2.28	0.67
1:A:337:LEU:C	1:A:339:PRO:HD3	2.16	0.66
2:B:30:LEU:HD22	2:B:172:PRO:HD3	1.76	0.66
3:C:50:SER:OG	3:C:51:THR:N	2.27	0.65
1:A:589:ILE:HG22	1:A:590:PRO:HD3	1.77	0.65
2:B:54:ASN:ND2	2:B:118:SER:OG	2.29	0.65
3:C:211:SER:HA	3:C:229:PHE:O	1.97	0.65
1:A:337:LEU:C	1:A:339:PRO:CD	2.65	0.64
3:C:52:ALA:CB	3:C:111:HIS:CE1	2.82	0.62
2:B:192:PRO:HD3	3:C:184:THR:HG22	1.81	0.62
1:A:437:ASP:N	1:A:437:ASP:OD1	2.32	0.62
1:A:454:PHE:C	1:A:457:VAL:HG12	2.18	0.62
1:A:161:ILE:CG1	1:A:589:ILE:HD12	2.29	0.62
1:A:147:CYS:H	1:A:449:ALA:CB	2.12	0.61
2:B:177:VAL:HA	2:B:221:SER:O	2.01	0.61
3:C:49:VAL:HG22	3:C:112:TYR:CE1	2.35	0.61
1:A:454:PHE:C	1:A:457:VAL:CG1	2.70	0.60
1:A:112:ASN:O	1:A:117:PHE:HB2	2.01	0.60
3:C:171:ASP:OD2	3:C:209:HIS:ND1	2.33	0.60
1:A:152:ARG:HE	1:A:159:LYS:HZ2	1.49	0.60
1:A:146:GLY:HA3	1:A:449:ALA:HA	1.82	0.59
1:A:588:CYS:O	1:A:592:TYR:HB2	2.02	0.59
1:A:273:GLY:HA2	1:A:462:ARG:CZ	2.31	0.59
1:A:454:PHE:O	1:A:457:VAL:HG13	2.02	0.59
1:A:454:PHE:O	1:A:457:VAL:HG12	2.02	0.59
1:A:101:ASN:ND2	1:A:372:SER:OG	2.34	0.59
1:A:458:TRP:CZ3	1:A:465:PHE:HB2	2.39	0.58
3:C:74:ARG:HH21	3:C:83:THR:HG22	1.67	0.58
1:A:586:PHE:O	1:A:589:ILE:HG22	2.02	0.58
1:A:86:VAL:HG13	1:A:90:LEU:HD11	1.85	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:224:HIS:O	2:B:228:SER:N	2.37	0.57
1:A:87:ASP:O	1:A:91:SER:HB2	2.03	0.56
1:A:236:VAL:HG13	1:A:237:LEU:N	2.20	0.55
1:A:85:LYS:HE2	1:A:355:ASN:HD21	1.71	0.55
1:A:456:HIS:N	1:A:458:TRP:O	2.35	0.55
3:C:49:VAL:HG13	3:C:112:TYR:CD1	2.41	0.55
1:A:454:PHE:CB	1:A:457:VAL:HG11	2.34	0.55
1:A:577:LEU:HD13	6:A:703:CLR:H151	1.89	0.55
1:A:352:LYS:HB2	1:A:355:ASN:HB2	1.90	0.53
1:A:440:PHE:O	1:A:444:GLU:HB2	2.08	0.53
2:B:32:LYS:HG2	2:B:138:SER:HA	1.90	0.52
1:A:573:TRP:CE3	6:A:703:CLR:H71	2.43	0.52
1:A:454:PHE:HB3	1:A:457:VAL:HG13	1.88	0.52
1:A:86:VAL:HA	1:A:89:LEU:HB3	1.92	0.52
2:B:71:ASN:O	2:B:75:GLY:N	2.43	0.52
1:A:197:TRP:HB2	1:A:228:ALA:HA	1.91	0.51
1:A:336:SER:OG	1:A:368:ASN:ND2	2.38	0.51
1:A:583:THR:CG2	7:A:704:C14:H081	2.38	0.51
1:A:184:LEU:HD21	1:A:261:LEU:HD23	1.92	0.51
3:C:49:VAL:HG12	3:C:49:VAL:O	2.11	0.51
1:A:161:ILE:HG13	1:A:589:ILE:CD1	2.34	0.51
1:A:460:LYS:HG3	1:A:461:ARG:N	2.25	0.50
1:A:478:LEU:HD23	1:A:481:LEU:HD12	1.94	0.50
2:B:59:SER:HB2	2:B:62:LYS:HB2	1.94	0.49
2:B:177:VAL:HG22	2:B:222:VAL:HG22	1.92	0.49
1:A:151:TRP:HZ2	1:A:508:GLU:HG2	1.77	0.49
3:C:55:TRP:HB2	3:C:68:ILE:HB	1.95	0.49
1:A:457:VAL:HG13	1:A:458:TRP:N	2.28	0.49
1:A:456:HIS:N	1:A:458:TRP:H	2.11	0.48
3:C:165:ASN:HB3	3:C:217:THR:HB	1.94	0.48
3:C:130:ASP:HB3	3:C:220:THR:HG22	1.96	0.48
3:C:49:VAL:HG11	3:C:52:ALA:O	2.13	0.48
1:A:163:TYR:O	1:A:166:CYS:HB2	2.14	0.48
1:A:580:ALA:HB1	6:A:703:CLR:H241	1.96	0.48
1:A:363:VAL:O	1:A:367:VAL:HG23	2.14	0.47
1:A:106:PRO:HG3	1:A:376:GLY:HA2	1.97	0.47
1:A:573:TRP:CZ3	6:A:703:CLR:H71	2.50	0.47
1:A:341:PHE:HD2	1:A:343:VAL:HG23	1.80	0.47
1:A:152:ARG:HH21	1:A:159:LYS:HZ1	1.62	0.46
2:B:193:ALA:HA	2:B:202:MET:HB3	1.97	0.46
1:A:236:VAL:HG13	1:A:237:LEU:H	1.80	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:451:LEU:HD23	1:A:458:TRP:HB3	1.96	0.46
2:B:163:LEU:HB3	2:B:235:LEU:HD22	1.98	0.46
1:A:259:ILE:HG21	1:A:481:LEU:HD11	1.98	0.46
1:A:165:ILE:O	1:A:168:ILE:HB	2.16	0.46
3:C:164:ILE:HB	3:C:218:HIS:HD2	1.79	0.46
1:A:250:GLY:H	1:A:483:PHE:HE2	1.62	0.46
1:A:613:THR:HA	1:A:614:PRO:HD2	1.73	0.46
1:A:81:THR:OG1	1:A:82:TRP:N	2.48	0.46
1:A:266:ILE:HA	1:A:440:PHE:HE1	1.80	0.45
3:C:186:GLN:HE21	3:C:191:SER:HB3	1.82	0.45
2:B:149:LEU:HD11	2:B:166:LEU:HB2	1.98	0.45
1:A:456:HIS:HA	1:A:458:TRP:O	2.17	0.45
1:A:156:PRO:O	1:A:159:LYS:HB2	2.16	0.45
7:A:704:C14:H122	7:A:704:C14:H081	1.99	0.45
2:B:57:LYS:HB2	2:B:67:ILE:HD11	1.98	0.45
2:B:224:HIS:CE1	2:B:226:ALA:HB3	2.51	0.44
3:C:231:ARG:O	3:C:233:GLU:N	2.49	0.44
1:A:219:THR:OG1	5:A:706:NAG:H61	2.18	0.44
1:A:503:THR:O	1:A:507:ILE:HG12	2.17	0.44
1:A:195:LEU:H	1:A:195:LEU:HD12	1.83	0.43
1:A:453:GLU:HG3	1:A:454:PHE:CD1	2.53	0.43
1:A:447:ILE:HA	1:A:465:PHE:HE2	1.82	0.43
3:C:57:GLN:O	3:C:65:LYS:N	2.39	0.43
2:B:80:ASN:OD1	2:B:81:GLN:N	2.51	0.43
6:A:703:CLR:H162	6:A:703:CLR:H231	2.01	0.43
2:B:183:SER:HA	2:B:184:LEU:HA	1.51	0.43
3:C:215:GLU:HA	3:C:225:ILE:O	2.19	0.43
1:A:171:TYR:O	1:A:174:SER:HB2	2.18	0.43
1:A:277:SER:O	1:A:281:VAL:HG21	2.12	0.42
1:A:85:LYS:NZ	1:A:355:ASN:OD1	2.47	0.42
1:A:451:LEU:CD2	1:A:458:TRP:HB3	2.49	0.42
2:B:52:TYR:HE1	2:B:71:ASN:HB2	1.84	0.42
3:C:55:TRP:CD2	3:C:93:PHE:HB2	2.54	0.42
3:C:212:TYR:HB2	3:C:229:PHE:CE1	2.54	0.42
1:A:394:VAL:O	1:A:397:VAL:CG1	2.63	0.41
1:A:600:THR:HA	1:A:601:PRO:HD3	1.89	0.41
1:A:426:ILE:O	1:A:430:MET:HB2	2.20	0.41
1:A:518:ILE:HD11	1:A:541:TRP:CE3	2.54	0.41
1:A:546:PRO:O	1:A:550:LEU:HB2	2.20	0.41
2:B:188:VAL:HG22	2:B:189:HIS:N	2.35	0.41
2:B:169:GLY:HA2	2:B:199:LEU:HB3	2.01	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:212:TYR:O	3:C:228:SER:HA	2.20	0.41
1:A:298:ARG:O	1:A:302:LEU:HG	2.20	0.41
1:A:335:PHE:HE2	4:A:701:68P:N04	2.18	0.41
1:A:95:TYR:CD1	1:A:343:VAL:HG11	2.55	0.41
1:A:437:ASP:HA	1:A:440:PHE:CD2	2.56	0.41
1:A:89:LEU:O	1:A:92:VAL:HG12	2.21	0.41
1:A:184:LEU:HA	1:A:432:ILE:HD11	2.01	0.41
1:A:570:TYR:HA	1:A:571:PRO:HD3	1.94	0.41
7:A:704:C14:H072	7:A:704:C14:H031	2.02	0.41
3:C:135:VAL:HA	3:C:155:PHE:O	2.21	0.41
3:C:179:VAL:HA	3:C:198:THR:O	2.21	0.41
3:C:139:PRO:HB3	3:C:229:PHE:CE2	2.56	0.41
2:B:191:PHE:HA	2:B:192:PRO:HD3	1.87	0.40
1:A:90:LEU:O	1:A:93:ILE:N	2.54	0.40
3:C:50:SER:OG	3:C:51:THR:HG23	2.20	0.40
1:A:314:LYS:HA	1:A:315:PRO:HD3	1.88	0.40
1:A:127:PHE:HB3	1:A:544:ILE:HG21	2.03	0.40
3:C:213:THR:HA	3:C:227:LYS:O	2.22	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	538/549 (98%)	520 (97%)	18 (3%)	0	100	100
2	B	216/221 (98%)	207 (96%)	9 (4%)	0	100	100
3	C	212/214 (99%)	197 (93%)	15 (7%)	0	100	100
All	All	966/984 (98%)	924 (96%)	42 (4%)	0	100	100

There are no Ramachandran outliers to report.

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	428/462 (93%)	423 (99%)	5 (1%)	78 92
2	B	190/193 (98%)	190 (100%)	0	100 100
3	C	189/190 (100%)	188 (100%)	1 (0%)	92 97
All	All	807/845 (96%)	801 (99%)	6 (1%)	88 96

All (6) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	217	ASN
1	A	271	TRP
1	A	400	ASP
1	A	437	ASP
1	A	551	PHE
3	C	109	GLN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

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 (i)

Of 9 ligands modelled in this entry, 2 are monoatomic - leaving 7 for Mogul analysis.

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	$\#\|Z\| > 2$
4	68P	A	701	-	24,26,26	5.84	14 (58%)	31,37,37	1.33	5 (16%)
5	NAG	A	702	1	14,14,15	0.42	0	15,19,21	0.41	0
6	CLR	A	703	-	31,31,31	0.81	0	48,48,48	1.24	4 (8%)
7	C14	A	704	-	13,13,13	0.14	0	12,12,12	0.63	0
4	68P	A	705	-	24,26,26	5.86	14 (58%)	31,37,37	1.13	1 (3%)
5	NAG	A	706	1	14,14,15	0.22	0	15,19,21	0.29	0
9	ACA	A	709	-	5,8,8	0.30	0	5,8,8	0.80	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
4	68P	A	701	-	-	0/15/27/27	0/3/3/3
5	NAG	A	702	1	-	0/6/23/26	0/1/1/1
6	CLR	A	703	-	-	0/10/68/68	0/4/4/4
7	C14	A	704	-	-	0/11/11/11	0/0/0/0
4	68P	A	705	-	-	0/15/27/27	0/3/3/3
5	NAG	A	706	1	-	0/6/23/26	0/1/1/1
9	ACA	A	709	-	-	0/4/6/6	0/0/0/0

All (28) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	701	68P	C18-C24	3.57	1.53	1.44
4	A	705	68P	C18-C24	3.66	1.53	1.44
4	A	705	68P	O02-C11	3.70	1.49	1.44
4	A	701	68P	O02-C11	4.04	1.50	1.44
4	A	701	68P	C17-C18	4.95	1.50	1.39
4	A	705	68P	C17-C18	5.16	1.50	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	705	68P	C08-C07	6.04	1.48	1.39
4	A	701	68P	C08-C07	6.04	1.48	1.39
4	A	701	68P	C13-C17	7.00	1.52	1.38
4	A	705	68P	C13-C17	7.11	1.52	1.38
4	A	705	68P	C14-C18	7.53	1.53	1.39
4	A	701	68P	C14-C18	7.57	1.53	1.39
4	A	701	68P	C19-C21	7.62	1.52	1.37
4	A	705	68P	C19-C21	7.64	1.52	1.37
4	A	705	68P	C16-C20	7.75	1.54	1.38
4	A	705	68P	C15-C19	7.81	1.54	1.38
4	A	701	68P	C16-C20	7.92	1.54	1.38
4	A	701	68P	C15-C19	7.96	1.54	1.38
4	A	705	68P	C20-C21	8.15	1.53	1.37
4	A	705	68P	C16-C10	8.24	1.52	1.39
4	A	701	68P	C16-C10	8.27	1.52	1.39
4	A	701	68P	C20-C21	8.32	1.53	1.37
4	A	705	68P	C15-C10	9.13	1.53	1.39
4	A	705	68P	C14-C08	9.18	1.55	1.39
4	A	701	68P	C15-C10	9.20	1.53	1.39
4	A	701	68P	C14-C08	9.39	1.55	1.39
4	A	701	68P	C13-C07	10.92	1.54	1.39
4	A	705	68P	C13-C07	11.62	1.55	1.39

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
6	A	703	CLR	C8-C7-C6	-2.87	108.33	112.76
4	A	701	68P	C10-C05-C07	-2.72	108.80	115.42
4	A	701	68P	C09-C06-C05	-2.60	110.59	115.23
6	A	703	CLR	C13-C14-C8	-2.48	110.50	114.36
4	A	701	68P	C19-C21-C20	-2.29	119.53	122.87
4	A	701	68P	C11-C08-C14	2.02	133.64	129.40
6	A	703	CLR	C4-C5-C10	2.14	119.52	116.41
6	A	703	CLR	C9-C10-C5	2.64	114.21	109.67
4	A	701	68P	O02-C11-C08	2.81	107.99	104.68
4	A	705	68P	O02-C11-C08	3.19	108.43	104.68

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

4 monomers are involved in 11 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	701	68P	1	0
6	A	703	CLR	5	0
7	A	704	C14	4	0
5	A	706	NAG	1	0

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	540/549 (98%)	0.59	47 (8%) 13 8	83, 146, 214, 351	0
2	B	218/221 (98%)	1.03	43 (19%) 1 1	93, 173, 323, 427	0
3	C	214/214 (100%)	1.24	57 (26%) 1 1	100, 206, 375, 496	0
All	All	972/984 (98%)	0.83	147 (15%) 3 2	83, 159, 313, 496	0

All (147) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	151	PRO	23.9
2	B	150	ALA	13.6
2	B	155	ASP	10.7
2	B	152	GLY	10.6
3	C	203	LYS	8.6
3	C	214	CYS	7.0
3	C	227	LYS	6.7
2	B	204	SER	6.6
2	B	236	GLU	6.5
3	C	153	VAL	6.3
3	C	201	LEU	6.1
3	C	229	PHE	6.1
2	B	156	THR	6.1
1	A	134	TYR	6.0
2	B	188	VAL	5.9
3	C	228	SER	5.8
3	C	152	VAL	5.7
3	C	138	PHE	5.7
3	C	170	ILE	5.6
3	C	226	VAL	5.6
3	C	155	PHE	5.4
1	A	401	ALA	5.3
3	C	200	THR	5.3

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Mol	Chain	Res	Type	RSRZ
2	B	154	GLY	5.3
3	C	95	ILE	5.2
3	C	225	ILE	5.1
3	C	106	TYR	5.0
1	A	400	ASP	5.0
2	B	208	VAL	4.9
3	C	93	PHE	4.9
2	B	163	LEU	4.8
3	C	41	ILE	4.8
2	B	153	CYS	4.8
2	B	190	THR	4.8
3	C	207	GLU	4.8
1	A	389	MET	4.5
2	B	237	PRO	4.5
2	B	149	LEU	4.4
1	A	390	ARG	4.3
2	B	205	SER	4.3
3	C	212	TYR	4.2
2	B	179	TRP	4.1
3	C	78	VAL	4.0
2	B	164	GLY	4.0
1	A	337	LEU	4.0
1	A	139	LEU	3.9
1	A	407	PHE	3.8
1	A	220	TRP	3.8
2	B	235	LEU	3.7
2	B	157	THR	3.7
1	A	103	TRP	3.7
3	C	79	PRO	3.7
3	C	206	TYR	3.6
3	C	172	GLY	3.6
3	C	124	LEU	3.6
2	B	165	CYS	3.6
3	C	151	SER	3.5
3	C	139	PRO	3.5
1	A	80	GLU	3.5
3	C	94	THR	3.5
1	A	147	CYS	3.4
1	A	405	LEU	3.4
3	C	141	SER	3.4
2	B	121	ARG	3.4
3	C	112	TYR	3.3

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Mol	Chain	Res	Type	RSRZ
3	C	82	PHE	3.3
3	C	122	THR	3.3
2	B	233	LYS	3.3
2	B	65	GLU	3.3
3	C	169	LYS	3.2
1	A	406	LEU	3.1
1	A	137	LEU	3.0
3	C	202	THR	3.0
1	A	133	PHE	3.0
3	C	104	ALA	3.0
3	C	198	THR	3.0
1	A	414	ILE	3.0
2	B	66	TRP	2.9
3	C	55	TRP	2.9
1	A	104	ARG	2.9
2	B	219	THR	2.9
2	B	189	HIS	2.9
3	C	53	VAL	2.9
1	A	386	MET	2.9
2	B	213	TRP	2.9
2	B	146	VAL	2.9
3	C	137	ILE	2.9
1	A	142	TYR	2.9
3	C	76	THR	2.9
2	B	206	VAL	2.8
1	A	341	PHE	2.8
3	C	143	GLU	2.8
3	C	164	ILE	2.8
3	C	40	SER	2.7
1	A	140	GLY	2.7
3	C	136	SER	2.7
1	A	345	LEU	2.7
3	C	116	ARG	2.6
2	B	220	CYS	2.6
3	C	54	ALA	2.6
1	A	566	PHE	2.6
1	A	464	ARG	2.6
3	C	39	VAL	2.6
3	C	123	LYS	2.6
1	A	494	GLU	2.6
2	B	177	VAL	2.6
1	A	231	PHE	2.5

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Mol	Chain	Res	Type	RSRZ
1	A	177	ASN	2.5
1	A	516	TYR	2.5
1	A	403	PRO	2.5
2	B	218	VAL	2.5
2	B	148	PRO	2.4
2	B	100	MET	2.4
2	B	83	PHE	2.4
2	B	166	LEU	2.4
1	A	138	ALA	2.4
2	B	124	TYR	2.4
3	C	150	ALA	2.4
1	A	512	VAL	2.3
1	A	145	ASN	2.3
2	B	212	THR	2.3
2	B	181	SER	2.3
3	C	74	ARG	2.3
1	A	426	ILE	2.3
1	A	146	GLY	2.2
1	A	99	LEU	2.2
1	A	576	ILE	2.2
1	A	132	LEU	2.2
2	B	234	LYS	2.2
2	B	207	THR	2.2
3	C	98	VAL	2.2
1	A	357	CYS	2.2
1	A	218	ILE	2.2
3	C	193	TYR	2.1
1	A	467	LEU	2.1
3	C	189	LYS	2.1
3	C	168	TRP	2.1
1	A	344	LEU	2.1
3	C	199	LEU	2.1
1	A	79	ARG	2.0
1	A	107	TYR	2.0
2	B	125	PHE	2.0
1	A	415	ALA	2.0
3	C	204	ASP	2.0
1	A	469	VAL	2.0
3	C	213	THR	2.0
1	A	515	PHE	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
5	NAG	A	706	14/15	0.85	0.97	6.17	266,279,291,294	0
4	68P	A	701	24/24	0.91	1.01	5.40	134,148,167,180	0
4	68P	A	705	24/24	0.87	0.89	4.42	134,173,213,222	0
6	CLR	A	703	28/28	0.75	0.68	3.39	165,196,215,233	0
7	C14	A	704	14/14	0.91	0.44	1.14	103,104,109,109	14
5	NAG	A	702	14/15	0.94	0.24	0.28	82,111,149,154	0
8	NA	A	708	1/1	0.88	0.10	-1.58	130,130,130,130	0
8	NA	A	707	1/1	0.40	0.17	-1.60	260,260,260,260	0
9	ACA	A	709	9/9	0.79	0.51	-	118,144,199,204	0

6.5 Other polymers (i)

There are no such residues in this entry.