Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 10:24 PM GMT

PDB ID	:	4XP1
Title	:	X-ray structure of Drosophila dopamine transporter bound to neurotransmitter dopamine
Authors	:	Gouaux, E.; Penmatsa, A.; Wang, K.
Deposited on	:	2015-01-16
Resolution	:	2.89 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 ⓘ symbol.

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

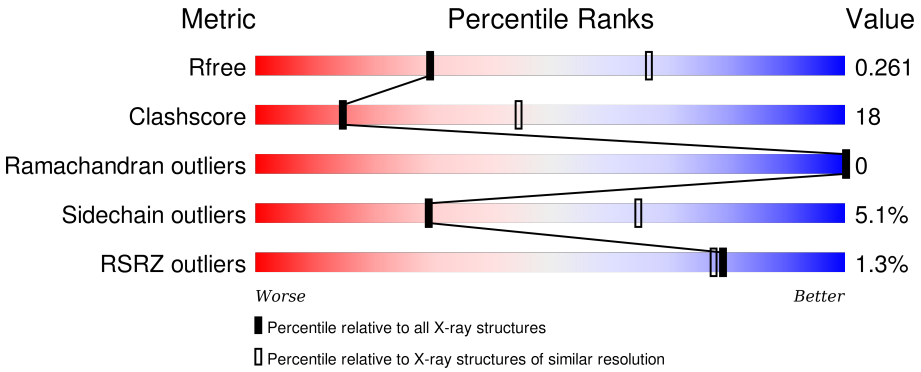
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)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

1 Overall quality at a glance

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.89 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	1451 (2.90-2.90)
Clashscore	102246	1668 (2.90-2.90)
Ramachandran outliers	100387	1630 (2.90-2.90)
Sidechain outliers	100360	1632 (2.90-2.90)
RSRZ outliers	91569	1456 (2.90-2.90)

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	535	63% 35%
2	L	214	71% 27%
3	H	219	5% 68% 32%

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	NA	L	301	-	-	-	X

2 Entry composition

There are 13 unique types of molecules in this entry. The entry contains 7680 atoms, of which 29 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 Dopamine transporter, isoform B.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	535	Total	C	N	O	S	0	1	0
			4230	2837	656	718	19			

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
			1616	1006	268	334	8			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	H	219	Total	C	N	O	S	0	0	0
			1631	1027	277	319	8			

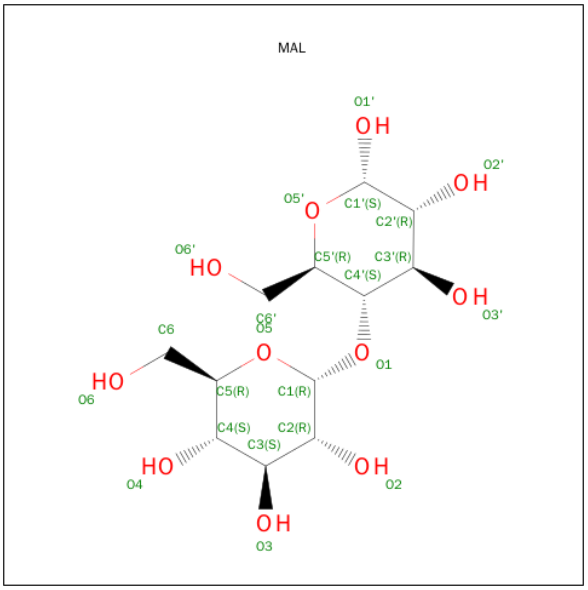
- Molecule 4 is SODIUM ION (three-letter code: NA) (formula: Na).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	2	Total	Na	0	0
			2	2		
4	L	1	Total	Na	0	0
			1	1		

- Molecule 5 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

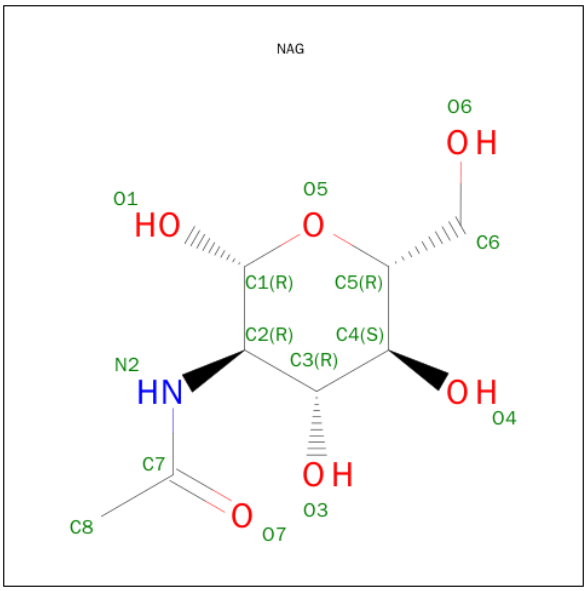
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	1	Total	Cl	0	0
			1	1		

- Molecule 6 is MALTOSE (three-letter code: MAL) (formula: $C_{12}H_{22}O_{11}$).



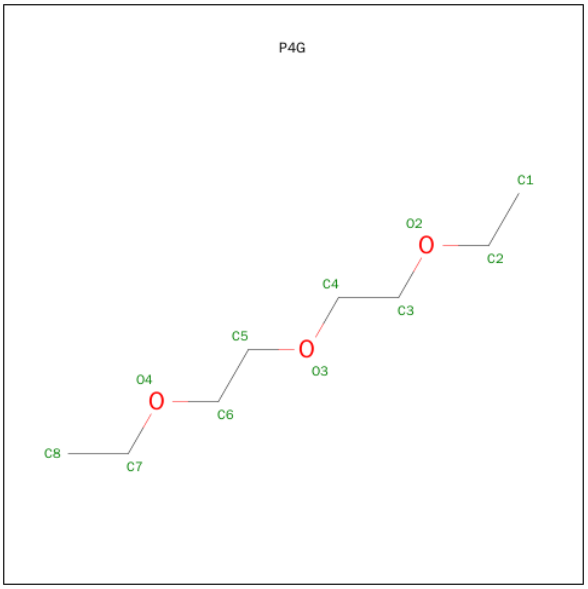
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	1	Total C O 23 12 11	0	0
6	A	1	Total C O 23 12 11	0	0

- Molecule 7 is N-ACETYL-D-GLUCOSAMINE (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).



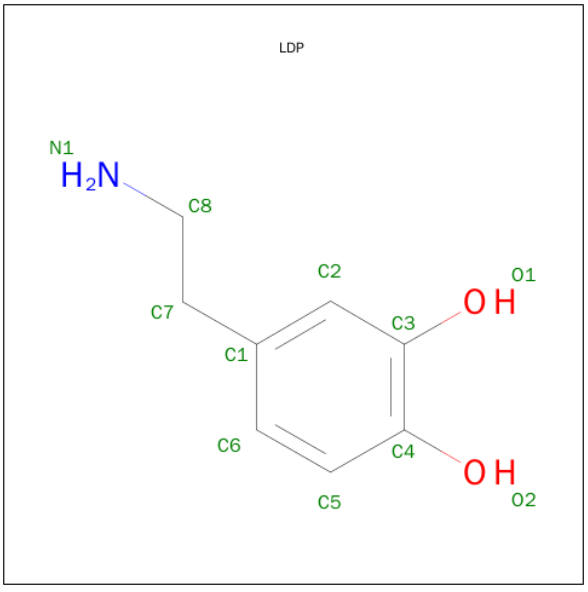
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	A	1	Total C N O 14 8 1 5	0	0

- Molecule 8 is 1-ETHOXY-2-(2-ETHOXYETHOXY)ETHANE (three-letter code: P4G) (formula: $C_8H_{18}O_3$).



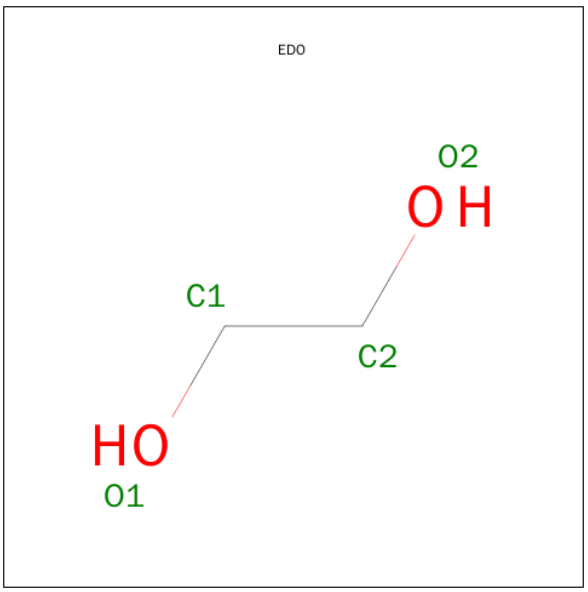
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
8	A	1	Total	C	H	O	0	0
			29	8	18	3		

- Molecule 9 is L-DOPAMINE (three-letter code: LDP) (formula: $C_8H_{11}NO_2$).



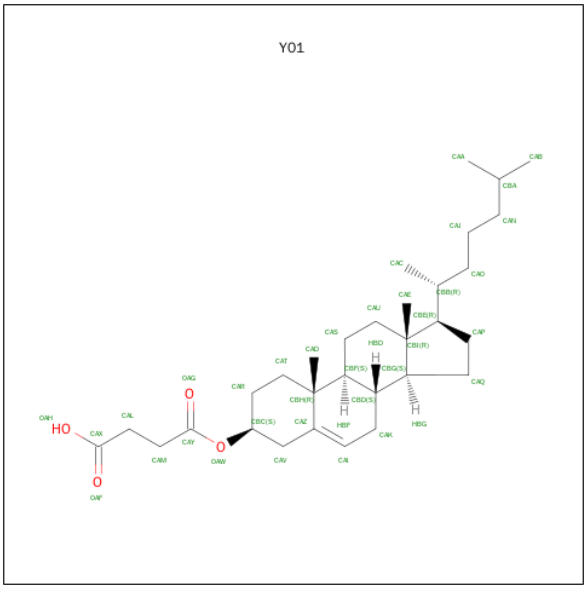
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
9	A	1	Total	C	H	N	O	0	0
			22	8	11	1	2		

- Molecule 10 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: $C_2H_6O_2$).



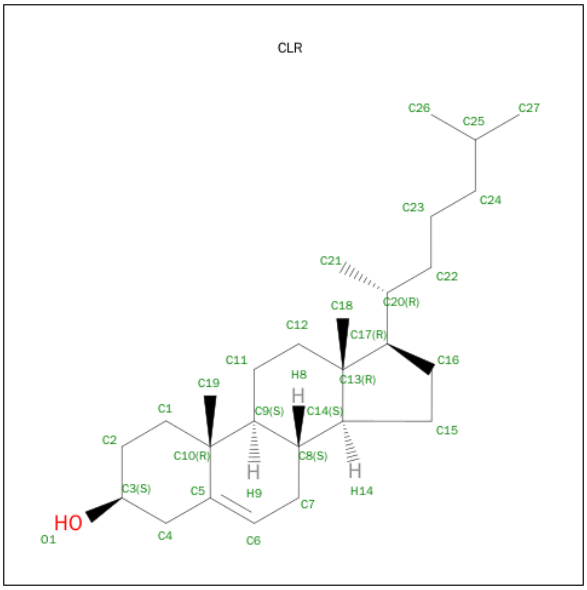
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
10	A	1	Total C O 4 2 2	0	0

- Molecule 11 is CHOLESTEROL HEMISUCCINATE (three-letter code: Y01) (formula: $C_{31}H_{50}O_4$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
11	A	1	Total C O 35 31 4	0	0

- Molecule 12 is CHOLESTEROL (three-letter code: CLR) (formula: $C_{27}H_{46}O$).



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

- Molecule 13 is water.

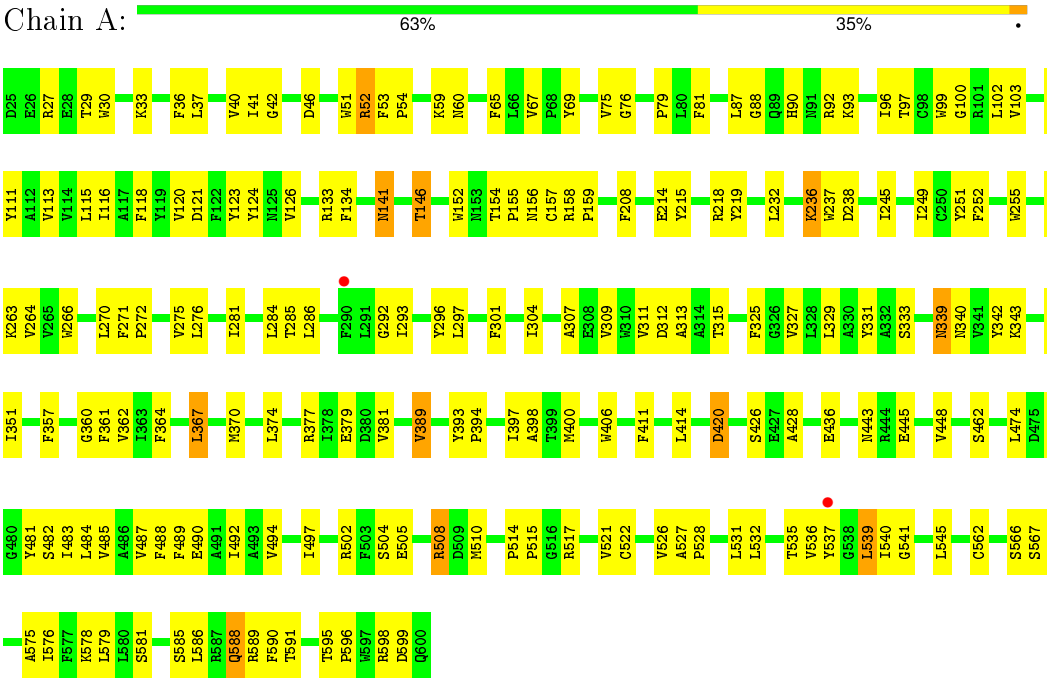
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
13	A	15	Total O 15 15	0	0
13	L	3	Total O 3 3	0	0
13	H	3	Total O 3 3	0	0

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.

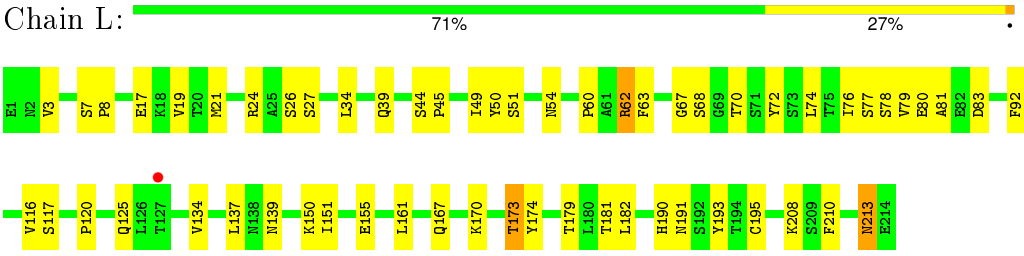
- Molecule 1: Dopamine transporter, isoform B

Chain A:



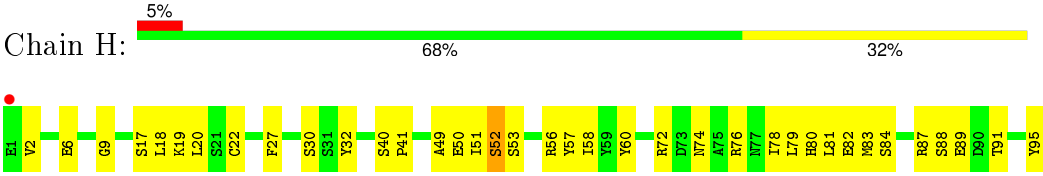
- Molecule 2: Antibody fragment light chain

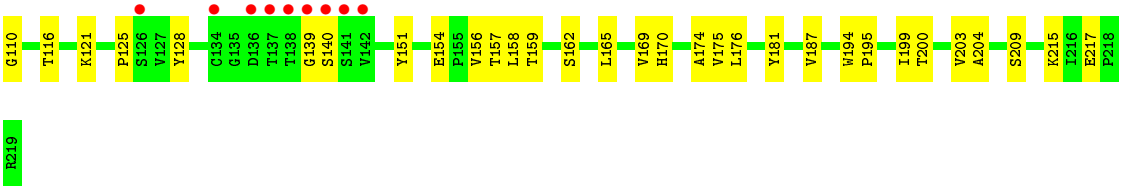
Chain L:



- Molecule 3: antibody fragment heavy chain

Chain H:




G110
T116
K121
P125
S126
V127
Y128
C134
G135
D136
T137
T138
G139
S140
S141
V142
Y151
E154
P155
V156
T157
L158
T159
S162
L165
V169
H170
A174
V175
L176
Y181
V187
W194
P195
I199
T200
V203
A204
S209
K215
I216
E217
P218
R219

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	96.80Å 140.18Å 166.19Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	44.98 – 2.89 44.98 – 2.89	Depositor EDS
% Data completeness (in resolution range)	96.7 (44.98-2.89) 96.4 (44.98-2.89)	Depositor EDS
R_{merge}	0.11	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.05 (at 2.91Å)	Xtriage
Refinement program	PHENIX	Depositor
R, R_{free}	0.218 , 0.256 0.224 , 0.261	Depositor DCC
R_{free} test set	2427 reflections (5.15%)	DCC
Wilson B-factor (Å^2)	82.7	Xtriage
Anisotropy	0.293	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.29 , 60.3	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.33$	Xtriage
Outliers	0 of 49563 reflections	Xtriage
F_o,F_c correlation	0.91	EDS
Total number of atoms	7680	wwPDB-VP
Average B, all atoms (Å^2)	75.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.02% 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: Y01, NAG, CL, P4G, NA, EDO, LDP, MAL, CLR

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	0.34	0/4375	0.51	0/5976
2	L	0.34	0/1654	0.54	0/2250
3	H	0.36	0/1670	0.53	0/2276
All	All	0.34	0/7699	0.52	0/10502

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	2
2	L	0	1
All	All	0	3

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	478	ALA	Peptide
1	A	479	ALA	Peptide
2	L	190	HIS	Peptide

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	4230	0	4155	164	0
2	L	1616	0	1520	50	0
3	H	1631	0	1568	55	0
4	A	2	0	0	0	0
4	L	1	0	0	0	0
5	A	1	0	0	0	0
6	A	46	0	44	5	0
7	A	14	0	13	0	0
8	A	11	18	18	0	0
9	A	11	11	11	0	0
10	A	4	0	6	0	0
11	A	35	0	49	5	0
12	A	28	0	46	4	0
13	A	15	0	0	1	0
13	H	3	0	0	0	0
13	L	3	0	0	0	0
All	All	7651	29	7430	266	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 18.

All (266) 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:200:THR:HG22	3:H:215:LYS:HA	1.50	0.92
1:A:487:VAL:HG12	1:A:531:LEU:HD11	1.53	0.88
11:A:710:Y01:HAO1	11:A:710:Y01:HAA1	1.54	0.88
2:L:134:VAL:HG22	2:L:179:THR:HG23	1.55	0.87
3:H:165:LEU:HD11	3:H:187:VAL:HG21	1.62	0.82
1:A:527:ALA:HB3	1:A:528:PRO:HD3	1.60	0.81
6:A:705:MAL:H5	6:A:705:MAL:H6'2	1.62	0.81
1:A:33:LYS:NZ	1:A:339:ASN:OD1	2.14	0.80
3:H:18:LEU:HD12	3:H:19:LYS:H	1.49	0.78
1:A:364:PHE:HA	1:A:367:LEU:HB2	1.64	0.78
1:A:123:TYR:O	1:A:126:VAL:HG12	1.83	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:75:VAL:HB	1:A:526:VAL:HG11	1.65	0.76
11:A:710:Y01:HAC1	11:A:710:Y01:HAU2	1.68	0.76
3:H:51:ILE:HG13	3:H:58:ILE:HD11	1.67	0.76
3:H:17:SER:HB3	3:H:84:SER:HA	1.68	0.74
1:A:293:ILE:HD12	1:A:361:PHE:HD1	1.51	0.74
3:H:200:THR:HG22	3:H:215:LYS:CA	2.17	0.74
1:A:46:ASP:OD1	1:A:124:TYR:OH	2.06	0.73
1:A:502:ARG:HG3	3:H:56:ARG:NH1	2.02	0.73
2:L:19:VAL:HG22	2:L:76:ILE:HB	1.71	0.73
1:A:251:TYR:CE1	1:A:448:VAL:HG23	2.24	0.73
2:L:34:LEU:HD22	2:L:72:TYR:CG	2.24	0.73
1:A:389:VAL:HG13	1:A:414:LEU:HD11	1.71	0.73
1:A:585:SER:O	1:A:589:ARG:HG2	1.88	0.73
1:A:141:ASN:ND2	1:A:141:ASN:H	1.86	0.72
1:A:53:PHE:HB3	1:A:54:PRO:HD3	1.72	0.70
1:A:237:TRP:HD1	6:A:705:MAL:H62	1.56	0.69
3:H:51:ILE:HD13	3:H:72:ARG:HB2	1.73	0.69
3:H:91:THR:HG23	3:H:116:THR:HA	1.74	0.69
1:A:90:HIS:HB2	1:A:510:MET:CE	2.23	0.69
1:A:293:ILE:HD12	1:A:361:PHE:CD1	2.26	0.69
2:L:151:ILE:HG22	2:L:193:TYR:CD1	2.28	0.69
1:A:370:MET:HG2	1:A:374:LEU:HD12	1.75	0.68
1:A:393:TYR:CE2	1:A:397:ILE:HD11	2.30	0.67
1:A:579:LEU:HD21	1:A:590:PHE:HE1	1.58	0.67
1:A:60:ASN:O	1:A:65:PHE:HB2	1.96	0.66
2:L:34:LEU:HD22	2:L:72:TYR:CD2	2.31	0.66
1:A:297:LEU:HD11	1:A:361:PHE:CZ	2.30	0.66
1:A:93:LYS:HG2	1:A:97:THR:HG21	1.78	0.66
1:A:96:ILE:HD12	1:A:111:TYR:CD1	2.31	0.65
3:H:2:VAL:HG13	3:H:27:PHE:CD1	2.31	0.65
1:A:37:LEU:O	1:A:41:ILE:HG12	1.97	0.65
6:A:705:MAL:C6'	6:A:705:MAL:H5	2.27	0.64
3:H:22:CYS:HB3	3:H:79:LEU:HB3	1.78	0.64
1:A:585:SER:HB3	1:A:588:GLN:HG2	1.78	0.63
1:A:301:PHE:O	1:A:304:ILE:HG22	1.98	0.63
1:A:340:ASN:ND2	1:A:343:LYS:HB2	2.14	0.63
3:H:51:ILE:HG13	3:H:58:ILE:CD1	2.28	0.62
1:A:237:TRP:CD1	6:A:705:MAL:H62	2.33	0.62
2:L:161:LEU:HD11	3:H:175:VAL:HB	1.81	0.62
1:A:27:ARG:NH1	1:A:92:ARG:O	2.32	0.62
2:L:139:ASN:HA	2:L:173:THR:CG2	2.30	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:578:LYS:HA	1:A:581:SER:OG	1.99	0.62
1:A:157:CYS:HB2	1:A:214:GLU:OE1	1.99	0.62
1:A:146:THR:HG23	1:A:398:ALA:HB1	1.81	0.61
1:A:286:LEU:HD11	1:A:400:MET:CE	2.30	0.61
1:A:52:ARG:HH12	1:A:315:THR:HG23	1.66	0.61
2:L:120:PRO:HB3	2:L:210:PHE:CZ	2.36	0.61
1:A:109:ILE:HD11	1:A:489:PHE:HB3	1.83	0.60
1:A:103:VAL:HG11	1:A:497:ILE:HG21	1.83	0.60
3:H:157:THR:HB	3:H:204:ALA:HB3	1.82	0.60
1:A:88:GLY:CA	1:A:329:LEU:HD12	2.31	0.60
3:H:19:LYS:HE2	3:H:80:HIS:ND1	2.17	0.60
2:L:161:LEU:HD21	3:H:175:VAL:CG2	2.32	0.60
11:A:710:Y01:CAO	11:A:710:Y01:HAA1	2.32	0.59
2:L:134:VAL:CG2	2:L:179:THR:HG23	2.28	0.59
1:A:508:ARG:NE	3:H:100:GLU:O	2.36	0.59
1:A:532:LEU:HA	1:A:535:THR:OG1	2.02	0.59
2:L:109:ARG:NH1	2:L:110:ALA:O	2.36	0.59
2:L:49:ILE:HD12	2:L:74:LEU:HD12	1.85	0.59
3:H:194:TRP:CD1	3:H:199:ILE:HG13	2.38	0.59
1:A:42:GLY:O	1:A:420:ASP:HB2	2.03	0.58
1:A:517:ARG:O	1:A:521:VAL:HG23	2.03	0.58
1:A:99:TRP:HH2	1:A:494:VAL:HG23	1.69	0.58
2:L:50:TYR:O	2:L:54:ASN:HB2	2.03	0.58
3:H:40:SER:HB2	3:H:41:PRO:HD2	1.85	0.58
2:L:17:GLU:O	2:L:79:VAL:HG23	2.03	0.58
1:A:397:ILE:HG23	1:A:406:TRP:HB2	1.86	0.57
2:L:44:SER:HB2	3:H:95:TYR:CE1	2.39	0.57
1:A:485:VAL:HG21	1:A:568:VAL:CG1	2.35	0.57
1:A:141:ASN:ND2	1:A:141:ASN:N	2.51	0.57
1:A:489:PHE:CD1	1:A:571:ILE:HG21	2.40	0.56
1:A:40:VAL:HG12	1:A:348:THR:HG21	1.87	0.56
1:A:484:LEU:HD13	1:A:535:THR:CG2	2.35	0.56
1:A:445:GLU:OE1	1:A:445:GLU:N	2.29	0.56
1:A:236:LYS:NZ	1:A:236:LYS:HB3	2.19	0.56
2:L:63:PHE:CE1	2:L:76:ILE:HG12	2.41	0.56
3:H:81:LEU:HD23	3:H:83:MET:HE3	1.86	0.56
1:A:281:ILE:O	1:A:285:THR:HG23	2.05	0.56
1:A:502:ARG:HG3	3:H:56:ARG:CZ	2.37	0.55
1:A:481:TYR:O	1:A:485:VAL:HG13	2.05	0.55
1:A:115:LEU:O	1:A:118:PHE:HB3	2.06	0.55
1:A:60:ASN:HB3	1:A:309:VAL:HG22	1.88	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:L:3:VAL:HG13	2:L:26:SER:HB3	1.88	0.55
1:A:393:TYR:CD2	1:A:397:ILE:HD11	2.42	0.55
1:A:75:VAL:HG23	1:A:76:GLY:N	2.22	0.54
3:H:32:TYR:O	3:H:72:ARG:NH2	2.39	0.54
2:L:167:GLN:HB2	2:L:174:TYR:CE2	2.43	0.54
12:A:711:CLR:H183	12:A:711:CLR:H212	1.89	0.54
1:A:115:LEU:HD23	1:A:567:SER:HA	1.88	0.54
1:A:245:ILE:O	1:A:249:ILE:HG13	2.08	0.54
1:A:271:PHE:CE2	1:A:275:VAL:HG21	2.43	0.54
3:H:19:LYS:HG3	3:H:82:GLU:HG2	1.89	0.54
1:A:505:GLU:OE1	3:H:56:ARG:HD3	2.08	0.54
2:L:81:ALA:HA	2:L:107:MET:SD	2.48	0.54
1:A:508:ARG:O	1:A:508:ARG:HD2	2.08	0.53
2:L:213:ASN:N	2:L:213:ASN:OD1	2.39	0.53
1:A:389:VAL:HG13	1:A:414:LEU:CD1	2.38	0.53
2:L:19:VAL:HG13	2:L:79:VAL:HG21	1.91	0.53
1:A:271:PHE:HB3	1:A:272:PRO:HD3	1.91	0.53
1:A:152:TRP:O	1:A:218:ARG:HD3	2.09	0.53
1:A:476:ARG:CD	1:A:545:LEU:HD13	2.40	0.52
3:H:125:PRO:HB3	3:H:151:TYR:HB3	1.92	0.52
1:A:40:VAL:CG1	1:A:348:THR:HG21	2.39	0.52
3:H:151:TYR:CE2	3:H:156:VAL:HG13	2.44	0.52
3:H:9:GLY:HA2	3:H:18:LEU:HD21	1.91	0.52
1:A:87:LEU:HD22	1:A:102:LEU:HD21	1.92	0.52
1:A:67:VAL:HG11	1:A:304:ILE:HD11	1.91	0.52
1:A:69:TYR:HA	1:A:313:ALA:HB1	1.90	0.52
1:A:490:GLU:O	1:A:494:VAL:HG23	2.10	0.52
3:H:165:LEU:HD11	3:H:187:VAL:CG2	2.38	0.51
2:L:60:PRO:HG2	2:L:63:PHE:CD2	2.45	0.51
2:L:150:LYS:HG2	2:L:155:GLU:HA	1.92	0.51
1:A:585:SER:N	1:A:588:GLN:HG3	2.26	0.51
1:A:251:TYR:HE1	1:A:448:VAL:HG23	1.73	0.51
1:A:99:TRP:CZ2	1:A:490:GLU:HG2	2.46	0.51
3:H:81:LEU:HD23	3:H:83:MET:CE	2.41	0.51
1:A:591:THR:O	1:A:595:THR:HG23	2.11	0.51
2:L:109:ARG:HG3	2:L:110:ALA:O	2.11	0.51
1:A:585:SER:HB3	1:A:588:GLN:CG	2.40	0.50
2:L:116:VAL:O	2:L:208:LYS:HE3	2.11	0.50
1:A:585:SER:H	1:A:588:GLN:HG3	1.77	0.49
1:A:88:GLY:O	1:A:333:SER:HA	2.12	0.49
1:A:393:TYR:HB3	1:A:394:PRO:HD3	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:67:VAL:CG1	1:A:304:ILE:HD11	2.42	0.49
1:A:479:ALA:HB1	1:A:483:ILE:H	1.76	0.49
1:A:96:ILE:HG21	1:A:436:GLU:HG3	1.95	0.49
1:A:75:VAL:O	1:A:79:PRO:HG2	2.13	0.49
2:L:151:ILE:HG22	2:L:193:TYR:CE1	2.47	0.49
1:A:485:VAL:HG21	1:A:568:VAL:HG11	1.93	0.49
3:H:158:LEU:HD23	3:H:159:THR:N	2.27	0.49
1:A:357:PHE:CE2	1:A:361:PHE:HE2	2.30	0.49
1:A:571:ILE:HB	1:A:572:PRO:CD	2.43	0.49
1:A:133:ARG:NH2	6:A:704:MAL:O3'	2.46	0.49
1:A:30:TRP:CD1	1:A:36:PHE:HB2	2.48	0.48
2:L:139:ASN:HA	2:L:173:THR:HG21	1.94	0.48
1:A:476:ARG:HD2	1:A:545:LEU:HD13	1.94	0.48
1:A:598:ARG:NH1	1:A:598:ARG:HB2	2.28	0.48
1:A:292:GLY:HA3	1:A:364:PHE:O	2.13	0.48
1:A:146:THR:CG2	1:A:398:ALA:HB1	2.43	0.48
2:L:139:ASN:HA	2:L:173:THR:HG23	1.95	0.48
1:A:571:ILE:HB	1:A:572:PRO:HD3	1.95	0.48
1:A:154:THR:HB	1:A:155:PRO:HD2	1.95	0.48
1:A:508:ARG:NH2	3:H:50:GLU:OE2	2.37	0.47
1:A:342:TYR:CZ	1:A:346:LEU:HD11	2.49	0.47
3:H:20:LEU:HD12	3:H:83:MET:HE3	1.96	0.47
2:L:151:ILE:HG22	2:L:193:TYR:HD1	1.76	0.47
1:A:484:LEU:HD13	1:A:535:THR:HG22	1.94	0.47
1:A:351:ILE:HD13	12:A:711:CLR:H72	1.95	0.47
1:A:296:TYR:CZ	1:A:360:GLY:HA3	2.49	0.47
2:L:77:SER:OG	2:L:78:SER:N	2.47	0.47
1:A:59:LYS:HG2	1:A:60:ASN:OD1	2.14	0.47
2:L:60:PRO:HG2	2:L:63:PHE:HD2	1.79	0.47
2:L:68:SER:HA	2:L:72:TYR:CZ	2.49	0.47
2:L:161:LEU:HD21	3:H:175:VAL:HG21	1.95	0.47
2:L:125:GLN:HG3	3:H:128:TYR:CE2	2.49	0.47
1:A:158:ARG:HB2	1:A:159:PRO:HD2	1.94	0.47
1:A:575:ALA:O	1:A:579:LEU:HB2	2.15	0.47
1:A:81:PHE:HZ	1:A:348:THR:HG21	1.79	0.47
3:H:49:ALA:HB2	3:H:60:TYR:CD1	2.50	0.47
2:L:67:GLY:HA3	2:L:72:TYR:HA	1.98	0.46
1:A:90:HIS:HB2	1:A:510:MET:HE1	1.94	0.46
3:H:76:ARG:HG2	3:H:76:ARG:HH11	1.81	0.46
2:L:19:VAL:CG2	2:L:76:ILE:HB	2.43	0.46
1:A:484:LEU:HD13	1:A:535:THR:HG23	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:H:194:TRP:CG	3:H:195:PRO:HA	2.51	0.46
3:H:139:GLY:HA2	3:H:140:SER:C	2.35	0.46
1:A:276:LEU:HD22	1:A:362:VAL:HG21	1.97	0.46
1:A:487:VAL:HG12	1:A:531:LEU:CD1	2.37	0.46
2:L:19:VAL:HG21	2:L:76:ILE:HD12	1.96	0.46
1:A:576:ILE:HD13	1:A:576:ILE:HA	1.74	0.46
1:A:134:PHE:HB3	1:A:411:PHE:CE2	2.51	0.46
3:H:200:THR:CG2	3:H:215:LYS:HA	2.35	0.46
1:A:488:PHE:O	1:A:492:ILE:HG12	2.15	0.46
3:H:51:ILE:HA	3:H:58:ILE:HD13	1.97	0.45
1:A:260:THR:O	1:A:264:VAL:HG23	2.16	0.45
2:L:39:GLN:NE2	2:L:45:PRO:HD3	2.32	0.45
1:A:535:THR:O	1:A:539:LEU:HB2	2.16	0.45
3:H:51:ILE:CD1	3:H:72:ARG:HB2	2.46	0.45
1:A:393:TYR:HE2	1:A:397:ILE:HD11	1.79	0.45
3:H:30:SER:HA	3:H:74:ASN:OD1	2.16	0.45
1:A:585:SER:H	1:A:588:GLN:CG	2.30	0.45
1:A:252:PHE:HA	1:A:255:TRP:HB2	1.98	0.45
2:L:7:SER:HA	2:L:8:PRO:C	2.36	0.45
1:A:562:CYS:O	1:A:566:SER:N	2.49	0.45
1:A:215:TYR:O	1:A:219:TYR:HB3	2.15	0.45
3:H:157:THR:O	3:H:203:VAL:HA	2.17	0.45
1:A:527:ALA:HB3	1:A:528:PRO:CD	2.39	0.44
1:A:595:THR:HA	1:A:596:PRO:HD3	1.75	0.44
3:H:78:ILE:HG22	3:H:79:LEU:N	2.32	0.44
1:A:325:PHE:HB2	1:A:327:VAL:HG23	2.00	0.44
3:H:154:GLU:OE1	3:H:174:ALA:HB3	2.17	0.44
3:H:18:LEU:HD12	3:H:19:LYS:N	2.26	0.44
2:L:62:ARG:NH1	2:L:83:ASP:OD1	2.50	0.44
1:A:52:ARG:HH12	1:A:315:THR:CG2	2.31	0.44
1:A:116:ILE:HG23	1:A:479:ALA:HB2	2.00	0.44
3:H:176:LEU:HB2	3:H:181:TYR:CE1	2.53	0.44
1:A:286:LEU:HD11	1:A:400:MET:HE1	2.00	0.43
1:A:497:ILE:HD12	1:A:497:ILE:H	1.83	0.43
1:A:327:VAL:HG22	1:A:428:ALA:HB2	1.99	0.43
1:A:156:ASN:HB3	1:A:208:PHE:CD2	2.53	0.43
1:A:487:VAL:CG1	1:A:531:LEU:HD11	2.37	0.43
1:A:531:LEU:HD23	1:A:531:LEU:HA	1.84	0.43
1:A:123:TYR:HB3	1:A:474:LEU:HD12	1.99	0.43
1:A:93:LYS:HG2	1:A:97:THR:CG2	2.45	0.43
2:L:116:VAL:HG22	2:L:137:LEU:HD22	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:H:6:GLU:OE2	3:H:110:GLY:HA3	2.19	0.43
1:A:351:ILE:HD13	12:A:711:CLR:C7	2.49	0.43
1:A:113:VAL:HG13	1:A:325:PHE:C	2.38	0.43
1:A:377:ARG:NE	1:A:379:GLU:OE2	2.51	0.43
1:A:263:LYS:HD3	1:A:263:LYS:HA	1.73	0.43
1:A:598:ARG:HD2	3:H:56:ARG:NH2	2.34	0.43
2:L:62:ARG:NH1	2:L:83:ASP:OD2	2.51	0.43
2:L:139:ASN:OD1	3:H:170:HIS:NE2	2.48	0.43
1:A:426:SER:OG	13:A:801:HOH:O	2.20	0.43
2:L:24:ARG:HA	2:L:70:THR:O	2.19	0.43
1:A:536:VAL:HG12	1:A:537:TYR:N	2.33	0.43
2:L:3:VAL:CG1	2:L:26:SER:HB3	2.48	0.43
1:A:232:LEU:HD23	1:A:232:LEU:HA	1.81	0.42
1:A:103:VAL:CG1	1:A:497:ILE:HG21	2.47	0.42
1:A:297:LEU:CD1	1:A:361:PHE:CZ	3.01	0.42
1:A:370:MET:HE3	1:A:381:VAL:HB	2.01	0.42
1:A:27:ARG:NH1	1:A:93:LYS:HD2	2.34	0.42
1:A:286:LEU:HD11	1:A:400:MET:HE2	2.00	0.42
1:A:312:ASP:O	1:A:315:THR:HG22	2.19	0.42
1:A:307:ALA:O	1:A:311:VAL:HG23	2.20	0.42
1:A:540:ILE:C	1:A:540:ILE:HD12	2.40	0.42
3:H:52:SER:OG	3:H:57:TYR:HB2	2.19	0.42
1:A:312:ASP:HA	1:A:315:THR:HG22	2.00	0.42
1:A:271:PHE:N	1:A:272:PRO:CD	2.83	0.42
1:A:238:ASP:N	1:A:238:ASP:OD1	2.53	0.42
3:H:87:ARG:HD2	3:H:89:GLU:OE2	2.20	0.42
1:A:99:TRP:CH2	1:A:494:VAL:HG23	2.54	0.41
12:A:711:CLR:H121	12:A:711:CLR:H212	2.02	0.41
2:L:19:VAL:HG13	2:L:79:VAL:CG2	2.50	0.41
11:A:710:Y01:HAC1	11:A:710:Y01:HAE2	2.02	0.41
1:A:522:CYS:HA	1:A:526:VAL:HB	2.03	0.41
1:A:75:VAL:HG23	1:A:76:GLY:H	1.86	0.41
1:A:585:SER:OG	1:A:586:LEU:N	2.52	0.41
1:A:539:LEU:HA	1:A:539:LEU:HD13	1.67	0.41
1:A:476:ARG:HD3	1:A:545:LEU:HD13	2.02	0.41
1:A:540:ILE:HD12	1:A:541:GLY:N	2.35	0.41
1:A:514:PRO:HA	1:A:515:PRO:HD3	1.98	0.41
11:A:710:Y01:HAE1	11:A:710:Y01:HAS2	1.89	0.41
3:H:17:SER:HB2	3:H:83:MET:O	2.21	0.41
2:L:170:LYS:HA	2:L:170:LYS:HD2	1.78	0.41
1:A:331:TYR:HA	1:A:331:TYR:HD1	1.78	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:284:LEU:HD23	1:A:284:LEU:HA	1.89	0.41
2:L:79:VAL:HG12	2:L:80:GLU:N	2.36	0.41
2:L:107:MET:HA	2:L:107:MET:CE	2.51	0.41
1:A:100:GLY:HA2	1:A:107:LYS:HB2	2.03	0.41
1:A:502:ARG:NH1	1:A:599:ASP:OD2	2.54	0.40
1:A:116:ILE:O	1:A:120:VAL:HG23	2.21	0.40
1:A:266:TRP:O	1:A:270:LEU:HB2	2.21	0.40
2:L:80:GLU:O	2:L:83:ASP:HB2	2.21	0.40
3:H:169:VAL:HG22	3:H:187:VAL:HG23	2.03	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	534/535 (100%)	519 (97%)	15 (3%)	0	100	100
2	L	212/214 (99%)	202 (95%)	10 (5%)	0	100	100
3	H	217/219 (99%)	210 (97%)	7 (3%)	0	100	100
All	All	963/968 (100%)	931 (97%)	32 (3%)	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	434/440 (99%)	414 (95%)	20 (5%)	33	69
2	L	181/187 (97%)	169 (93%)	12 (7%)	21	51
3	H	177/187 (95%)	169 (96%)	8 (4%)	34	70
All	All	792/814 (97%)	752 (95%)	40 (5%)	29	65

All (40) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	29	THR
1	A	51	TRP
1	A	52	ARG
1	A	121	ASP
1	A	141	ASN
1	A	146	THR
1	A	236	LYS
1	A	259	SER
1	A	261	SER
1	A	339	ASN
1	A	367	LEU
1	A	389	VAL
1	A	420	ASP
1	A	443	ASN
1	A	462	SER
1	A	482	SER
1	A	504	SER
1	A	508	ARG
1	A	539	LEU
1	A	588	GLN
2	L	21	MET
2	L	27	SER
2	L	51	SER
2	L	62	ARG
2	L	92	PHE
2	L	117	SER
2	L	173	THR
2	L	181	THR
2	L	182	LEU
2	L	191	ASN
2	L	195	CYS
2	L	213	ASN
3	H	52	SER
3	H	53	SER

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Mol	Chain	Res	Type
3	H	88	SER
3	H	96	CYS
3	H	121	LYS
3	H	162	SER
3	H	209	SER
3	H	217	GLU

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

Of 12 ligands modelled in this entry, 4 are monoatomic - leaving 8 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	$\#\|Z\| > 2$
6	MAL	A	704	-	24,24,24	0.49	0	35,35,35	1.26	5 (14%)
6	MAL	A	705	-	24,24,24	0.51	0	35,35,35	0.97	1 (2%)
7	NAG	A	706	1	14,14,15	0.60	0	15,19,21	0.71	0
8	P4G	A	707	-	10,10,10	0.79	0	9,9,9	0.43	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
9	LDP	A	708	-	10,11,11	1.08	2 (20%)	13,14,14	0.79	0
10	EDO	A	709	-	3,3,3	0.51	0	2,2,2	0.32	0
11	Y01	A	710	-	35,38,38	4.09	13 (37%)	54,57,57	1.82	14 (25%)
12	CLR	A	711	-	31,31,31	0.67	0	48,48,48	1.38	5 (10%)

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
6	MAL	A	704	-	-	0/8/48/48	0/2/2/2
6	MAL	A	705	-	-	0/8/48/48	0/2/2/2
7	NAG	A	706	1	-	0/6/23/26	0/1/1/1
8	P4G	A	707	-	-	0/8/8/8	0/0/0/0
9	LDP	A	708	-	-	0/3/3/3	0/1/1/1
10	EDO	A	709	-	-	0/1/1/1	0/0/0/0
11	Y01	A	710	-	-	0/17/77/77	0/4/4/4
12	CLR	A	711	-	-	0/10/68/68	0/4/4/4

All (15) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	A	710	Y01	CBB-CBE	-9.44	1.36	1.54
11	A	710	Y01	CAU-CBI	-6.57	1.41	1.54
11	A	710	Y01	CBH-CAZ	-4.08	1.44	1.52
11	A	710	Y01	CBD-CBF	-2.22	1.49	1.53
9	A	708	LDP	O1-C3	2.31	1.41	1.36
9	A	708	LDP	O2-C4	2.35	1.41	1.36
11	A	710	Y01	CAQ-CBG	2.49	1.60	1.54
11	A	710	Y01	CAO-CBB	2.56	1.61	1.54
11	A	710	Y01	OAW-CAY	3.38	1.44	1.34
11	A	710	Y01	CBI-CBE	4.56	1.64	1.55
11	A	710	Y01	CAU-CAS	5.04	1.64	1.53
11	A	710	Y01	CAP-CBE	5.04	1.66	1.54
11	A	710	Y01	CAK-CBD	5.45	1.62	1.53
11	A	710	Y01	CBH-CBF	6.93	1.68	1.56
11	A	710	Y01	CAI-CAZ	15.37	1.71	1.33

All (25) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
11	A	710	Y01	CBI-CBE-CBB	-3.64	113.15	119.46
11	A	710	Y01	CAE-CBI-CBE	-3.52	104.86	111.75
12	A	711	CLR	C19-C10-C9	-3.42	107.29	111.67
11	A	710	Y01	CAE-CBI-CAU	-3.12	105.22	110.54
11	A	710	Y01	CAE-CBI-CBG	-3.07	105.75	111.75
6	A	704	MAL	C1'-C2'-C3'	-2.86	106.18	110.43
11	A	710	Y01	CAK-CAI-CAZ	-2.84	118.90	125.01
11	A	710	Y01	CBH-CAZ-CAI	-2.77	117.79	122.92
12	A	711	CLR	C8-C7-C6	-2.63	108.78	112.75
6	A	704	MAL	O3'-C3'-C2'	-2.58	104.54	110.34
12	A	711	CLR	C4-C5-C6	-2.50	116.33	120.57
11	A	710	Y01	CAD-CBH-CBF	-2.38	108.62	111.67
12	A	711	CLR	C2-C3-C4	-2.11	106.56	110.32
11	A	710	Y01	CBC-CAV-CAZ	-2.07	108.13	111.52
11	A	710	Y01	CBG-CBI-CBE	2.13	102.59	100.09
6	A	704	MAL	O5-C5-C6	2.21	111.94	106.36
11	A	710	Y01	CBF-CBH-CAZ	2.44	113.47	109.67
6	A	705	MAL	O1-C4'-C3'	2.47	113.54	107.17
6	A	704	MAL	O1-C1-C2	2.48	114.13	108.10
11	A	710	Y01	CAK-CBD-CBF	2.62	113.29	109.71
6	A	704	MAL	O1-C4'-C3'	3.37	115.87	107.17
11	A	710	Y01	CAU-CBI-CBE	3.64	123.02	116.56
11	A	710	Y01	CAU-CBI-CBG	4.10	113.98	107.31
11	A	710	Y01	OAW-CAY-CAM	4.32	120.92	111.53
12	A	711	CLR	C4-C5-C10	5.20	124.00	116.43

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

4 monomers are involved in 14 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	A	704	MAL	1	0
6	A	705	MAL	4	0
11	A	710	Y01	5	0
12	A	711	CLR	4	0

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95^{th} percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled 'Q< 0.9' lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
1	A	535/535 (100%)	-0.19	2 (0%)	93	92	58, 74, 98, 151	0
2	L	214/214 (100%)	-0.26	1 (0%)	91	90	47, 69, 100, 116	0
3	H	219/219 (100%)	-0.06	10 (4%)	36	30	54, 69, 110, 154	0
All	All	968/968 (100%)	-0.18	13 (1%)	79	78	47, 72, 100, 154	0

All (13) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	H	138	THR	6.9
3	H	142	VAL	3.3
1	A	537	TYR	3.2
3	H	140	SER	3.0
3	H	137	THR	2.9
3	H	139	GLY	2.9
1	A	290	PHE	2.8
2	L	127	THR	2.6
3	H	134	CYS	2.5
3	H	141	SER	2.3
3	H	1	GLU	2.1
3	H	136	ASP	2.1
3	H	126	SER	2.0

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
4	NA	L	301	1/1	0.96	0.23	2.63	95,95,95,95	0
12	CLR	A	711	28/28	0.93	0.26	1.90	70,80,87,88	0
9	LDP	A	708	11/11	0.97	0.25	1.79	64,78,94,103	0
6	MAL	A	704	23/23	0.79	0.26	1.78	93,107,120,123	0
6	MAL	A	705	23/23	0.84	0.23	1.60	89,111,119,125	0
10	EDO	A	709	4/4	0.85	0.28	1.37	82,86,88,93	0
11	Y01	A	710	35/35	0.92	0.23	0.79	70,85,111,120	0
4	NA	A	702	1/1	0.95	0.26	0.51	69,69,69,69	0
5	CL	A	703	1/1	0.97	0.20	-0.77	72,72,72,72	0
8	P4G	A	707	11/11	0.79	0.13	-0.85	96,117,139,142	0
4	NA	A	701	1/1	0.96	0.18	-1.52	69,69,69,69	0
7	NAG	A	706	14/15	0.79	0.27	-	89,109,117,120	0

6.5 Other polymers

There are no such residues in this entry.