Full wwPDB X-ray Structure Validation Report (i)

Jan 31, 2016 – 08:13 PM GMT

PDB ID	:	1JDP
Title	:	Crystal Structure of Hormone/Receptor Complex
Authors	:	He, X.-L.; Chow, D.-C.; Martick, M.M.; Garcia, K.C.
Deposited on	:	2001-06-14
Resolution	:	2.00 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.
We welcome your comments at validation@mail.wwpdb.org
A user guide is available at
http://wwpdb.org/validation/2016/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

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

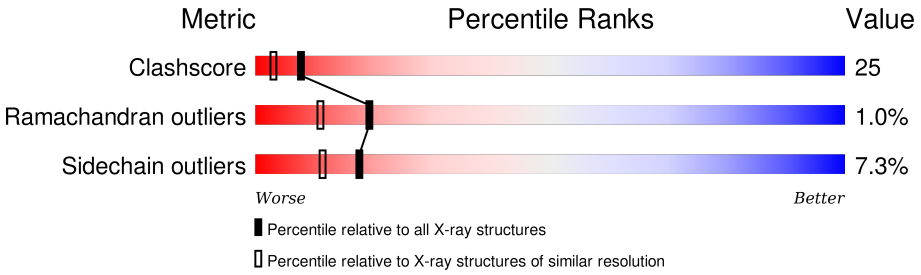
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
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 2.00 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))
Clashscore	102246	7340 (2.00-2.00)
Ramachandran outliers	100387	7248 (2.00-2.00)
Sidechain outliers	100360	7247 (2.00-2.00)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5% The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	441	58% 29% • 10%
1	B	441	61% 26% • 10%
2	H	22	36% 36% 9% 18%

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
3	NDG	A	501	-	-	X	-

2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 7041 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.

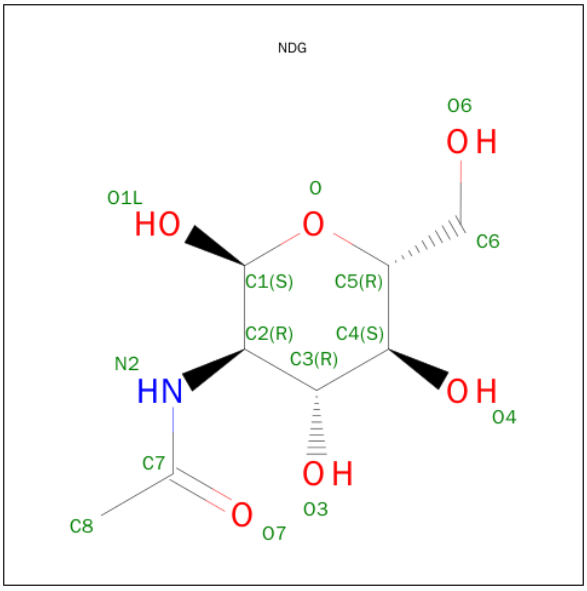
- Molecule 1 is a protein called ATRIAL NATRIURETIC PEPTIDE CLEARANCE RECEPTOR.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	396	Total	C	N	O	S	0	0	0
			3130	1983	537	594	16			
1	B	395	Total	C	N	O	S	0	0	0
			3121	1978	536	591	16			

- Molecule 2 is a protein called C-TYPE NATRIURETIC PEPTIDE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	H	18	Total	C	N	O	S	0	18	0
			248	152	44	46	6			

- Molecule 3 is SUGAR (N-ACETYL-D-GLUCOSAMINE) (three-letter code: NDG) (formula: $C_8H_{15}NO_6$).

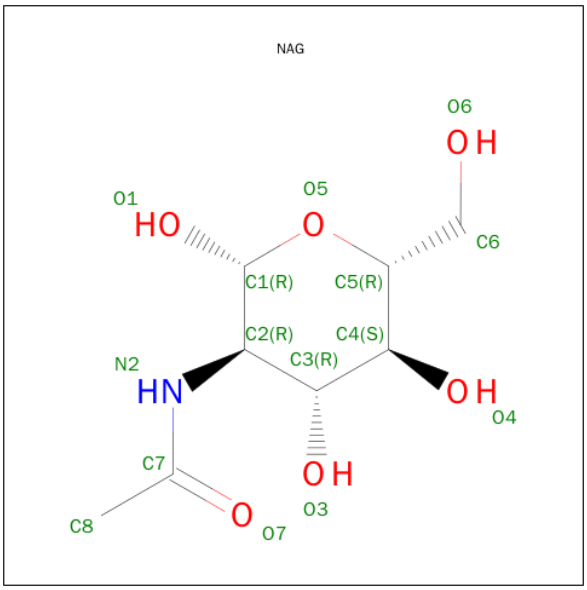


Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total C N O 14 8 1 5	0	0
3	A	1	Total C N O 14 8 1 5	0	0

- Molecule 4 is a polymer of unknown type called SUGAR (2-MER).

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

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



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

- Molecule 6 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	B	1	Total Cl 1 1	0	0
6	A	1	Total Cl 1 1	0	0

- Molecule 7 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	A	217	Total O 217 217	0	0
7	B	238	Total O 238 238	0	0
7	H	15	Total O 15 15	0	0

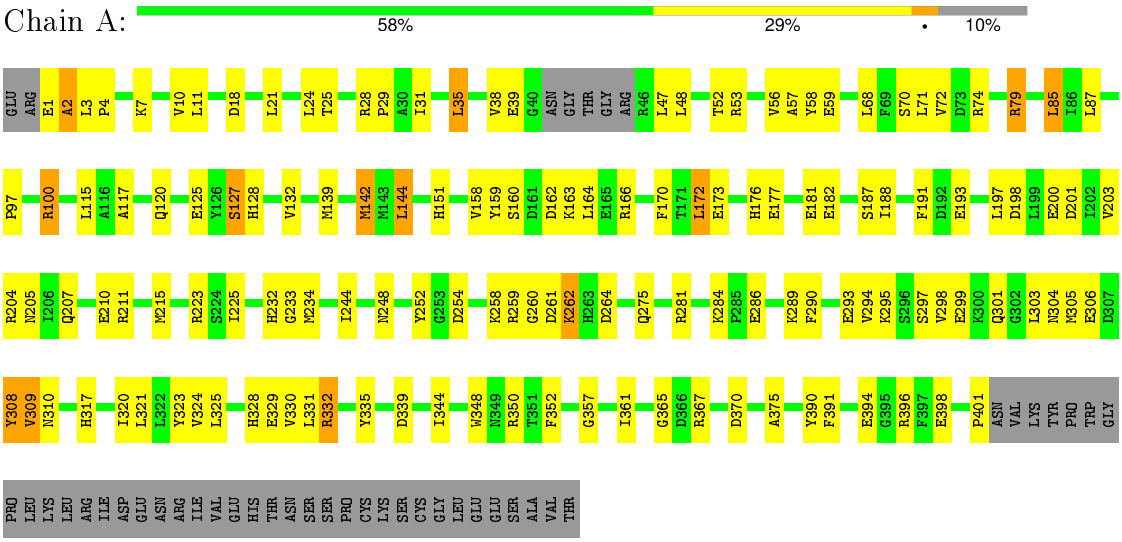
3 Residue-property plots (i)

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.

Note EDS was not executed.

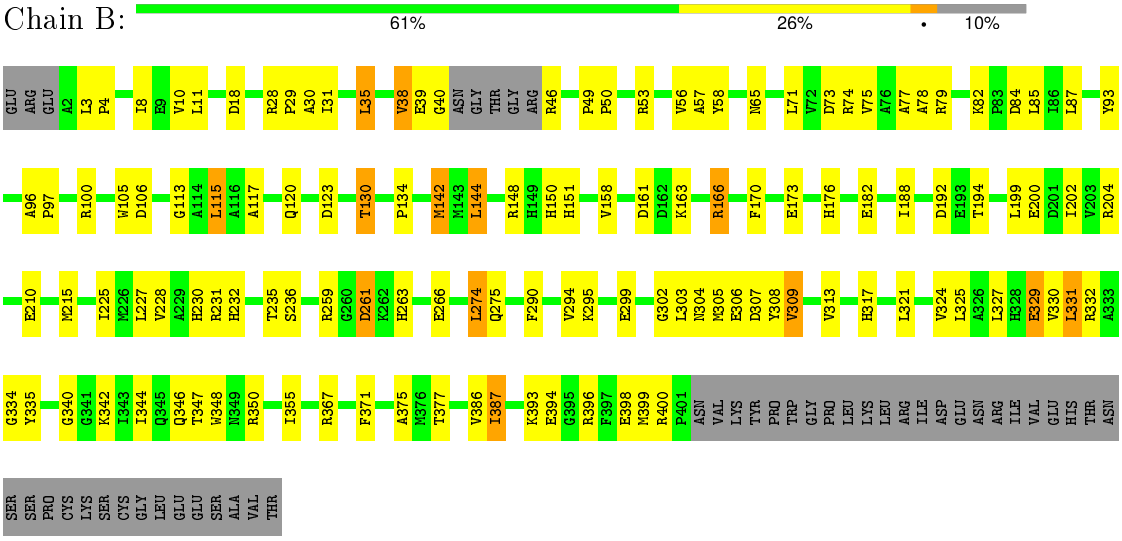
• Molecule 1: ATRIAL NATRIURETIC PEPTIDE CLEARANCE RECEPTOR

Chain A:



• Molecule 1: ATRIAL NATRIURETIC PEPTIDE CLEARANCE RECEPTOR

Chain B:



• Molecule 2: C-TYPE NATRIURETIC PEPTIDE

Chain H:


36%
36%
9%
18%
GLY
LEU
SER
LYS
G5
C6
F7
G8
L9
K10
L11
D12
R13
I14
G15
S16
M17
S18
G19
L20
G21
C22

4 Data and refinement statistics (i)

Xtriage (Phenix) and EDS were not executed - this section will therefore be incomplete.

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	56.80Å 136.46Å 137.59Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	50.00 – 2.00	Depositor
% Data completeness (in resolution range)	97.7 (50.00-2.00)	Depositor
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	CNS	Depositor
R, R_{free}	0.227 , 0.248	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	7041	wwPDB-VP
Average B, all atoms (Å^2)	44.0	wwPDB-VP

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: NAG, NDG, 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	0.45	0/3199	0.70	2/4323 (0.0%)
1	B	0.46	0/3190	0.71	2/4311 (0.0%)
2	H	0.45	0/248	0.88	2/320 (0.6%)
All	All	0.46	0/6637	0.71	6/8954 (0.1%)

There are no bond length outliers.

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	166	ARG	NE-CZ-NH1	-7.79	116.41	120.30
1	A	127	SER	N-CA-C	-5.48	96.21	111.00
2	H	11[A]	LEU	CA-CB-CG	5.39	127.69	115.30
2	H	11[B]	LEU	CA-CB-CG	5.39	127.69	115.30
1	A	100	ARG	NE-CZ-NH1	-5.08	117.76	120.30
1	B	274	LEU	CA-CB-CG	5.08	126.99	115.30

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3130	0	3035	144	0
1	B	3121	0	3027	128	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	H	248	0	248	115	0
3	A	28	0	26	8	0
4	B	28	0	25	0	0
5	B	14	0	13	0	0
6	A	1	0	0	0	0
6	B	1	0	0	0	0
7	A	217	0	0	17	0
7	B	238	0	0	9	0
7	H	15	0	0	5	0
All	All	7041	0	6374	326	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 25.

All (326) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:21:LEU:HD21	3:A:501:NDG:C8	1.82	1.10
1:A:21:LEU:HD21	3:A:501:NDG:H8C2	1.14	1.07
1:A:163:LYS:HE2	2:H:10[B]:LYS:HG3	1.05	1.04
1:B:163:LYS:HG3	2:H:10[A]:LYS:HB2	1.40	1.03
1:B:163:LYS:NZ	2:H:10[A]:LYS:HE2	1.76	1.00
1:A:163:LYS:CE	2:H:10[B]:LYS:HG3	1.91	0.99
1:B:100:ARG:HH22	2:H:16[A]:SER:HB2	1.32	0.94
1:A:163:LYS:HG3	2:H:10[B]:LYS:HB2	1.50	0.93
1:A:21:LEU:CD2	3:A:501:NDG:H8C2	2.00	0.91
1:B:100:ARG:HH22	2:H:16[A]:SER:CB	1.84	0.91
1:A:163:LYS:HE2	2:H:10[B]:LYS:CG	1.97	0.90
1:A:248:ASN:ND2	3:A:501:NDG:H8C1	1.87	0.88
1:A:204:ARG:HH12	1:A:232:HIS:HE1	1.21	0.88
1:B:100:ARG:HH12	2:H:16[A]:SER:C	1.77	0.87
1:B:163:LYS:HZ1	2:H:10[A]:LYS:HE2	1.40	0.87
1:B:38:VAL:HG21	1:B:324:VAL:HG21	1.55	0.86
1:A:100:ARG:HH12	2:H:16[B]:SER:CA	1.87	0.86
1:A:100:ARG:HH12	2:H:16[B]:SER:CB	1.89	0.85
2:H:11[A]:LEU:CD2	2:H:14[A]:ILE:HB	2.06	0.85
2:H:11[B]:LEU:CD2	2:H:14[B]:ILE:HB	2.07	0.85
1:A:100:ARG:HH12	2:H:16[B]:SER:HA	1.46	0.81
1:B:163:LYS:HA	1:B:166:ARG:HD3	1.63	0.80
1:B:163:LYS:HG3	2:H:10[A]:LYS:CB	2.11	0.80
1:A:100:ARG:HD3	1:A:125:GLU:OE2	1.81	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:163:LYS:CE	2:H:10[A]:LYS:HG3	2.13	0.79
1:A:100:ARG:HH12	2:H:16[B]:SER:HB2	1.47	0.79
1:A:128:HIS:HA	1:A:344:ILE:HG13	1.65	0.79
1:B:148:ARG:HG3	1:B:148:ARG:HH21	1.48	0.78
1:A:284:LYS:HE3	1:A:357:GLY:HA2	1.67	0.77
2:H:11[B]:LEU:HD22	2:H:14[B]:ILE:HB	1.68	0.75
2:H:13[A]:ARG:HH21	2:H:13[A]:ARG:HG2	1.50	0.75
2:H:13[B]:ARG:HG2	2:H:13[B]:ARG:HH21	1.51	0.74
1:B:130:THR:HG21	1:B:347:THR:OG1	1.88	0.74
1:A:163:LYS:HB3	2:H:11[B]:LEU:H	1.52	0.74
2:H:11[A]:LEU:HD22	2:H:14[A]:ILE:HB	1.68	0.73
1:A:31:ILE:HG23	1:A:320:ILE:CD1	2.17	0.73
2:H:20[A]:LEU:HG	2:H:21[A]:GLY:N	2.04	0.73
1:A:159:TYR:HB3	1:A:172:LEU:HD22	1.71	0.73
2:H:20[B]:LEU:HG	2:H:21[B]:GLY:N	2.03	0.72
1:A:193:GLU:HA	1:A:197:LEU:HD21	1.72	0.71
1:A:127:SER:O	1:A:128:HIS:HB2	1.89	0.71
1:B:163:LYS:CD	2:H:10[A]:LYS:HG3	2.20	0.71
1:B:130:THR:HG22	1:B:348:TRP:HE1	1.56	0.70
1:A:100:ARG:NH1	2:H:16[B]:SER:HA	2.05	0.70
1:B:230:HIS:CD2	1:B:266:GLU:HG3	2.27	0.70
1:A:198:ASP:OD2	1:A:201:ASP:HB2	1.91	0.70
1:A:3:LEU:HB3	1:A:4:PRO:HD2	1.74	0.69
1:B:215:MET:CE	1:B:225:ILE:HG21	2.23	0.69
1:B:161:ASP:OD2	1:B:166:ARG:HD2	1.93	0.68
1:B:290:PHE:O	1:B:294:VAL:HG23	1.93	0.68
1:B:202:ILE:HG21	1:B:225:ILE:HD12	1.74	0.68
1:A:47:LEU:O	1:A:328:HIS:ND1	2.20	0.68
1:A:289:LYS:HE2	1:A:293:GLU:OE2	1.94	0.68
1:A:163:LYS:NZ	2:H:10[B]:LYS:HE2	2.09	0.67
1:B:40:GLY:O	1:B:46:ARG:HG2	1.95	0.67
1:B:325:LEU:O	1:B:329:GLU:HG2	1.94	0.67
1:A:258:LYS:HD3	1:A:259:ARG:N	2.09	0.67
1:A:187:SER:C	1:A:188:ILE:HD12	2.16	0.67
1:B:327:LEU:O	1:B:330:VAL:HG12	1.95	0.66
1:B:100:ARG:HH22	2:H:16[A]:SER:CA	2.08	0.66
1:A:48:LEU:HD13	1:A:324:VAL:HG13	1.76	0.66
1:B:166:ARG:HH11	2:H:14[B]:ILE:HD11	1.60	0.66
1:A:100:ARG:NH1	2:H:16[B]:SER:HB2	2.09	0.66
1:A:188:ILE:HB	2:H:5[A]:GLY:HA2	1.78	0.66
1:A:10:VAL:CG2	1:A:56:VAL:HG22	2.26	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:177:GLU:OE1	2:H:9[A]:LEU:HB3	1.96	0.65
1:A:306:GLU:CD	1:A:306:GLU:H	1.98	0.65
1:B:163:LYS:HG3	2:H:10[A]:LYS:HG3	1.79	0.65
1:A:31:ILE:HG23	1:A:320:ILE:HD11	1.79	0.65
1:B:227:LEU:HD22	1:B:266:GLU:HG2	1.79	0.64
1:A:204:ARG:HH11	1:A:204:ARG:HG3	1.62	0.64
1:B:148:ARG:NH2	1:B:148:ARG:HG3	2.10	0.64
1:A:401:PRO:HD2	7:A:648:HOH:O	1.97	0.63
1:B:161:ASP:OD1	1:B:163:LYS:HE3	1.99	0.63
1:B:166:ARG:NH1	2:H:14[B]:ILE:HD11	2.12	0.63
1:B:3:LEU:HD23	1:B:4:PRO:HD2	1.79	0.62
1:B:227:LEU:CD2	1:B:266:GLU:HG2	2.30	0.62
1:A:48:LEU:HD23	1:A:52:THR:HG21	1.80	0.62
3:A:501:NDG:H8C1	3:A:501:NDG:C1	2.28	0.62
1:A:163:LYS:HG3	2:H:10[B]:LYS:CB	2.29	0.62
1:B:100:ARG:HH12	2:H:17[A]:MET:N	1.97	0.61
1:A:35:LEU:HD13	1:A:320:ILE:HG21	1.81	0.61
1:B:176:HIS:CD2	2:H:7[B]:PHE:HB3	2.35	0.61
1:A:170:PHE:CE1	2:H:14[A]:ILE:HD13	2.34	0.61
1:B:100:ARG:HH12	2:H:16[A]:SER:CA	2.13	0.61
1:A:325:LEU:O	1:A:329:GLU:HG3	2.00	0.61
2:H:18[B]:SER:HB3	7:H:152:HOH:O	2.00	0.61
1:B:28:ARG:HB3	1:B:29:PRO:HD3	1.82	0.60
2:H:8[A]:GLY:C	2:H:10[A]:LYS:HD2	2.21	0.60
1:B:96:ALA:HB3	1:B:97:PRO:HD3	1.83	0.60
1:A:262:LYS:HG2	1:A:262:LYS:O	2.00	0.60
1:B:163:LYS:HG3	2:H:10[A]:LYS:CG	2.31	0.60
1:B:215:MET:HE1	1:B:225:ILE:HG21	1.84	0.60
1:B:18:ASP:OD1	1:B:303:LEU:HD11	2.00	0.60
1:B:295:LYS:O	1:B:299:GLU:HG3	2.02	0.60
1:A:394:GLU:OE1	1:A:396:ARG:NH1	2.35	0.59
2:H:8[B]:GLY:C	2:H:10[B]:LYS:HD2	2.21	0.59
1:B:163:LYS:CG	2:H:10[A]:LYS:HG3	2.33	0.58
1:A:10:VAL:HG23	1:A:56:VAL:HG13	1.85	0.58
1:A:163:LYS:HZ3	2:H:10[B]:LYS:HE2	1.67	0.58
1:B:3:LEU:HD22	1:B:49:PRO:HG2	1.85	0.58
1:B:117:ALA:O	1:B:120:GLN:HB2	2.03	0.58
1:B:161:ASP:OD2	1:B:166:ARG:CD	2.51	0.58
1:B:192:ASP:OD1	1:B:194:THR:HB	2.03	0.58
1:B:100:ARG:NH2	2:H:16[A]:SER:HB2	2.11	0.58
1:B:215:MET:HE3	1:B:225:ILE:HG21	1.85	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:25:THR:HG23	7:A:603:HOH:O	2.03	0.58
1:B:309:VAL:HG11	1:B:313:VAL:HG11	1.86	0.58
1:B:100:ARG:NH1	2:H:16[A]:SER:HA	2.19	0.58
1:B:100:ARG:NH2	2:H:16[A]:SER:HA	2.18	0.58
1:B:39:GLU:OE1	1:B:53:ARG:NH1	2.36	0.58
1:A:330:VAL:CG1	1:A:335:TYR:HB2	2.33	0.58
7:A:621:HOH:O	2:H:9[A]:LEU:HD13	2.03	0.57
1:A:176:HIS:CD2	2:H:7[A]:PHE:HB3	2.39	0.57
1:A:100:ARG:NH1	2:H:16[B]:SER:CB	2.62	0.57
1:B:123:ASP:HB2	7:B:660:HOH:O	2.04	0.57
1:B:394:GLU:HG3	7:B:667:HOH:O	2.04	0.57
1:A:7:LYS:HE3	1:A:53:ARG:HD2	1.85	0.57
1:B:170:PHE:CE1	2:H:14[B]:ILE:HD13	2.39	0.57
1:B:38:VAL:CG2	1:B:324:VAL:HG21	2.29	0.57
1:B:3:LEU:HD23	1:B:4:PRO:CD	2.34	0.57
2:H:14[A]:ILE:HG23	2:H:14[A]:ILE:O	2.05	0.57
1:A:204:ARG:HH12	1:A:232:HIS:CE1	2.12	0.56
2:H:14[B]:ILE:O	2:H:14[B]:ILE:HG23	2.05	0.56
1:A:290:PHE:O	1:A:294:VAL:HG23	2.04	0.56
1:A:68:LEU:HD23	7:A:659:HOH:O	2.04	0.56
2:H:13[A]:ARG:NH2	7:H:310:HOH:O	2.38	0.56
1:A:10:VAL:HG22	1:A:56:VAL:HG22	1.88	0.56
2:H:18[A]:SER:HB3	7:H:269:HOH:O	2.06	0.56
1:A:284:LYS:CE	1:A:357:GLY:HA2	2.34	0.55
1:A:132:VAL:O	1:A:367:ARG:HD2	2.06	0.55
1:A:298:VAL:HG12	1:A:303:LEU:HB2	1.88	0.55
7:B:640:HOH:O	2:H:17[A]:MET:HA	2.07	0.55
1:A:163:LYS:HD3	7:A:641:HOH:O	2.07	0.55
1:B:100:ARG:HH22	2:H:16[A]:SER:HA	1.72	0.55
1:A:100:ARG:HD2	1:B:65:ASN:ND2	2.23	0.54
1:B:386:VAL:HG11	1:B:400:ARG:CZ	2.38	0.54
1:B:231:ARG:HG3	7:B:681:HOH:O	2.07	0.54
1:B:46:ARG:NH1	1:B:50:PRO:HB3	2.23	0.54
1:A:258:LYS:HD3	1:A:260:GLY:H	1.73	0.54
1:A:48:LEU:CD1	1:A:324:VAL:HG13	2.38	0.54
1:B:163:LYS:CE	2:H:10[A]:LYS:HE2	2.36	0.53
1:A:166:ARG:NH2	2:H:14[A]:ILE:HD11	2.24	0.53
1:B:163:LYS:NZ	2:H:10[A]:LYS:CE	2.64	0.53
1:A:352:PHE:HE1	1:A:361:ILE:HD11	1.72	0.53
1:B:163:LYS:HZ3	2:H:10[A]:LYS:HE2	1.68	0.53
1:A:204:ARG:HG3	1:A:204:ARG:NH1	2.24	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:330:VAL:HG22	1:B:335:TYR:HB2	1.89	0.53
1:A:215:MET:CE	1:A:225:ILE:HG21	2.39	0.53
1:A:127:SER:O	1:A:128:HIS:CB	2.57	0.52
1:B:134:PRO:HD2	7:B:549:HOH:O	2.10	0.52
3:A:501:NDG:C8	3:A:501:NDG:C1	2.85	0.52
1:B:331:LEU:HD12	1:B:335:TYR:O	2.10	0.52
1:B:31:ILE:HG22	1:B:35:LEU:HD22	1.92	0.52
1:B:130:THR:HG22	1:B:344:ILE:HG23	1.91	0.52
1:B:275:GLN:HG2	1:B:375:ALA:HB2	1.90	0.52
1:A:295:LYS:HE3	1:A:299:GLU:OE1	2.09	0.52
1:B:100:ARG:HH12	2:H:16[A]:SER:HA	1.73	0.52
1:A:252:TYR:C	1:A:254:ASP:H	2.13	0.51
1:B:200:GLU:HG3	1:B:204:ARG:NE	2.24	0.51
1:A:159:TYR:HB3	1:A:172:LEU:CD2	2.40	0.51
1:A:132:VAL:O	1:A:367:ARG:CD	2.58	0.51
1:A:284:LYS:HE3	1:A:357:GLY:CA	2.39	0.51
1:A:10:VAL:CG2	1:A:56:VAL:HG13	2.40	0.51
1:B:163:LYS:HE2	2:H:10[A]:LYS:HG3	1.90	0.51
1:A:35:LEU:HA	1:A:38:VAL:HG22	1.92	0.51
1:A:204:ARG:NH1	1:A:232:HIS:HE1	2.00	0.50
1:A:295:LYS:HG3	1:A:305:MET:HE2	1.93	0.50
1:A:275:GLN:HG2	1:A:375:ALA:HB2	1.93	0.50
1:A:10:VAL:HG21	1:A:56:VAL:HG22	1.93	0.50
1:B:130:THR:HG23	1:B:344:ILE:HD12	1.93	0.50
1:A:85:LEU:HG	1:A:323:TYR:CD1	2.47	0.50
1:A:39:GLU:O	1:A:39:GLU:HG3	2.12	0.50
2:H:16[A]:SER:O	2:H:17[A]:MET:CB	2.60	0.50
1:A:144:LEU:HD11	1:A:182:GLU:HG3	1.94	0.50
1:A:74:ARG:HD3	7:A:596:HOH:O	2.11	0.50
2:H:13[A]:ARG:HH21	2:H:13[A]:ARG:CG	2.24	0.49
1:A:173:GLU:HB2	2:H:7[A]:PHE:CE1	2.47	0.49
1:A:142:MET:HB2	1:A:390:TYR:CD2	2.46	0.49
1:A:317:HIS:HE1	1:A:321:LEU:HD11	1.78	0.49
1:B:28:ARG:HG3	1:B:58:TYR:CZ	2.47	0.49
1:A:233:GLY:HA2	7:A:551:HOH:O	2.12	0.49
2:H:16[B]:SER:O	2:H:17[B]:MET:CB	2.60	0.49
1:A:335:TYR:HB3	1:A:339:ASP:OD1	2.13	0.49
1:B:73:ASP:O	1:B:77:ALA:HB2	2.13	0.49
1:B:100:ARG:CZ	2:H:16[A]:SER:HA	2.43	0.49
1:A:330:VAL:HG12	1:A:335:TYR:HB2	1.95	0.49
1:A:21:LEU:HD21	3:A:501:NDG:H8C3	1.87	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:46:ARG:CZ	1:B:50:PRO:HB3	2.43	0.48
1:A:261:ASP:OD2	1:A:262:LYS:N	2.44	0.48
1:B:30:ALA:HB2	1:B:313:VAL:HG13	1.95	0.48
1:B:188:ILE:HB	2:H:5[B]:GLY:HA2	1.95	0.48
1:A:332:ARG:HD2	1:A:332:ARG:N	2.29	0.48
1:B:74:ARG:NH1	7:B:535:HOH:O	2.41	0.48
1:B:387:ILE:HG23	1:B:399:MET:CE	2.44	0.47
1:A:57:ALA:HB1	1:A:74:ARG:NH2	2.30	0.47
1:A:100:ARG:HG2	1:A:125:GLU:HG3	1.97	0.47
2:H:13[B]:ARG:CG	2:H:13[B]:ARG:HH21	2.25	0.47
1:A:163:LYS:CG	2:H:10[B]:LYS:HB2	2.33	0.47
1:B:377:THR:CG2	1:B:387:ILE:HD11	2.45	0.47
1:A:151:HIS:HE1	7:A:544:HOH:O	1.98	0.47
1:B:142:MET:HG3	1:B:371:PHE:HB2	1.97	0.47
2:H:12[B]:ASP:OD1	2:H:12[B]:ASP:C	2.54	0.46
1:B:321:LEU:O	1:B:325:LEU:HD13	2.15	0.46
1:A:215:MET:HE1	1:A:225:ILE:HG21	1.97	0.46
1:A:158:VAL:HB	1:A:215:MET:HG2	1.97	0.46
2:H:12[A]:ASP:C	2:H:12[A]:ASP:OD1	2.52	0.46
1:A:163:LYS:HD2	1:A:163:LYS:N	2.31	0.46
1:B:148:ARG:NH1	1:B:182:GLU:OE1	2.38	0.46
7:B:641:HOH:O	2:H:22[A]:CYS:HA	2.16	0.46
1:A:1:GLU:O	1:A:2:ALA:C	2.54	0.46
1:A:3:LEU:HA	7:A:647:HOH:O	2.14	0.46
2:H:13[B]:ARG:O	2:H:15[B]:GLY:N	2.49	0.46
1:B:294:VAL:HG11	1:B:309:VAL:HG11	1.98	0.46
1:A:325:LEU:HD13	7:A:609:HOH:O	2.16	0.45
2:H:12[A]:ASP:C	2:H:14[A]:ILE:H	2.19	0.45
1:A:170:PHE:HE1	2:H:14[A]:ILE:HD13	1.81	0.45
1:A:35:LEU:O	1:A:38:VAL:HG22	2.17	0.45
1:B:113:GLY:C	1:B:115:LEU:HD13	2.37	0.45
2:H:12[B]:ASP:O	2:H:14[B]:ILE:N	2.50	0.45
2:H:12[A]:ASP:O	2:H:14[A]:ILE:N	2.50	0.45
1:B:261:ASP:HB3	1:B:263:HIS:H	1.82	0.45
1:A:28:ARG:HB3	1:A:29:PRO:HD3	1.98	0.45
2:H:8[A]:GLY:O	2:H:10[A]:LYS:HD2	2.16	0.45
1:A:3:LEU:HD23	7:A:647:HOH:O	2.16	0.45
1:A:370:ASP:OD1	1:A:391:PHE:HA	2.16	0.45
2:H:13[A]:ARG:O	2:H:15[A]:GLY:N	2.50	0.44
2:H:8[B]:GLY:O	2:H:10[B]:LYS:HD2	2.17	0.44
2:H:8[B]:GLY:O	2:H:9[B]:LEU:C	2.56	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:166:ARG:NH1	2:H:14[B]:ILE:CD1	2.78	0.44
1:A:188:ILE:HD12	1:A:188:ILE:N	2.32	0.44
1:B:163:LYS:NZ	2:H:10[A]:LYS:HG3	2.32	0.44
2:H:12[B]:ASP:C	2:H:14[B]:ILE:H	2.19	0.44
2:H:8[A]:GLY:O	2:H:9[A]:LEU:C	2.56	0.44
1:B:144:LEU:HD11	1:B:148:ARG:NH1	2.33	0.44
1:B:235:THR:O	1:B:236:SER:CB	2.65	0.44
1:A:139:MET:HE2	1:A:244:ILE:HG21	1.99	0.44
1:A:79:ARG:NH1	1:B:78:ALA:O	2.51	0.44
1:B:194:THR:HG22	1:B:194:THR:O	2.18	0.44
1:A:330:VAL:HG13	1:A:335:TYR:HB2	2.00	0.44
1:B:393:LYS:HB3	7:B:667:HOH:O	2.18	0.44
2:H:13[A]:ARG:HG2	2:H:13[A]:ARG:NH2	2.24	0.43
1:A:298:VAL:CG1	1:A:303:LEU:HB2	2.47	0.43
1:A:72:VAL:HG11	1:B:105:TRP:CZ2	2.53	0.43
1:B:332:ARG:HH11	1:B:332:ARG:HG2	1.83	0.43
1:A:160:SER:HA	1:A:191:PHE:O	2.17	0.43
1:A:398:GLU:HG3	7:A:558:HOH:O	2.18	0.43
1:A:211:ARG:HD2	7:A:690:HOH:O	2.17	0.43
1:A:18:ASP:OD2	1:A:303:LEU:HD11	2.18	0.43
1:B:106:ASP:O	1:B:340:GLY:HA3	2.17	0.43
1:B:199:LEU:HB3	1:B:228:VAL:HG21	2.00	0.43
1:A:223:ARG:CZ	1:A:259:ARG:HG3	2.48	0.43
1:B:75:VAL:CG1	1:B:82:LYS:HD3	2.48	0.43
2:H:16[B]:SER:O	2:H:17[B]:MET:HB2	2.19	0.43
1:A:204:ARG:HA	1:A:207:GLN:HG2	2.00	0.43
1:A:31:ILE:HG23	1:A:320:ILE:HD12	2.00	0.43
1:B:227:LEU:HA	1:B:227:LEU:HD23	1.85	0.43
2:H:18[A]:SER:CB	7:H:269:HOH:O	2.66	0.43
1:B:396:ARG:NH1	1:B:398:GLU:OE1	2.44	0.43
1:B:130:THR:CG2	1:B:344:ILE:HD12	2.49	0.43
1:B:173:GLU:HB2	2:H:7[B]:PHE:CE1	2.54	0.43
1:A:181:GLU:HG3	7:A:586:HOH:O	2.17	0.43
2:H:10[B]:LYS:HG2	2:H:11[B]:LEU:N	2.33	0.43
1:B:200:GLU:HG3	1:B:204:ARG:CZ	2.48	0.43
2:H:18[B]:SER:CB	7:H:152:HOH:O	2.65	0.42
1:A:294:VAL:O	1:A:298:VAL:HG23	2.19	0.42
3:A:502:NDG:C8	3:A:502:NDG:H3	2.49	0.42
1:A:117:ALA:O	1:A:120:GLN:HB2	2.19	0.42
1:A:3:LEU:HB3	1:A:4:PRO:CD	2.46	0.42
1:B:332:ARG:C	1:B:334:GLY:H	2.22	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:342:LYS:HD3	7:B:619:HOH:O	2.18	0.42
2:H:16[A]:SER:O	2:H:17[A]:MET:HB2	2.18	0.42
2:H:13[B]:ARG:NH2	2:H:13[B]:ARG:HG2	2.25	0.42
1:B:327:LEU:C	1:B:330:VAL:HG12	2.39	0.42
1:A:100:ARG:NH1	2:H:16[B]:SER:CA	2.66	0.42
1:A:97:PRO:HG3	7:A:574:HOH:O	2.19	0.42
1:B:346:GLN:O	1:B:350:ARG:HD2	2.19	0.42
1:A:162:ASP:HB3	1:A:164:LEU:HB2	2.02	0.42
1:B:163:LYS:HZ3	2:H:10[A]:LYS:HG3	1.85	0.42
1:B:28:ARG:HG3	1:B:58:TYR:CE2	2.55	0.42
1:A:24:LEU:HD22	1:A:58:TYR:HB3	2.02	0.42
2:H:10[A]:LYS:HG2	2:H:11[A]:LEU:N	2.33	0.42
1:A:215:MET:HE3	1:A:225:ILE:HG21	2.02	0.42
1:A:396:ARG:NH2	1:A:398:GLU:OE1	2.53	0.42
1:B:317:HIS:ND1	1:B:355:ILE:HG13	2.35	0.42
1:B:259:ARG:HB2	1:B:261:ASP:HB2	2.02	0.42
1:A:201:ASP:O	1:A:205:ASN:ND2	2.52	0.41
2:H:11[A]:LEU:CD2	2:H:11[A]:LEU:O	2.68	0.41
1:A:172:LEU:HA	1:A:172:LEU:HD12	1.71	0.41
1:A:286:GLU:N	1:A:286:GLU:OE2	2.39	0.41
1:A:59:GLU:HG2	1:A:70:SER:HB3	2.02	0.41
1:B:163:LYS:HB3	2:H:11[A]:LEU:H	1.85	0.41
1:A:10:VAL:HG22	1:A:56:VAL:HA	2.02	0.41
1:A:47:LEU:HD13	1:A:325:LEU:HD12	2.03	0.41
2:H:5[B]:GLY:C	2:H:7[B]:PHE:H	2.24	0.41
1:B:144:LEU:O	1:B:148:ARG:HG2	2.20	0.41
1:B:57:ALA:HB1	1:B:74:ARG:NH2	2.35	0.41
2:H:16[A]:SER:O	2:H:17[A]:MET:CG	2.68	0.41
1:B:329:GLU:H	1:B:329:GLU:HG2	1.45	0.41
2:H:18[B]:SER:O	2:H:19[B]:GLY:C	2.57	0.41
1:B:317:HIS:CE1	1:B:355:ILE:HG13	2.55	0.41
2:H:12[A]:ASP:OD1	2:H:12[A]:ASP:O	2.38	0.41
2:H:5[A]:GLY:C	2:H:7[A]:PHE:H	2.24	0.41
1:A:297:SER:O	1:A:301:GLN:HB2	2.21	0.41
1:B:93:TYR:CD1	2:H:15[B]:GLY:HA2	2.56	0.41
1:B:158:VAL:O	1:B:215:MET:HA	2.21	0.41
2:H:18[A]:SER:O	2:H:19[A]:GLY:C	2.57	0.41
7:A:585:HOH:O	2:H:22[B]:CYS:HA	2.19	0.41
1:B:228:VAL:O	1:B:232:HIS:HD2	2.04	0.41
1:A:308:TYR:O	1:A:309:VAL:C	2.58	0.41
1:B:194:THR:CG2	1:B:194:THR:O	2.68	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:295:LYS:HE3	1:A:299:GLU:CD	2.41	0.41
2:H:13[A]:ARG:NH2	2:H:13[A]:ARG:CG	2.82	0.40
1:A:252:TYR:C	1:A:254:ASP:N	2.75	0.40
2:H:6[B]:CYS:SG	2:H:22[B]:CYS:OXT	2.80	0.40
2:H:11[B]:LEU:CD2	2:H:11[B]:LEU:O	2.69	0.40
2:H:16[B]:SER:O	2:H:17[B]:MET:CG	2.68	0.40
1:B:10:VAL:HB	1:B:56:VAL:HG22	2.02	0.40
1:A:281:ARG:HH12	1:A:310:ASN:HA	1.85	0.40
1:B:150:HIS:O	1:B:151:HIS:HB2	2.21	0.40
1:B:100:ARG:NH1	2:H:17[A]:MET:N	2.68	0.40
1:B:38:VAL:CG1	1:B:39:GLU:N	2.85	0.40
1:B:8:ILE:HG23	1:B:84:ASP:HB2	2.03	0.40
1:A:348:TRP:CE2	1:A:365:GLY:HA3	2.56	0.40
1:A:166:ARG:HA	7:A:524:HOH:O	2.20	0.40
1:A:203:VAL:CG1	1:A:234:MET:SD	3.10	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	392/441 (89%)	377 (96%)	13 (3%)	2 (0%)	34 26
1	B	391/441 (89%)	373 (95%)	17 (4%)	1 (0%)	46 41
2	H	32/22 (146%)	10 (31%)	12 (38%)	10 (31%)	0 0
All	All	815/904 (90%)	760 (93%)	42 (5%)	13 (2%)	19 5

All (13) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	H	13[A]	ARG
2	H	13[B]	ARG

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Mol	Chain	Res	Type
2	H	17[A]	MET
2	H	17[B]	MET
1	A	2	ALA
1	A	309	VAL
1	B	302	GLY
2	H	8[A]	GLY
2	H	8[B]	GLY
2	H	21[A]	GLY
2	H	21[B]	GLY
2	H	14[A]	ILE
2	H	14[B]	ILE

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	331/371 (89%)	312 (94%)	19 (6%)	25 19
1	B	330/371 (89%)	306 (93%)	24 (7%)	17 11
2	H	26/16 (162%)	14 (54%)	12 (46%)	0 0
All	All	687/758 (91%)	632 (92%)	55 (8%)	17 9

All (55) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	11	LEU
1	A	35	LEU
1	A	71	LEU
1	A	79	ARG
1	A	85	LEU
1	A	87	LEU
1	A	115	LEU
1	A	142	MET
1	A	144	LEU
1	A	172	LEU
1	A	200	GLU

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Mol	Chain	Res	Type
1	A	210	GLU
1	A	262	LYS
1	A	264	ASP
1	A	304	ASN
1	A	308	TYR
1	A	331	LEU
1	A	332	ARG
1	A	350	ARG
1	B	11	LEU
1	B	35	LEU
1	B	38	VAL
1	B	71	LEU
1	B	79	ARG
1	B	85	LEU
1	B	87	LEU
1	B	115	LEU
1	B	130	THR
1	B	142	MET
1	B	144	LEU
1	B	210	GLU
1	B	261	ASP
1	B	274	LEU
1	B	304	ASN
1	B	305	MET
1	B	306	GLU
1	B	307	ASP
1	B	308	TYR
1	B	309	VAL
1	B	329	GLU
1	B	331	LEU
1	B	367	ARG
1	B	387	ILE
2	H	6[A]	CYS
2	H	6[B]	CYS
2	H	9[A]	LEU
2	H	9[B]	LEU
2	H	10[A]	LYS
2	H	10[B]	LYS
2	H	13[A]	ARG
2	H	13[B]	ARG
2	H	17[A]	MET
2	H	17[B]	MET

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Mol	Chain	Res	Type
2	H	22[A]	CYS
2	H	22[B]	CYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (6) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	232	HIS
1	B	151	HIS
1	B	232	HIS
1	B	304	ASN
1	B	345	GLN
1	B	346	GLN

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

2 carbohydrates are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the chemical component dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
4	NAG	B	501	1,4	14,14,15	0.53	0	15,19,21	0.73	1 (6%)
4	NAG	B	502	4	14,14,15	0.45	0	15,19,21	0.74	1 (6%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the chemical

component dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	NAG	B	501	1,4	-	0/6/23/26	0/1/1/1
4	NAG	B	502	4	-	0/6/23/26	0/1/1/1

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	B	502	NAG	C2-N2-C7	-2.43	119.92	123.04
4	B	501	NAG	C2-N2-C7	-2.18	120.24	123.04

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.6 Ligand geometry

Of 5 ligands modelled in this entry, 2 are monoatomic - leaving 3 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	$\#\|Z\| > 2$
3	NDG	A	501	1	14,14,15	0.57	0	15,19,21	0.72	1 (6%)
3	NDG	A	502	1	14,14,15	0.74	1 (7%)	15,19,21	0.78	0
5	NAG	B	503	1	14,14,15	0.53	0	15,19,21	0.81	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
3	NDG	A	501	1	-	2/6/23/26	0/1/1/1
3	NDG	A	502	1	-	0/6/23/26	0/1/1/1
5	NAG	B	503	1	-	1/6/23/26	0/1/1/1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	502	NDG	C1-C2	2.16	1.55	1.52

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	A	501	NDG	C2-N2-C7	-2.04	120.42	123.04

There are no chirality outliers.

All (3) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	B	503	NAG	O7-C7-N2-C2
3	A	501	NDG	O7-C7-N2-C2
3	A	501	NDG	C8-C7-N2-C2

There are no ring outliers.

2 monomers are involved in 8 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	501	NDG	7	0
3	A	502	NDG	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

EDS was not executed - this section will therefore be empty.

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

EDS was not executed - this section will therefore be empty.

6.3 Carbohydrates

EDS was not executed - this section will therefore be empty.

6.4 Ligands

EDS was not executed - this section will therefore be empty.

6.5 Other polymers

EDS was not executed - this section will therefore be empty.