Full wwPDB X-ray Structure Validation Report (i)

Feb 1, 2016 – 10:23 PM GMT

PDB ID	:	4XNX
Title	:	X-ray structure of Drosophila dopamine transporter in complex with reboxetine
Authors	:	Aravind, P.; Wang, K.; Gouaux, E.
Deposited on	:	2015-01-16
Resolution	:	3.00 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:

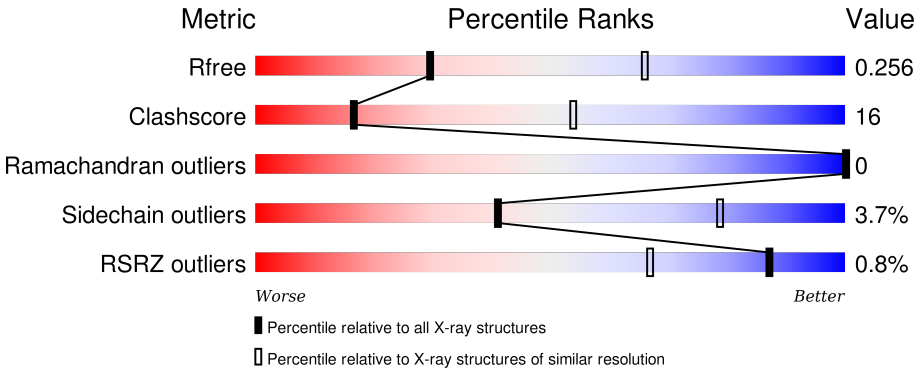
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	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 3.00 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	1578 (3.00-3.00)
Clashscore	102246	1912 (3.00-3.00)
Ramachandran outliers	100387	1853 (3.00-3.00)
Sidechain outliers	100360	1856 (3.00-3.00)
RSRZ outliers	91569	1592 (3.00-3.00)

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	536	68% 32%
2	L	214	66% 31%
3	H	240	3% 63% 25% 10%

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
6	NA	A	704	-	-	-	X

2 Entry composition

There are 9 unique types of molecules in this entry. The entry contains 7536 atoms, of which 22 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 Transporter.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	536	Total	C	N	O	S	0	1	0
			4189	2807	646	718	18			

There are 43 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	74	ALA	VAL	engineered mutation	UNP A0A0B4KEX2
A	?	-	SER	deletion	UNP A0A0B4KEX2
A	?	-	GLN	deletion	UNP A0A0B4KEX2
A	?	-	ASN	deletion	UNP A0A0B4KEX2
A	?	-	ALA	deletion	UNP A0A0B4KEX2
A	?	-	SER	deletion	UNP A0A0B4KEX2
A	?	-	ARG	deletion	UNP A0A0B4KEX2
A	?	-	VAL	deletion	UNP A0A0B4KEX2
A	?	-	PRO	deletion	UNP A0A0B4KEX2
A	?	-	VAL	deletion	UNP A0A0B4KEX2
A	?	-	ILE	deletion	UNP A0A0B4KEX2
A	?	-	GLY	deletion	UNP A0A0B4KEX2
A	?	-	ASN	deletion	UNP A0A0B4KEX2
A	?	-	TYR	deletion	UNP A0A0B4KEX2
A	?	-	SER	deletion	UNP A0A0B4KEX2
A	?	-	ASP	deletion	UNP A0A0B4KEX2
A	?	-	LEU	deletion	UNP A0A0B4KEX2
A	?	-	TYR	deletion	UNP A0A0B4KEX2
A	?	-	ALA	deletion	UNP A0A0B4KEX2
A	?	-	MET	deletion	UNP A0A0B4KEX2
A	?	-	GLY	deletion	UNP A0A0B4KEX2
A	?	-	ASN	deletion	UNP A0A0B4KEX2
A	?	-	GLN	deletion	UNP A0A0B4KEX2
A	?	-	SER	deletion	UNP A0A0B4KEX2
A	?	-	LEU	deletion	UNP A0A0B4KEX2
A	?	-	LEU	deletion	UNP A0A0B4KEX2
A	?	-	TYR	deletion	UNP A0A0B4KEX2

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Chain	Residue	Modelled	Actual	Comment	Reference
A	?	-	ASN	deletion	UNP A0A0B4KEX2
A	?	-	GLU	deletion	UNP A0A0B4KEX2
A	?	-	THR	deletion	UNP A0A0B4KEX2
A	?	-	TYR	deletion	UNP A0A0B4KEX2
A	?	-	MET	deletion	UNP A0A0B4KEX2
A	?	-	ASN	deletion	UNP A0A0B4KEX2
A	?	-	GLY	deletion	UNP A0A0B4KEX2
A	?	-	SER	deletion	UNP A0A0B4KEX2
A	?	-	SER	deletion	UNP A0A0B4KEX2
A	?	-	LEU	deletion	UNP A0A0B4KEX2
A	?	-	ASP	deletion	UNP A0A0B4KEX2
A	?	-	THR	deletion	UNP A0A0B4KEX2
A	?	-	SER	deletion	UNP A0A0B4KEX2
A	?	-	ALA	deletion	UNP A0A0B4KEX2
A	?	-	VAL	deletion	UNP A0A0B4KEX2
A	415	ALA	LEU	engineered mutation	UNP A0A0B4KEX2

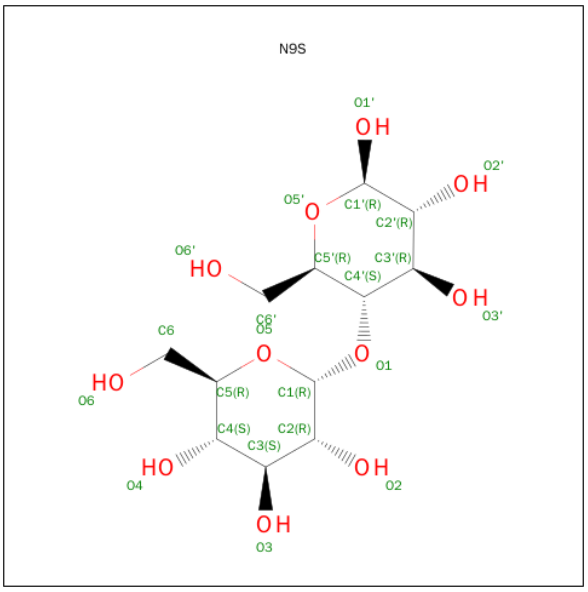
- Molecule 2 is a protein called antibody fragment light chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	L	214	Total	C	N	O	S	0	0	0
			1613	1002	265	338	8			

- Molecule 3 is a protein called Antibody fragment heavy chain.

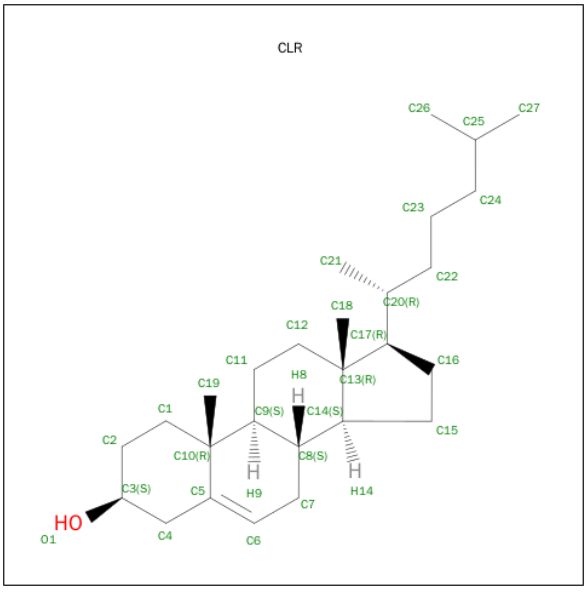
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	H	216	Total	C	N	O	S	0	0	0
			1601	1010	270	313	8			

- Molecule 4 is 4-O-alpha-D-Glucopyranosyl-beta-D-glucopyranose (three-letter code: N9S) (formula: $C_{12}H_{22}O_{11}$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	1	Total	C	H	O	0	0
			45	12	22	11		

- Molecule 5 is CHOLESTEROL (three-letter code: CLR) (formula: $C_{27}H_{46}O$).



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

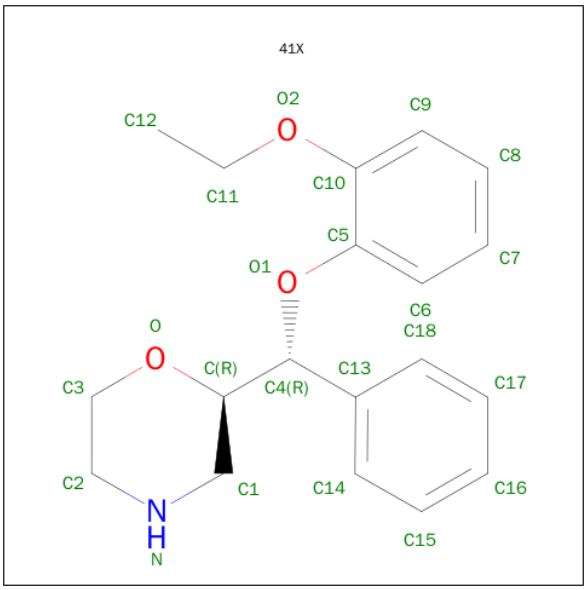
- Molecule 6 is SODIUM ION (three-letter code: NA) (formula: Na).

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

- Molecule 7 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	A	1	Total Cl 1 1	0	0

- Molecule 8 is (2R)-2-[(R)-(2-ethoxyphenoxy)(phenyl)methyl]morpholine (three-letter code: 41X) (formula: $C_{19}H_{23}NO_3$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
8	A	1	Total C N O 23 19 1 3	0	0

- Molecule 9 is water.

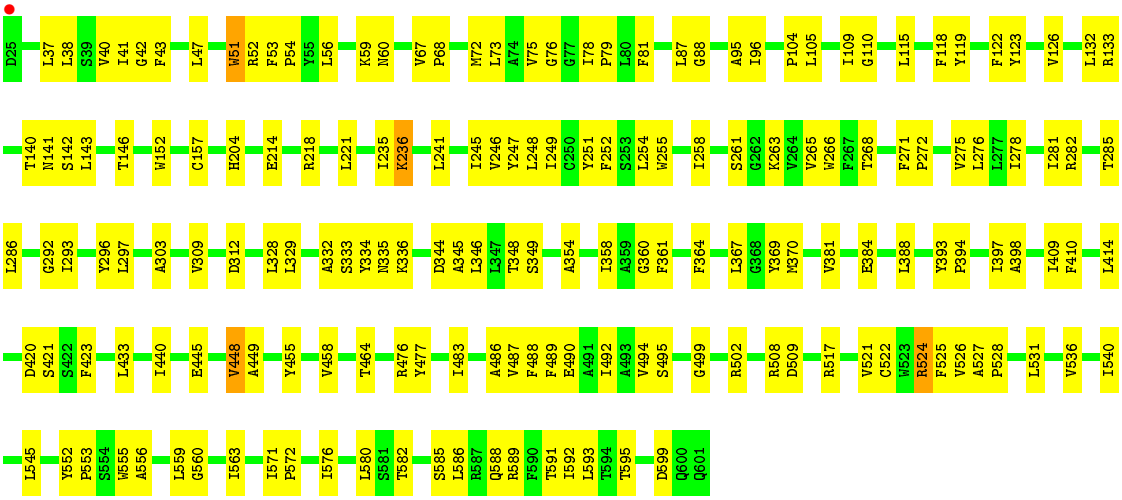
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
9	A	5	Total O 5 5	0	0
9	L	1	Total O 1 1	0	0

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.

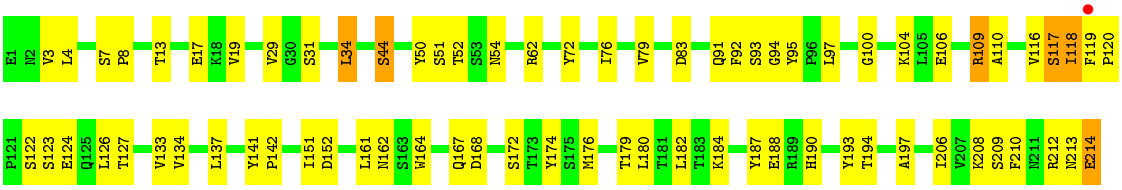
- Molecule 1: Transporter

Chain A:



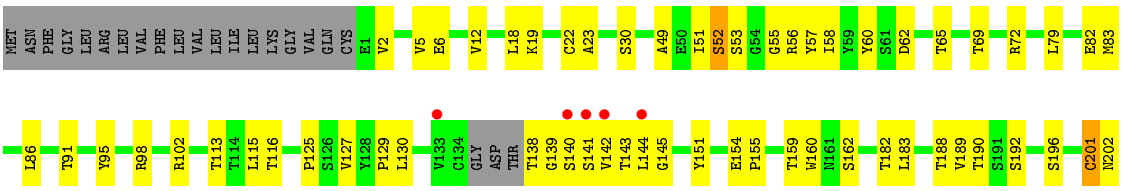
- Molecule 2: antibody fragment light chain

Chain L:



- Molecule 3: Antibody fragment heavy chain

Chain H:




T210
K211
K214
K215
I216
R219
GLY
PRO

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	97.67Å 141.04Å 167.25Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	48.42 – 3.00 48.42 – 3.00	Depositor EDS
% Data completeness (in resolution range)	98.1 (48.42-3.00) 93.7 (48.42-3.00)	Depositor EDS
R_{merge}	0.11	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	3.66 (at 3.01Å)	Xtriage
Refinement program	PHENIX	Depositor
R, R_{free}	0.217 , 0.258 0.221 , 0.256	Depositor DCC
R_{free} test set	1996 reflections (4.73%)	DCC
Wilson B-factor (Å^2)	105.2	Xtriage
Anisotropy	0.265	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.29 , 68.9	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Outliers	1 of 46792 reflections (0.002%)	Xtriage
F_o,F_c correlation	0.93	EDS
Total number of atoms	7536	wwPDB-VP
Average B, all atoms (Å^2)	110.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.89% 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: NA, N9S, 41X, CLR, CL

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	0/4333	0.45	0/5929
2	L	0.28	0/1651	0.48	0/2248
3	H	0.28	0/1639	0.47	0/2234
All	All	0.29	0/7623	0.46	0/10411

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
3	H	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
3	H	98	ARG	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	4189	0	4056	126	0
2	L	1613	0	1504	66	0
3	H	1601	0	1532	56	0
4	A	23	22	22	1	0
5	A	56	0	92	4	0
6	A	2	0	0	0	0
7	A	1	0	0	0	0
8	A	23	0	23	1	0
9	A	5	0	0	0	0
9	L	1	0	0	0	0
All	All	7514	22	7229	243	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 16.

All (243) 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)
3:H:51:ILE:HD13	3:H:72:ARG:HG3	1.39	1.04
2:L:134:VAL:HG12	2:L:179:THR:HG23	1.57	0.85
2:L:19:VAL:HG13	2:L:79:VAL:HG21	1.59	0.84
1:A:527:ALA:HB3	1:A:528:PRO:HD3	1.62	0.81
2:L:34:LEU:HB3	2:L:52:THR:HG22	1.62	0.79
2:L:188:GLU:HG2	2:L:212:ARG:NH2	1.98	0.79
2:L:91:GLN:HE21	2:L:94:GLY:H	1.29	0.78
1:A:140:THR:HG22	1:A:142:SER:H	1.47	0.78
1:A:582:THR:O	1:A:589:ARG:NE	2.17	0.77
3:H:5:VAL:CG2	3:H:23:ALA:HB3	2.14	0.76
2:L:126:LEU:O	2:L:184:LYS:NZ	2.16	0.76
3:H:91:THR:HG23	3:H:116:THR:HA	1.68	0.76
2:L:118:ILE:HD11	2:L:208:LYS:C	2.08	0.73
1:A:52:ARG:NH1	1:A:384:GLU:OE1	2.22	0.72
2:L:34:LEU:HB3	2:L:52:THR:CG2	2.18	0.72
1:A:146:THR:HG22	1:A:398:ALA:HB1	1.70	0.72
2:L:91:GLN:NE2	2:L:94:GLY:H	1.88	0.71
3:H:5:VAL:HG23	3:H:23:ALA:HB3	1.72	0.71
3:H:51:ILE:HG13	3:H:58:ILE:CD1	2.21	0.70
1:A:75:VAL:O	1:A:79:PRO:HG2	1.91	0.70
1:A:59:LYS:NZ	1:A:312:ASP:OD2	2.24	0.69
1:A:487:VAL:HG12	1:A:531:LEU:HD11	1.73	0.69
3:H:139:GLY:HA2	3:H:140:SER:C	2.11	0.69
2:L:119:PHE:HB2	2:L:134:VAL:HG22	1.76	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:L:19:VAL:HG22	2:L:76:ILE:HB	1.76	0.67
1:A:152:TRP:O	1:A:218:ARG:HD3	1.94	0.67
3:H:83:MET:HB3	3:H:86:LEU:HD21	1.76	0.67
2:L:120:PRO:HB3	2:L:210:PHE:CE2	2.31	0.66
3:H:159:THR:OG1	3:H:202:ASN:OD1	2.15	0.65
3:H:51:ILE:CD1	3:H:72:ARG:HG3	2.24	0.65
2:L:116:VAL:HG22	2:L:137:LEU:HD22	1.79	0.65
3:H:125:PRO:HB3	3:H:151:TYR:HB3	1.79	0.64
1:A:235:ILE:HG12	1:A:464:THR:HG22	1.79	0.64
1:A:251:TYR:CE2	1:A:449:ALA:HB2	2.33	0.64
1:A:433:LEU:HB3	1:A:440:ILE:HD11	1.80	0.63
3:H:12:VAL:CG2	3:H:18:LEU:HD12	2.29	0.63
1:A:502:ARG:HG3	3:H:56:ARG:NH2	2.14	0.63
2:L:214:GLU:OE1	2:L:214:GLU:N	2.32	0.63
1:A:143:LEU:O	1:A:146:THR:HG23	1.99	0.62
2:L:188:GLU:HG2	2:L:212:ARG:HH21	1.64	0.62
2:L:116:VAL:HG22	2:L:137:LEU:CD2	2.30	0.62
1:A:109:ILE:HA	1:A:571:ILE:HD11	1.82	0.62
2:L:193:TYR:HB2	2:L:210:PHE:CE1	2.36	0.60
3:H:6:GLU:HB3	3:H:113:THR:HG22	1.84	0.60
1:A:252:PHE:HA	1:A:255:TRP:CD1	2.37	0.60
2:L:19:VAL:HG13	2:L:79:VAL:CG2	2.31	0.60
3:H:22:CYS:HB3	3:H:79:LEU:HB3	1.83	0.60
1:A:524:ARG:HG3	1:A:525:PHE:CD2	2.37	0.59
1:A:591:THR:O	1:A:595:THR:HG23	2.03	0.59
3:H:18:LEU:HD23	3:H:19:LYS:N	2.16	0.59
1:A:524:ARG:HG3	1:A:525:PHE:N	2.18	0.59
3:H:12:VAL:HG21	3:H:18:LEU:HD12	1.85	0.59
1:A:53:PHE:HB3	1:A:54:PRO:HD3	1.84	0.59
2:L:182:LEU:HD11	2:L:187:TYR:HB2	1.84	0.59
1:A:75:VAL:HG23	1:A:76:GLY:H	1.68	0.59
1:A:292:GLY:HA3	1:A:364:PHE:O	2.02	0.59
1:A:370:MET:HE1	1:A:381:VAL:HB	1.85	0.58
1:A:502:ARG:HG3	3:H:56:ARG:CZ	2.33	0.58
2:L:123:SER:O	2:L:127:THR:HG23	2.04	0.58
1:A:75:VAL:HG23	1:A:76:GLY:N	2.18	0.58
3:H:18:LEU:HD23	3:H:19:LYS:H	1.68	0.58
2:L:162:ASN:HB3	2:L:176:MET:CE	2.33	0.58
2:L:194:THR:HG23	2:L:209:SER:HB2	1.85	0.58
1:A:588:GLN:O	1:A:592:ILE:HG12	2.04	0.58
1:A:75:VAL:HB	1:A:526:VAL:HG11	1.86	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:297:LEU:HD11	1:A:361:PHE:CZ	2.38	0.57
1:A:96:ILE:HA	1:A:110:GLY:HA3	1.87	0.57
1:A:293:ILE:HD12	1:A:361:PHE:CD2	2.40	0.57
2:L:34:LEU:HD22	2:L:72:TYR:CD2	2.40	0.56
1:A:571:ILE:HB	1:A:572:PRO:HD3	1.87	0.56
2:L:19:VAL:CG1	2:L:79:VAL:HG21	2.32	0.56
1:A:251:TYR:HE2	1:A:449:ALA:HB2	1.70	0.56
1:A:571:ILE:HB	1:A:572:PRO:CD	2.36	0.56
3:H:210:THR:C	3:H:211:LYS:HD2	2.27	0.55
1:A:123:TYR:O	1:A:126:VAL:HG12	2.06	0.55
1:A:42:GLY:C	1:A:420:ASP:HB3	2.27	0.55
3:H:129:PRO:HD3	3:H:214:LYS:CD	2.36	0.55
3:H:162:SER:H	3:H:202:ASN:HD21	1.53	0.55
1:A:109:ILE:HA	1:A:571:ILE:CD1	2.37	0.55
3:H:211:LYS:HD2	3:H:211:LYS:N	2.22	0.55
2:L:95:TYR:OH	3:H:102:ARG:NH2	2.40	0.55
1:A:364:PHE:HA	1:A:367:LEU:HB2	1.89	0.54
2:L:4:LEU:HB2	2:L:100:GLY:HA2	1.90	0.54
1:A:95:ALA:HA	1:A:329:LEU:CD2	2.38	0.54
1:A:40:VAL:CG1	1:A:348:THR:HG21	2.39	0.53
2:L:117:SER:HB2	2:L:119:PHE:HE1	1.74	0.53
1:A:95:ALA:HA	1:A:329:LEU:HD23	1.91	0.53
1:A:553:PRO:HB2	1:A:555:TRP:CD1	2.44	0.53
2:L:29:VAL:HG13	2:L:93:SER:HB2	1.90	0.53
1:A:40:VAL:HG11	1:A:348:THR:HG21	1.90	0.53
1:A:241:LEU:O	1:A:245:ILE:HG13	2.08	0.53
1:A:508:ARG:O	1:A:508:ARG:HD2	2.08	0.53
2:L:164:TRP:CD1	2:L:176:MET:HG3	2.43	0.53
1:A:132:LEU:HD12	1:A:246:VAL:HG23	1.91	0.52
1:A:275:VAL:HG13	1:A:409:ILE:HD12	1.90	0.52
1:A:56:LEU:O	1:A:60:ASN:HB2	2.09	0.52
1:A:236:LYS:NZ	1:A:236:LYS:HB3	2.24	0.52
2:L:44:SER:HB3	3:H:95:TYR:CE1	2.45	0.52
3:H:6:GLU:HB3	3:H:113:THR:CG2	2.40	0.52
3:H:192:SER:O	3:H:196:SER:OG	2.24	0.52
1:A:599:ASP:OD1	3:H:56:ARG:HD2	2.10	0.52
2:L:109:ARG:NH1	2:L:110:ALA:O	2.43	0.51
1:A:43:PHE:HA	1:A:421:SER:HA	1.92	0.51
1:A:410:PHE:CE2	1:A:414:LEU:HD11	2.45	0.51
2:L:17:GLU:O	2:L:79:VAL:HG23	2.10	0.51
2:L:161:LEU:HD13	3:H:182:THR:HB	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:433:LEU:CB	1:A:440:ILE:HD11	2.41	0.51
1:A:38:LEU:HD13	1:A:266:TRP:HA	1.91	0.51
1:A:488:PHE:O	1:A:492:ILE:HG12	2.12	0.50
3:H:6:GLU:N	3:H:6:GLU:OE1	2.43	0.50
3:H:69:THR:HB	3:H:82:GLU:HG3	1.93	0.50
3:H:62:ASP:O	3:H:65:THR:HG22	2.11	0.50
2:L:182:LEU:CD1	2:L:187:TYR:HB2	2.41	0.50
1:A:303:ALA:HB1	1:A:309:VAL:HG21	1.94	0.50
2:L:162:ASN:HB3	2:L:176:MET:HE2	1.94	0.50
1:A:140:THR:HG22	1:A:141:ASN:N	2.27	0.49
3:H:140:SER:O	3:H:190:THR:HA	2.12	0.49
1:A:489:PHE:CD2	1:A:571:ILE:HG21	2.48	0.49
2:L:91:GLN:HG2	2:L:93:SER:H	1.78	0.49
1:A:81:PHE:CZ	1:A:348:THR:HG22	2.48	0.49
2:L:167:GLN:HB2	2:L:174:TYR:CE2	2.48	0.49
2:L:13:THR:HG21	2:L:19:VAL:CG1	2.43	0.49
3:H:51:ILE:HG13	3:H:58:ILE:HD11	1.91	0.49
1:A:37:LEU:O	1:A:41:ILE:HG12	2.13	0.49
1:A:476:ARG:CD	1:A:545:LEU:HD13	2.43	0.49
1:A:73:LEU:O	1:A:78:ILE:HG12	2.12	0.49
1:A:81:PHE:CE2	1:A:328:LEU:HD11	2.48	0.49
3:H:129:PRO:HD3	3:H:214:LYS:HD3	1.95	0.49
3:H:130:LEU:HB2	3:H:145:GLY:C	2.32	0.48
1:A:296:TYR:CZ	1:A:360:GLY:HA3	2.48	0.48
2:L:44:SER:HB3	3:H:95:TYR:HE1	1.79	0.48
1:A:157:CYS:HB2	1:A:214:GLU:OE1	2.12	0.48
3:H:49:ALA:HB2	3:H:60:TYR:HD1	1.78	0.48
1:A:245:ILE:O	1:A:249:ILE:HG13	2.13	0.48
1:A:119:TYR:O	1:A:122:PHE:HB2	2.13	0.48
1:A:115:LEU:O	1:A:118:PHE:HB3	2.14	0.48
2:L:197:ALA:O	2:L:206:ILE:HG22	2.13	0.48
1:A:410:PHE:O	1:A:414:LEU:HG	2.14	0.47
2:L:62:ARG:HD2	2:L:83:ASP:OD2	2.14	0.47
1:A:51:TRP:HA	1:A:388:LEU:HD23	1.95	0.47
1:A:585:SER:OG	1:A:586:LEU:N	2.47	0.47
1:A:281:ILE:O	1:A:285:THR:HG23	2.13	0.47
5:A:703:CLR:H273	5:A:703:CLR:H231	1.61	0.47
2:L:31:SER:O	2:L:52:THR:HG23	2.15	0.47
2:L:118:ILE:HD11	2:L:209:SER:N	2.30	0.47
3:H:130:LEU:HB2	3:H:145:GLY:O	2.15	0.47
1:A:522:CYS:HA	1:A:526:VAL:HB	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:H:83:MET:CB	3:H:86:LEU:HD21	2.45	0.47
2:L:162:ASN:HB3	2:L:176:MET:HE3	1.96	0.47
5:A:702:CLR:H183	5:A:702:CLR:H212	1.97	0.47
1:A:476:ARG:HD3	1:A:545:LEU:HD13	1.95	0.46
1:A:393:TYR:HB3	1:A:394:PRO:HD3	1.97	0.46
1:A:263:LYS:HA	1:A:266:TRP:CD1	2.50	0.46
2:L:141:TYR:CG	2:L:142:PRO:HA	2.50	0.46
2:L:50:TYR:O	2:L:54:ASN:HB2	2.14	0.46
2:L:52:THR:HG21	2:L:72:TYR:CE2	2.50	0.46
1:A:282:ARG:O	1:A:286:LEU:HG	2.16	0.46
3:H:51:ILE:HG12	3:H:55:GLY:HA2	1.98	0.46
1:A:105:LEU:HB2	1:A:593:LEU:HB3	1.97	0.46
1:A:517:ARG:O	1:A:521:VAL:HG23	2.15	0.46
2:L:151:ILE:HD12	2:L:193:TYR:CD1	2.50	0.46
2:L:34:LEU:HD22	2:L:72:TYR:CG	2.51	0.45
1:A:88:GLY:O	1:A:333:SER:HA	2.16	0.45
3:H:160:TRP:CZ3	3:H:201:CYS:HB2	2.51	0.45
2:L:50:TYR:C	2:L:52:THR:H	2.19	0.45
1:A:254:LEU:HD11	1:A:423:PHE:HA	1.98	0.45
1:A:354:ALA:O	1:A:358:ILE:HG12	2.17	0.45
2:L:124:GLU:OE1	2:L:124:GLU:N	2.40	0.45
1:A:293:ILE:HD12	1:A:361:PHE:HD2	1.79	0.45
1:A:477:TYR:CD2	1:A:560:GLY:HA3	2.52	0.45
1:A:42:GLY:CA	1:A:420:ASP:HB3	2.46	0.45
3:H:127:VAL:O	3:H:214:LYS:HD2	2.16	0.45
2:L:119:PHE:CD2	3:H:130:LEU:HB3	2.52	0.45
1:A:393:TYR:CE2	1:A:397:ILE:HD11	2.52	0.45
3:H:144:LEU:HD13	3:H:216:ILE:HG21	1.99	0.45
1:A:67:VAL:HB	1:A:68:PRO:CD	2.47	0.45
2:L:116:VAL:O	2:L:208:LYS:HD2	2.18	0.44
1:A:54:PRO:HB3	1:A:360:GLY:HA2	1.99	0.44
2:L:161:LEU:CD1	3:H:182:THR:HB	2.47	0.44
5:A:703:CLR:H162	5:A:703:CLR:H222	1.78	0.44
5:A:702:CLR:H121	5:A:702:CLR:H212	2.00	0.44
1:A:104:PRO:HD2	1:A:593:LEU:O	2.16	0.44
1:A:344:ASP:O	1:A:348:THR:HB	2.18	0.44
1:A:495:SER:O	1:A:499:GLY:HA2	2.18	0.44
2:L:19:VAL:HG21	2:L:76:ILE:HD12	1.99	0.44
1:A:72:MET:HE2	1:A:72:MET:HA	1.99	0.44
1:A:332:ALA:O	1:A:335:ASN:HB2	2.18	0.44
3:H:30:SER:O	3:H:53:SER:HB2	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:251:TYR:CD2	1:A:448:VAL:HG23	2.53	0.44
1:A:433:LEU:HB3	1:A:440:ILE:CD1	2.48	0.43
1:A:81:PHE:CZ	1:A:348:THR:CG2	3.02	0.43
1:A:133:ARG:NH2	4:A:701:N9S:H2	2.33	0.43
3:H:154:GLU:CB	3:H:155:PRO:HA	2.48	0.43
3:H:142:VAL:N	3:H:189:VAL:O	2.51	0.43
1:A:81:PHE:HZ	1:A:348:THR:CG2	2.31	0.43
1:A:87:LEU:HD11	1:A:494:VAL:HG21	2.00	0.43
1:A:47:LEU:H	1:A:47:LEU:HD12	1.82	0.43
1:A:258:ILE:HD11	1:A:334:TYR:CD2	2.53	0.43
2:L:62:ARG:NH1	2:L:83:ASP:OD1	2.51	0.43
1:A:263:LYS:HA	1:A:266:TRP:HD1	1.83	0.43
1:A:536:VAL:O	1:A:540:ILE:HG12	2.18	0.43
3:H:143:THR:OG1	3:H:188:THR:HG22	2.19	0.43
2:L:168:ASP:O	2:L:172:SER:HA	2.18	0.43
1:A:367:LEU:HD12	1:A:370:MET:HE2	2.01	0.43
1:A:78:ILE:HB	1:A:79:PRO:HD3	1.99	0.43
1:A:51:TRP:C	1:A:51:TRP:CD1	2.92	0.43
8:A:707:41X:H4	8:A:707:41X:H6	1.71	0.43
1:A:509:ASP:O	3:H:102:ARG:NH1	2.51	0.42
1:A:272:PRO:O	1:A:276:LEU:HG	2.19	0.42
2:L:7:SER:HA	2:L:8:PRO:C	2.39	0.42
1:A:345:ALA:O	1:A:349:SER:OG	2.29	0.42
1:A:122:PHE:CE1	1:A:458:VAL:HG11	2.55	0.42
2:L:104:LYS:NZ	2:L:106:GLU:OE2	2.52	0.42
1:A:524:ARG:CG	1:A:525:PHE:N	2.82	0.42
1:A:553:PRO:HG2	1:A:556:ALA:HB2	2.02	0.42
2:L:109:ARG:HG3	2:L:110:ALA:N	2.34	0.42
3:H:154:GLU:HG2	3:H:155:PRO:HA	2.01	0.42
2:L:188:GLU:HA	2:L:212:ARG:HH21	1.83	0.42
1:A:78:ILE:N	1:A:79:PRO:CD	2.83	0.41
1:A:247:TYR:CZ	1:A:455:TYR:HB3	2.55	0.41
1:A:261:SER:O	1:A:265:VAL:HG13	2.18	0.41
2:L:122:SER:OG	2:L:124:GLU:OE1	2.37	0.41
1:A:483:ILE:HA	1:A:483:ILE:HD12	1.88	0.41
1:A:78:ILE:HD13	1:A:349:SER:HB3	2.03	0.41
1:A:67:VAL:HB	1:A:68:PRO:HD3	2.03	0.41
3:H:183:LEU:HD23	3:H:183:LEU:C	2.41	0.41
3:H:52:SER:OG	3:H:57:TYR:N	2.47	0.41
3:H:12:VAL:HG11	3:H:86:LEU:HD12	2.02	0.41
3:H:143:THR:HG23	3:H:188:THR:HG22	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:H:138:THR:HA	3:H:139:GLY:HA3	1.78	0.41
1:A:251:TYR:OH	1:A:445:GLU:O	2.23	0.41
2:L:164:TRP:HD1	2:L:176:MET:HB2	1.85	0.41
2:L:184:LYS:O	2:L:188:GLU:HG3	2.21	0.41
1:A:265:VAL:HA	1:A:268:THR:OG1	2.21	0.41
1:A:248:LEU:HD23	1:A:248:LEU:HA	1.92	0.41
1:A:576:ILE:O	1:A:580:LEU:HG	2.21	0.41
1:A:559:LEU:O	1:A:563:ILE:HG13	2.22	0.40
1:A:487:VAL:HG12	1:A:531:LEU:CD1	2.48	0.40
1:A:486:ALA:O	1:A:490:GLU:HG3	2.21	0.40
2:L:118:ILE:HD11	2:L:208:LYS:O	2.22	0.40
1:A:545:LEU:HG	1:A:552:TYR:CD1	2.56	0.40
1:A:271:PHE:N	1:A:272:PRO:CD	2.84	0.40
2:L:152:ASP:OD2	2:L:190:HIS:HB3	2.21	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	535/536 (100%)	520 (97%)	15 (3%)	0	100	100
2	L	212/214 (99%)	209 (99%)	3 (1%)	0	100	100
3	H	212/240 (88%)	208 (98%)	4 (2%)	0	100	100
All	All	959/990 (97%)	937 (98%)	22 (2%)	0	100	100

There are no Ramachandran outliers to report.

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	423/441 (96%)	413 (98%)	10 (2%)	57 87
2	L	181/187 (97%)	168 (93%)	13 (7%)	18 53
3	H	173/205 (84%)	167 (96%)	6 (4%)	43 80
All	All	777/833 (93%)	748 (96%)	29 (4%)	41 79

All (29) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	51	TRP
1	A	204	HIS
1	A	221	LEU
1	A	236	LYS
1	A	278	ILE
1	A	336	LYS
1	A	346	LEU
1	A	369	TYR
1	A	448	VAL
1	A	524	ARG
2	L	3	VAL
2	L	34	LEU
2	L	44	SER
2	L	51	SER
2	L	92	PHE
2	L	97	LEU
2	L	109	ARG
2	L	117	SER
2	L	118	ILE
2	L	133	VAL
2	L	180	LEU
2	L	213	ASN
2	L	214	GLU
3	H	2	VAL
3	H	52	SER
3	H	115	LEU

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Mol	Chain	Res	Type
3	H	141	SER
3	H	201	CYS
3	H	211	LYS

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

Mol	Chain	Res	Type
2	L	39	GLN
2	L	91	GLN
3	H	39	GLN
3	H	80	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

Of 7 ligands modelled in this entry, 3 are monoatomic - leaving 4 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	N9S	A	701	-	24,24,24	1.53	4 (16%)	35,35,35	1.44	7 (20%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
5	CLR	A	702	-	31,31,31	0.62	0	48,48,48	1.23	3 (6%)
5	CLR	A	703	-	31,31,31	0.58	0	48,48,48	0.96	2 (4%)
8	41X	A	707	-	25,25,25	0.68	0	26,32,32	1.50	6 (23%)

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	N9S	A	701	-	-	0/8/48/48	0/2/2/2
5	CLR	A	702	-	-	0/10/68/68	0/4/4/4
5	CLR	A	703	-	-	0/10/68/68	0/4/4/4
8	41X	A	707	-	-	0/15/23/23	0/3/3/3

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	701	N9S	O1-C1	-2.42	1.35	1.41
4	A	701	N9S	O5'-C5'	2.37	1.50	1.44
4	A	701	N9S	O3'-C3'	2.54	1.49	1.43
4	A	701	N9S	O5-C1	3.28	1.50	1.41

All (18) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
8	A	707	41X	C3-O-C	-4.75	105.65	112.01
5	A	702	CLR	C8-C7-C6	-3.43	107.58	112.75
4	A	701	N9S	C1-O1-C4'	-3.25	109.51	118.01
5	A	702	CLR	C19-C10-C9	-2.60	108.34	111.67
4	A	701	N9S	C1'-O5'-C5'	-2.32	109.18	113.47
8	A	707	41X	O2-C10-C9	-2.27	119.26	124.01
8	A	707	41X	O1-C5-C6	-2.27	117.91	123.93
5	A	703	CLR	C11-C12-C13	-2.14	109.02	112.84
4	A	701	N9S	O5'-C5'-C6'	2.01	111.43	106.36
4	A	701	N9S	C3-C4-C5	2.01	113.70	110.20
8	A	707	41X	C14-C13-C18	2.07	120.95	118.31
4	A	701	N9S	O5-C5-C4	2.09	113.61	109.68
4	A	701	N9S	C1-C2-C3	2.11	114.13	109.97
5	A	703	CLR	C4-C5-C10	2.24	119.69	116.43
8	A	707	41X	C5-O1-C4	2.34	124.24	118.02

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
8	A	707	41X	O2-C10-C5	2.48	120.99	115.78
4	A	701	N9S	O5-C1-C2	3.29	117.03	110.28
5	A	702	CLR	C4-C5-C10	4.28	122.67	116.43

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

4 monomers are involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	701	N9S	1	0
5	A	702	CLR	2	0
5	A	703	CLR	2	0
8	A	707	41X	1	0

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

The following chains have linkage breaks:

Mol	Chain	Number of breaks
3	H	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	H	134:CYS	C	138:THR	N	9.24

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	536/536 (100%)	-0.18	1 (0%)	95	87	86, 107, 134, 178	0
2	L	214/214 (100%)	-0.22	1 (0%)	91	76	88, 106, 138, 153	0
3	H	216/240 (90%)	-0.16	6 (2%)	56	27	89, 106, 147, 162	0
All	All	966/990 (97%)	-0.18	8 (0%)	87	67	86, 107, 139, 178	0

All (8) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	H	140	SER	3.5
3	H	133	VAL	3.1
3	H	141	SER	3.1
1	A	25	ASP	2.7
3	H	144	LEU	2.4
3	H	142	VAL	2.1
2	L	119	PHE	2.1
3	H	216	ILE	2.1

6.2 Non-standard residues in protein, DNA, RNA chains

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

6.3 Carbohydrates

There are no carbohydrates in this entry.

6.4 Ligands

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
6	NA	A	704	1/1	0.94	0.35	2.03	101,101,101,101	0
5	CLR	A	703	28/28	0.88	0.28	1.36	106,118,125,125	0
5	CLR	A	702	28/28	0.95	0.30	1.12	96,111,116,118	0
8	41X	A	707	23/23	0.93	0.30	1.01	87,98,106,131	0
6	NA	A	705	1/1	0.88	0.30	0.85	105,105,105,105	0
4	N9S	A	701	23/23	0.86	0.16	-0.53	131,156,184,197	0
7	CL	A	706	1/1	0.96	0.12	-5.10	104,104,104,104	0

6.5 Other polymers (i)

There are no such residues in this entry.