Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 04:43 PM GMT

PDB ID	:	4FVV
Title	:	Crystal structure of HCR/D-Sa-GBL1/C
Authors	:	Fu, Z.; Karalewitz, A.; Baldwin, M.R.; Kim, J.-J.P.; Barbieri, J.T.
Deposited on	:	2012-06-29
Resolution	:	2.70 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:

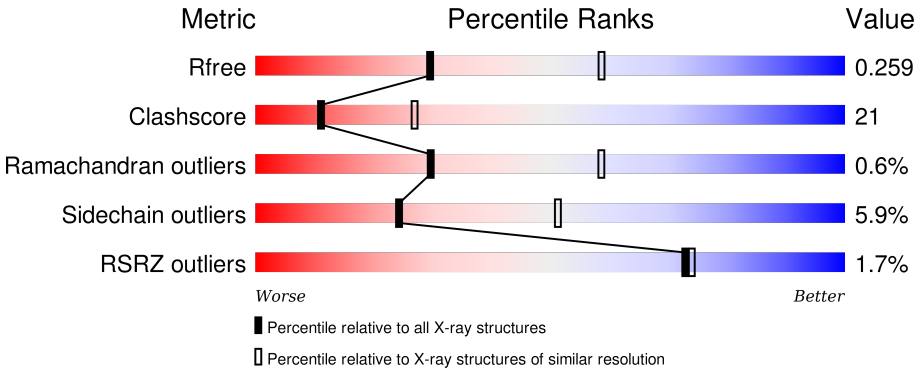
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)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

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 2.70 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	2103 (2.70-2.70)
Clashscore	102246	2422 (2.70-2.70)
Ramachandran outliers	100387	2382 (2.70-2.70)
Sidechain outliers	100360	2382 (2.70-2.70)
RSRZ outliers	91569	2107 (2.70-2.70)

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	423	2% 63% 30%
1	B	423	% 61% 33%

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	GOL	A	1304	-	-	-	X
3	GOL	B	1401	-	-	-	X

2 Entry composition (i)

There are 5 unique types of molecules in this entry. The entry contains 6985 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.

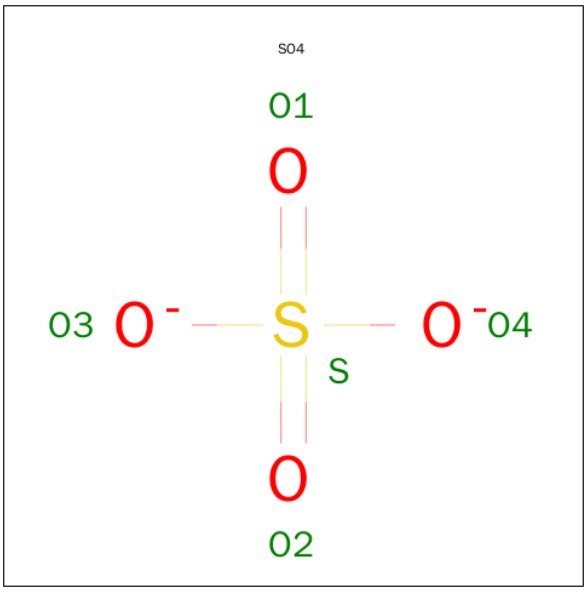
- Molecule 1 is a protein called Neurotoxin.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	412	Total	C	N	O	S	0	0	0
			3361	2156	561	630	14			
1	B	415	Total	C	N	O	S	0	0	0
			3380	2166	565	635	14			

There are 8 discrepancies between the modelled and reference sequences:

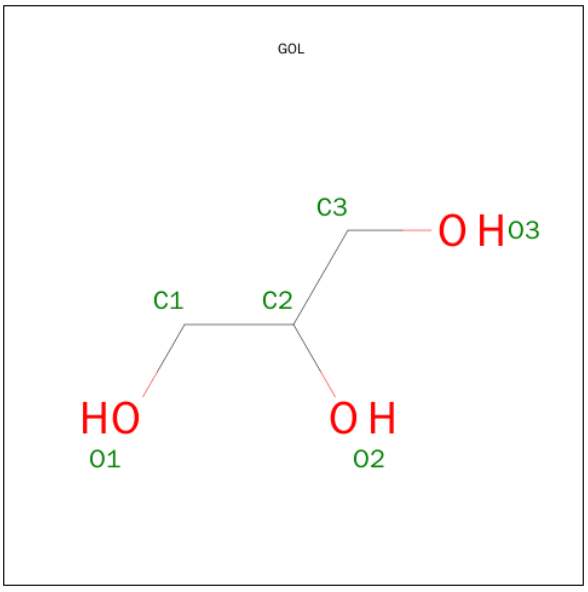
Chain	Residue	Modelled	Actual	Comment	Reference
A	1246	ARG	LYS	SEE REMARK 999	UNP Q9LBR1
A	1249	GLY	ASP	SEE REMARK 999	UNP Q9LBR1
A	1252	TYR	PHE	SEE REMARK 999	UNP Q9LBR1
A	1253	ARG	ASN	SEE REMARK 999	UNP Q9LBR1
B	1246	ARG	LYS	SEE REMARK 999	UNP Q9LBR1
B	1249	GLY	ASP	SEE REMARK 999	UNP Q9LBR1
B	1252	TYR	PHE	SEE REMARK 999	UNP Q9LBR1
B	1253	ARG	ASN	SEE REMARK 999	UNP Q9LBR1

- Molecule 2 is SULFATE ION (three-letter code: SO4) (formula: O_4S).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total O S 5 4 1	0	0
2	A	1	Total O S 5 4 1	0	0
2	A	1	Total O S 5 4 1	0	0

- Molecule 3 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total C O 6 3 3	0	0

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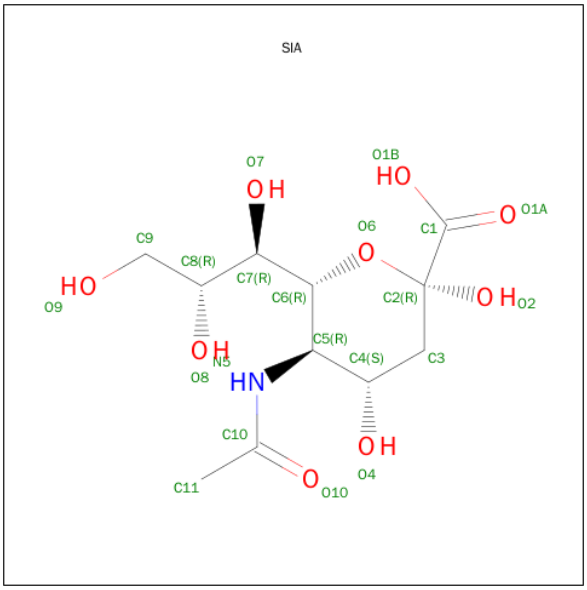
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	B	1	Total C O 6 3 3	0	0
3	B	1	Total C O 6 3 3	0	0

- Molecule 4 is SUGAR (O-SIALIC ACID) (three-letter code: SIA) (formula: $C_{11}H_{19}NO_9$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	B	1	Total C N O 21 11 1 9	0	0

- Molecule 5 is water.

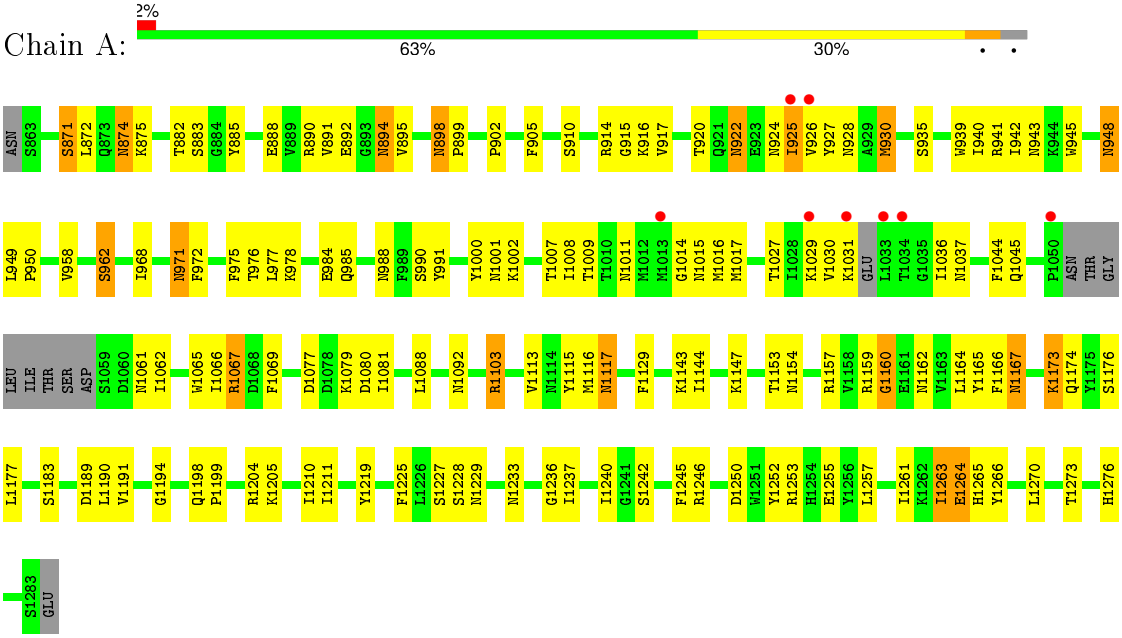
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	97	Total O 97 97	0	0
5	B	93	Total O 93 93	0	0

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.

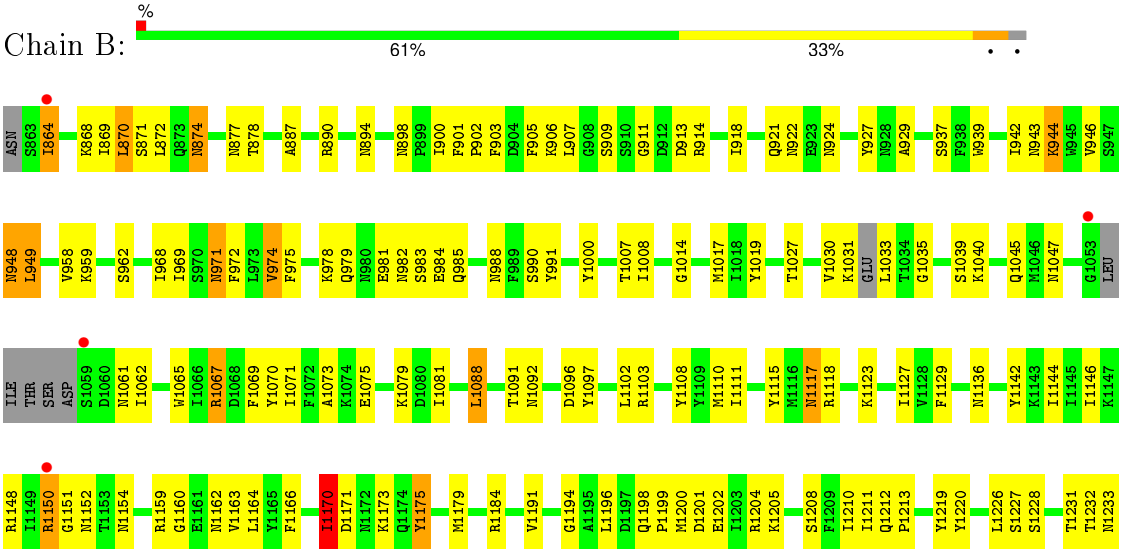
- Molecule 1: Neurotoxin

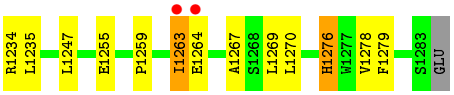
Chain A:



- Molecule 1: Neurotoxin

Chain B:




R1234
L1235
L1247
E1255
P1259
I1263
E1264
A1267
S1268
L1269
L1270
H1276
W1277
V1278
F1279
S1283
GLU

4 Data and refinement statistics (i)

Property	Value	Source
Space group	I 2 2 2	Depositor
Cell constants a, b, c, α, β, γ	82.60Å 154.63Å 181.03Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	39.38 – 2.70 39.37 – 2.70	Depositor EDS
% Data completeness (in resolution range)	90.0 (39.38-2.70) 90.0 (39.37-2.70)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.11	Depositor
$< I/\sigma(I) >$ [1]	2.01 (at 2.69Å)	Xtriage
Refinement program	CNS 1.3	Depositor
R, R_{free}	0.206 , 0.263 0.204 , 0.259	Depositor DCC
R_{free} test set	1429 reflections (5.17%)	DCC
Wilson B-factor (Å^2)	31.7	Xtriage
Anisotropy	0.202	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.34 , 46.4	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.31$	Xtriage
Outliers	0 of 29077 reflections	Xtriage
F_o,F_c correlation	0.92	EDS
Total number of atoms	6985	wwPDB-VP
Average B, all atoms (Å^2)	34.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.34% 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: GOL, SIA, SO4

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	0.40	0/3436	0.68	1/4647 (0.0%)
1	B	0.41	0/3455	0.66	0/4673
All	All	0.41	0/6891	0.67	1/9320 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	1264	GLU	N-CA-C	5.33	125.40	111.00

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	3361	0	3294	127	0
1	B	3380	0	3310	154	0
2	A	15	0	0	1	0
3	A	6	0	8	1	0
3	B	12	0	16	0	0
4	B	21	0	18	2	0
5	A	97	0	0	5	0
5	B	93	0	0	6	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
All	All	6985	0	6646	280	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 21.

All (280) 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:B:914:ARG:HH12	1:B:1047:ASN:ND2	1.58	1.00
1:B:944:LYS:NZ	1:B:944:LYS:HA	1.77	0.99
1:B:914:ARG:HH12	1:B:1047:ASN:HD22	1.05	0.97
1:B:921:GLN:HE21	1:B:1040:LYS:HD3	1.29	0.95
1:B:1159:ARG:H	1:B:1162:ASN:ND2	1.66	0.93
1:B:864:ILE:HD13	1:B:864:ILE:H	1.32	0.91
1:B:911:GLY:O	1:B:914:ARG:HD3	1.71	0.89
1:B:868:LYS:HD3	1:B:871:SER:HB2	1.54	0.88
1:B:1097:TYR:HD1	1:B:1278:VAL:HG21	1.40	0.85
1:A:1007:THR:HG21	1:A:1081:ILE:HG12	1.59	0.85
1:B:1199:PRO:HD2	1:B:1202:GLU:HG3	1.57	0.84
1:B:971:ASN:H	1:B:971:ASN:HD22	1.24	0.83
1:B:890:ARG:HB3	1:B:890:ARG:NH2	1.94	0.83
1:B:944:LYS:HZ1	1:B:944:LYS:HA	1.42	0.82
1:B:890:ARG:HH21	1:B:890:ARG:HB3	1.47	0.79
1:B:1007:THR:HG21	1:B:1081:ILE:HG12	1.64	0.79
1:B:1267:ALA:HA	1:B:1270:LEU:HD23	1.66	0.77
1:A:890:ARG:NH2	1:A:890:ARG:HB3	1.99	0.77
1:B:1117:ASN:H	1:B:1117:ASN:HD22	1.32	0.76
1:B:1198:GLN:HB2	1:B:1202:GLU:HB2	1.68	0.75
1:A:922:ASN:HD21	1:A:924:ASN:HB2	1.50	0.75
1:B:1097:TYR:CD1	1:B:1278:VAL:HG21	2.22	0.74
1:B:1269:LEU:HD21	4:B:1403:SIA:H112	1.70	0.72
1:B:1045:GLN:HG2	1:B:1047:ASN:HD21	1.54	0.72
1:A:1067:ARG:NH1	1:A:1088:LEU:O	2.22	0.71
1:B:921:GLN:HB2	1:B:927:TYR:CE2	2.26	0.70
1:B:1152:ASN:HD21	1:B:1154:ASN:HB2	1.55	0.69
1:B:874:ASN:HD21	1:B:877:ASN:HA	1.58	0.69
1:A:1117:ASN:H	1:A:1117:ASN:HD22	1.38	0.69
1:B:1115:TYR:HB3	1:B:1118:ARG:HG3	1.75	0.68
1:A:1219:TYR:OH	1:A:1276:HIS:HD2	1.78	0.67
1:A:978:LYS:HG2	1:A:984:GLU:OE2	1.95	0.67
1:A:890:ARG:HB3	1:A:890:ARG:HH21	1.59	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1117:ASN:N	1:B:1117:ASN:HD22	1.93	0.66
1:B:887:ALA:HA	5:B:1502:HOH:O	1.95	0.66
1:A:1236:GLY:HA2	1:A:1266:TYR:CD2	2.31	0.66
1:B:1198:GLN:HB2	1:B:1202:GLU:CB	2.24	0.65
1:B:1179:MET:HE3	1:B:1226:LEU:HD22	1.79	0.65
1:B:1045:GLN:HG2	1:B:1047:ASN:ND2	2.12	0.64
1:B:979:GLN:HG3	1:B:983:SER:OG	1.98	0.64
1:A:1017:MET:HE1	5:A:1577:HOH:O	1.96	0.64
1:A:1015:ASN:HD22	1:A:1029:LYS:HA	1.63	0.64
1:B:914:ARG:NH1	1:B:1047:ASN:ND2	2.40	0.64
1:B:864:ILE:CD1	1:B:864:ILE:H	2.09	0.63
1:A:1245:PHE:HA	1:A:1253:ARG:HG2	1.80	0.63
1:A:1015:ASN:ND2	1:A:1029:LYS:HA	2.13	0.63
1:A:1115:TYR:CD1	1:A:1240:ILE:HD13	2.33	0.63
1:B:942:ILE:HD13	1:B:968:ILE:HD13	1.80	0.63
1:A:871:SER:HB3	1:A:882:THR:OG1	2.00	0.62
1:B:944:LYS:HZ2	1:B:944:LYS:HA	1.62	0.61
1:B:944:LYS:HE3	1:B:946:VAL:HG13	1.83	0.61
1:B:943:ASN:O	1:B:944:LYS:HB3	2.00	0.61
1:A:890:ARG:CB	1:A:890:ARG:HH21	2.14	0.61
1:B:1136:ASN:HB3	5:B:1532:HOH:O	2.01	0.60
1:B:1148:ARG:HD2	1:B:1151:GLY:HA3	1.83	0.60
1:B:918:ILE:HD12	1:B:918:ILE:H	1.67	0.60
1:B:922:ASN:OD1	1:B:924:ASN:N	2.35	0.59
1:A:1183:SER:HB3	1:A:1246:ARG:O	2.01	0.59
1:B:1144:ILE:HD13	1:B:1166:PHE:HD2	1.67	0.59
1:B:1092:ASN:OD1	1:B:1160:GLY:HA3	2.02	0.59
1:B:1127:ILE:HG12	1:B:1194:GLY:HA2	1.85	0.59
1:A:939:TRP:HB2	1:A:1067:ARG:HD3	1.85	0.59
1:B:874:ASN:HD21	1:B:877:ASN:CA	2.16	0.58
1:A:1246:ARG:HG3	1:A:1253:ARG:HG3	1.84	0.58
1:B:1170:ILE:HG22	1:B:1171:ASP:N	2.17	0.58
1:A:1103:ARG:HD3	5:A:1591:HOH:O	2.03	0.58
1:B:1210:ILE:HD12	1:B:1234:ARG:HD3	1.86	0.58
1:B:1219:TYR:OH	1:B:1276:HIS:HD2	1.86	0.58
1:B:1219:TYR:OH	1:B:1276:HIS:CD2	2.57	0.57
1:B:918:ILE:HD12	1:B:918:ILE:N	2.19	0.57
1:B:1123:LYS:HG3	1:B:1247:LEU:HB3	1.85	0.57
1:A:1263:ILE:O	1:A:1264:GLU:HG2	2.05	0.57
1:A:1092:ASN:OD1	1:A:1160:GLY:HA3	2.04	0.57
1:B:981:GLU:HG3	1:B:982:ASN:ND2	2.19	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:910:SER:HB2	1:A:1061:ASN:CG	2.25	0.57
1:B:1103:ARG:HD3	5:B:1521:HOH:O	2.05	0.57
1:A:943:ASN:HB2	1:A:1065:TRP:CZ3	2.40	0.56
1:B:1017:MET:HG2	1:B:1027:THR:HB	1.87	0.56
1:A:1167:ASN:ND2	5:A:1572:HOH:O	2.35	0.56
1:B:959:LYS:HD3	5:B:1576:HOH:O	2.05	0.56
1:A:1157:ARG:HH12	3:A:1304:GOL:H2	1.69	0.56
1:A:898:ASN:HD22	1:A:899:PRO:HD2	1.70	0.56
1:A:902:PRO:HB2	1:A:1067:ARG:HD2	1.87	0.56
1:B:890:ARG:HH21	1:B:890:ARG:CB	2.16	0.56
1:A:1236:GLY:HA2	1:A:1266:TYR:CE2	2.40	0.55
1:A:971:ASN:O	1:A:990:SER:HA	2.06	0.55
1:A:924:ASN:HB3	1:A:927:TYR:CD2	2.42	0.55
1:A:1204:ARG:O	1:A:1229:ASN:HA	2.06	0.55
1:B:905:PHE:CE1	1:B:907:LEU:HD11	2.40	0.55
1:B:949:LEU:HD11	1:B:1062:ILE:HG21	1.88	0.55
1:B:1179:MET:HE1	1:B:1191:VAL:HG11	1.87	0.55
1:A:922:ASN:ND2	1:A:924:ASN:HB2	2.22	0.54
1:A:1154:ASN:N	1:A:1154:ASN:HD22	2.06	0.54
1:A:1253:ARG:HD2	2:A:1303:SO4:O4	2.07	0.54
1:A:1000:TYR:CE1	1:A:1002:LYS:HE3	2.42	0.54
1:A:1219:TYR:OH	1:A:1276:HIS:CD2	2.61	0.54
1:B:874:ASN:ND2	1:B:878:THR:H	2.06	0.54
1:B:1227:SER:HB2	1:B:1231:THR:O	2.08	0.53
1:A:948:ASN:HD22	1:A:948:ASN:N	2.06	0.53
1:A:922:ASN:ND2	1:A:924:ASN:H	2.07	0.53
1:A:948:ASN:HD22	1:A:948:ASN:H	1.57	0.53
1:B:1228:SER:HA	1:B:1235:LEU:HD11	1.90	0.53
1:B:1110:MET:HG3	1:B:1279:PHE:CE2	2.43	0.53
1:A:972:PHE:HD2	1:A:988:ASN:ND2	2.07	0.52
1:A:874:ASN:ND2	1:A:874:ASN:C	2.62	0.52
1:B:870:LEU:HD22	1:B:871:SER:N	2.24	0.52
1:B:1200:MET:HG3	1:B:1204:ARG:NH2	2.25	0.52
1:A:890:ARG:HH22	1:A:892:GLU:CG	2.22	0.52
1:B:948:ASN:H	1:B:948:ASN:HD22	1.58	0.52
1:A:1173:LYS:HD2	1:A:1174:GLN:H	1.75	0.52
1:A:1189:ASP:HB3	1:A:1263:ILE:O	2.09	0.52
1:B:937:SER:OG	1:B:1070:TYR:HB2	2.10	0.52
1:B:922:ASN:OD1	1:B:924:ASN:HB2	2.10	0.52
1:B:1150:ARG:HB3	1:B:1163:VAL:HB	1.91	0.52
1:B:1067:ARG:NH1	1:B:1088:LEU:O	2.42	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:922:ASN:HD22	1:A:922:ASN:C	2.12	0.51
1:A:1205:LYS:HA	1:A:1229:ASN:HD22	1.75	0.51
1:A:883:SER:HG	1:A:885:TYR:HD1	1.58	0.51
1:B:1117:ASN:H	1:B:1117:ASN:ND2	2.05	0.51
1:A:949:LEU:HD11	1:A:1062:ILE:HD13	1.92	0.51
1:A:1159:ARG:H	1:A:1162:ASN:ND2	2.08	0.51
1:A:935:SER:OG	1:A:1009:THR:HG22	2.10	0.51
1:A:890:ARG:HH22	1:A:892:GLU:HG3	1.75	0.51
1:B:872:LEU:HB3	1:B:1069:PHE:HB3	1.92	0.51
1:B:1175:TYR:HB3	1:B:1196:LEU:O	2.11	0.51
1:B:1196:LEU:HD22	1:B:1196:LEU:N	2.26	0.51
1:A:1144:ILE:HD12	1:A:1144:ILE:C	2.32	0.50
1:B:1199:PRO:HD2	1:B:1202:GLU:CG	2.35	0.50
1:A:874:ASN:HD22	1:A:874:ASN:C	2.13	0.50
1:B:907:LEU:N	1:B:907:LEU:HD12	2.27	0.50
1:A:971:ASN:HB2	1:A:991:TYR:CE1	2.46	0.49
1:A:1036:ILE:HG12	1:A:1037:ASN:H	1.77	0.49
1:B:975:PHE:CD2	1:B:1008:ILE:HD13	2.47	0.49
1:A:1154:ASN:N	1:A:1154:ASN:ND2	2.59	0.49
1:B:1152:ASN:ND2	1:B:1154:ASN:HB2	2.25	0.49
1:A:898:ASN:HD22	1:A:899:PRO:CD	2.23	0.49
1:B:985:GLN:CD	1:B:1031:LYS:HG3	2.33	0.49
1:B:929:ALA:HB2	5:B:1507:HOH:O	2.11	0.49
1:B:870:LEU:HB3	1:B:1071:ILE:HB	1.93	0.49
1:A:942:ILE:CG2	1:A:945:TRP:HB2	2.43	0.49
1:A:1117:ASN:N	1:A:1117:ASN:HD22	2.10	0.49
1:B:1142:TYR:CD1	1:B:1170:ILE:HD12	2.47	0.49
1:B:1211:ILE:HG12	1:B:1212:GLN:N	2.28	0.48
1:A:1067:ARG:NH1	1:A:1088:LEU:HB3	2.28	0.48
1:B:1173:LYS:HB2	1:B:1175:TYR:CE1	2.48	0.48
1:A:1166:PHE:O	1:A:1176:SER:HA	2.12	0.48
1:B:1144:ILE:C	1:B:1144:ILE:HD12	2.34	0.48
1:A:1160:GLY:O	1:A:1211:ILE:O	2.31	0.48
1:A:922:ASN:HD21	1:A:924:ASN:CB	2.24	0.48
1:B:1191:VAL:CG1	1:B:1263:ILE:HG13	2.44	0.48
1:A:874:ASN:HD22	1:A:875:LYS:N	2.12	0.48
1:B:921:GLN:NE2	1:B:1040:LYS:HD3	2.13	0.48
1:B:972:PHE:CD2	1:B:990:SER:HB3	2.49	0.48
1:A:928:ASN:C	1:A:930:MET:H	2.17	0.48
1:A:914:ARG:HG2	1:A:914:ARG:HH21	1.79	0.47
1:B:909:SER:H	1:B:1061:ASN:HD21	1.62	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:901:PHE:CD2	1:B:902:PRO:HA	2.49	0.47
1:B:944:LYS:O	1:B:944:LYS:HG3	2.14	0.47
1:A:942:ILE:N	1:A:942:ILE:HD12	2.29	0.47
1:B:1269:LEU:HD21	4:B:1403:SIA:C11	2.43	0.47
1:A:1036:ILE:HG12	1:A:1037:ASN:N	2.29	0.47
1:A:917:VAL:HB	1:A:1044:PHE:HB2	1.96	0.47
1:B:1045:GLN:CG	1:B:1047:ASN:HD21	2.25	0.47
1:A:1173:LYS:HD2	1:A:1174:GLN:N	2.30	0.47
1:A:1237:ILE:HG22	1:A:1266:TYR:HB2	1.97	0.47
1:A:943:ASN:HB2	1:A:1065:TRP:HZ3	1.78	0.47
1:A:928:ASN:C	1:A:930:MET:N	2.69	0.47
1:A:905:PHE:CZ	1:A:1066:ILE:HB	2.50	0.47
1:B:921:GLN:HG3	1:B:1040:LYS:CD	2.45	0.46
1:B:971:ASN:ND2	1:B:971:ASN:H	2.04	0.46
1:B:1150:ARG:HE	1:B:1232:THR:CG2	2.28	0.46
1:B:898:ASN:O	1:B:903:PHE:HA	2.15	0.46
1:A:1031:LYS:O	1:A:1031:LYS:HG3	2.16	0.46
1:B:1111:ILE:HB	1:B:1278:VAL:HG12	1.97	0.46
1:B:1129:PHE:CZ	1:B:1259:PRO:HD3	2.50	0.46
1:A:1129:PHE:HB2	1:A:1257:LEU:HD23	1.98	0.46
1:B:1220:TYR:O	1:B:1278:VAL:HG23	2.16	0.46
1:B:948:ASN:HD22	1:B:948:ASN:N	2.13	0.46
1:B:1175:TYR:CD1	1:B:1175:TYR:N	2.84	0.46
1:B:943:ASN:HB2	1:B:1065:TRP:CZ3	2.51	0.46
1:B:905:PHE:CD1	1:B:907:LEU:HD11	2.51	0.46
1:B:1014:GLY:O	1:B:1030:VAL:HG22	2.16	0.46
1:B:1150:ARG:HD2	1:B:1163:VAL:HG23	1.98	0.45
1:A:968:ILE:O	1:A:968:ILE:HG13	2.16	0.45
1:A:925:ILE:HD13	1:A:925:ILE:O	2.16	0.45
1:A:972:PHE:CD2	1:A:988:ASN:ND2	2.84	0.45
1:A:1210:ILE:HG13	1:A:1227:SER:HB2	1.98	0.45
1:B:944:LYS:HE3	1:B:946:VAL:CG1	2.46	0.45
1:B:985:GLN:HE22	1:B:1030:VAL:HA	1.82	0.45
1:A:985:GLN:HG3	1:A:1031:LYS:HE3	1.98	0.45
1:A:916:LYS:HD2	1:A:1045:GLN:NE2	2.31	0.45
1:A:885:TYR:CE2	1:A:926:VAL:HG11	2.52	0.45
1:A:1011:ASN:OD1	1:A:1014:GLY:N	2.50	0.45
1:A:1113:VAL:HA	1:A:1116:MET:CE	2.46	0.45
1:A:902:PRO:HB2	1:A:1067:ARG:CD	2.47	0.45
1:B:1096:ASP:HB2	1:B:1279:PHE:O	2.17	0.45
1:B:1007:THR:HB	1:B:1019:TYR:HB2	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1115:TYR:HB3	1:B:1118:ARG:CG	2.46	0.45
1:A:940:ILE:HG12	1:A:941:ARG:N	2.32	0.45
1:A:976:THR:HG22	1:A:977:LEU:N	2.32	0.45
1:B:1075:GLU:HG2	1:B:1075:GLU:O	2.17	0.44
1:A:872:LEU:HB3	1:A:1069:PHE:HB3	1.97	0.44
1:B:1179:MET:CE	1:B:1263:ILE:HD11	2.46	0.44
1:A:883:SER:OG	1:A:885:TYR:HD1	2.00	0.44
1:B:906:LYS:HD3	1:B:1065:TRP:NE1	2.32	0.44
1:B:1154:ASN:N	1:B:1154:ASN:HD22	2.16	0.44
1:A:1164:LEU:C	1:A:1164:LEU:HD12	2.37	0.44
1:A:978:LYS:HA	1:A:984:GLU:HB2	2.00	0.43
1:A:899:PRO:HB3	1:B:969:ILE:HD13	1.99	0.43
1:A:948:ASN:ND2	1:A:948:ASN:H	2.15	0.43
1:B:1017:MET:HG2	1:B:1027:THR:CB	2.48	0.43
1:B:1146:ILE:CG2	1:B:1164:LEU:HD22	2.49	0.43
1:B:921:GLN:HG3	1:B:1040:LYS:HD2	2.01	0.43
1:B:1173:LYS:HE3	1:B:1175:TYR:OH	2.19	0.43
1:B:869:ILE:HG21	1:B:1073:ALA:HB2	2.00	0.43
1:A:1198:GLN:HB2	1:A:1199:PRO:HD2	2.00	0.43
1:B:921:GLN:HG2	1:B:1040:LYS:O	2.19	0.43
1:A:888:GLU:HB3	1:A:920:THR:HB	1.99	0.43
1:A:1261:ILE:HG22	1:A:1263:ILE:HG22	2.00	0.43
1:A:1242:SER:OG	1:A:1255:GLU:OE2	2.36	0.43
1:A:894:ASN:C	1:A:894:ASN:ND2	2.72	0.43
1:A:891:VAL:HG13	1:A:895:VAL:HG21	2.01	0.43
1:A:1147:LYS:HB2	1:A:1165:TYR:CE1	2.53	0.43
1:B:1200:MET:HG3	1:B:1204:ARG:HH21	1.82	0.42
1:A:1205:LYS:HB3	1:A:1205:LYS:NZ	2.33	0.42
1:B:972:PHE:CE2	1:B:990:SER:HB3	2.54	0.42
1:B:874:ASN:ND2	1:B:878:THR:N	2.67	0.42
1:B:942:ILE:HD13	1:B:968:ILE:CD1	2.47	0.42
1:A:888:GLU:OE2	1:A:890:ARG:HD2	2.19	0.42
1:B:1191:VAL:HG11	1:B:1263:ILE:HG13	2.01	0.42
1:A:885:TYR:CD2	1:A:926:VAL:HG11	2.54	0.42
1:B:921:GLN:HB2	1:B:927:TYR:CZ	2.54	0.42
1:A:1077:ASP:N	1:A:1080:ASP:HB2	2.34	0.42
1:B:983:SER:OG	1:B:1031:LYS:HE2	2.20	0.42
1:B:874:ASN:HD22	1:B:874:ASN:C	2.22	0.42
1:A:1225:PHE:CE1	1:A:1237:ILE:HD12	2.55	0.42
1:B:1031:LYS:O	1:B:1033:LEU:HB3	2.20	0.42
1:A:924:ASN:HB3	1:A:927:TYR:HD2	1.85	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1228:SER:HB3	1:A:1233:ASN:HB3	2.01	0.42
1:A:1273:THR:HA	1:A:1276:HIS:CD2	2.55	0.41
1:B:978:LYS:HE2	1:B:984:GLU:OE2	2.20	0.41
1:B:874:ASN:ND2	1:B:874:ASN:C	2.74	0.41
1:B:1142:TYR:CZ	1:B:1170:ILE:HG23	2.54	0.41
1:B:1164:LEU:O	1:B:1208:SER:HA	2.20	0.41
1:B:943:ASN:HB2	1:B:1065:TRP:HZ3	1.83	0.41
1:A:949:LEU:HD12	1:A:950:PRO:HD2	2.03	0.41
1:A:985:GLN:CG	1:A:1031:LYS:HE3	2.50	0.41
1:A:1077:ASP:H	1:A:1080:ASP:HB2	1.85	0.41
1:A:1177:LEU:HA	1:A:1194:GLY:O	2.20	0.41
1:A:1264:GLU:HG3	1:A:1265:HIS:CE1	2.55	0.41
1:B:979:GLN:H	1:B:979:GLN:HG2	1.71	0.41
1:B:1136:ASN:HA	5:B:1532:HOH:O	2.21	0.41
1:B:1231:THR:OG1	1:B:1233:ASN:HB2	2.20	0.41
1:B:948:ASN:ND2	1:B:948:ASN:C	2.73	0.41
1:A:914:ARG:HG2	1:A:914:ARG:NH2	2.35	0.41
1:B:894:ASN:HB2	1:B:913:ASP:OD2	2.20	0.41
1:B:958:VAL:HA	1:B:962:SER:O	2.21	0.41
1:A:922:ASN:HB3	5:A:1580:HOH:O	2.20	0.41
1:B:1228:SER:HB2	1:B:1235:LEU:HD21	2.02	0.41
1:B:948:ASN:ND2	1:B:948:ASN:H	2.19	0.41
1:A:1016:MET:HB2	1:A:1030:VAL:HG22	2.02	0.41
1:A:958:VAL:HG13	1:A:962:SER:H	1.86	0.41
1:A:922:ASN:ND2	1:A:922:ASN:C	2.74	0.41
1:B:1179:MET:HE1	1:B:1263:ILE:HD11	2.03	0.41
1:A:1061:ASN:HD22	1:A:1062:ILE:N	2.19	0.41
1:B:959:LYS:HB2	1:B:1039:SER:HB2	2.03	0.41
1:B:1212:GLN:OE1	1:B:1213:PRO:HD2	2.21	0.41
1:A:1250:ASP:HB3	1:A:1252:TYR:O	2.21	0.41
1:B:974:VAL:HB	1:B:988:ASN:HB3	2.03	0.41
1:A:984:GLU:O	1:A:984:GLU:HG3	2.20	0.41
1:B:991:TYR:HB2	1:B:1000:TYR:CD1	2.56	0.41
1:A:898:ASN:HA	1:A:899:PRO:HD2	1.93	0.40
1:B:1079:LYS:HB3	1:B:1079:LYS:HE2	1.72	0.40
1:A:975:PHE:CD2	1:A:1008:ILE:HD13	2.56	0.40
1:B:948:ASN:HD22	1:B:948:ASN:C	2.24	0.40
1:B:939:TRP:HB2	1:B:1067:ARG:HD3	2.03	0.40
1:A:1077:ASP:O	1:A:1080:ASP:HB2	2.21	0.40
1:A:1017:MET:HE3	5:A:1511:HOH:O	2.20	0.40
1:B:1102:LEU:HD12	1:B:1108:TYR:CZ	2.56	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1201:ASP:O	1:B:1205:LYS:HD3	2.22	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	406/423 (96%)	357 (88%)	47 (12%)	2 (0%)	34	63
1	B	409/423 (97%)	367 (90%)	39 (10%)	3 (1%)	26	55
All	All	815/846 (96%)	724 (89%)	86 (11%)	5 (1%)	30	59

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	915	GLY
1	A	1160	GLY
1	B	1170	ILE
1	B	1035	GLY
1	B	1091	THR

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.

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	374/386 (97%)	350 (94%)	24 (6%)	22 47
1	B	376/386 (97%)	356 (95%)	20 (5%)	28 57
All	All	750/772 (97%)	706 (94%)	44 (6%)	24 51

All (44) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	871	SER
1	A	874	ASN
1	A	894	ASN
1	A	898	ASN
1	A	922	ASN
1	A	925	ILE
1	A	930	MET
1	A	948	ASN
1	A	962	SER
1	A	971	ASN
1	A	1001	ASN
1	A	1027	THR
1	A	1067	ARG
1	A	1079	LYS
1	A	1103	ARG
1	A	1117	ASN
1	A	1143	LYS
1	A	1153	THR
1	A	1167	ASN
1	A	1173	LYS
1	A	1190	LEU
1	A	1191	VAL
1	A	1263	ILE
1	A	1270	LEU
1	B	864	ILE
1	B	870	LEU
1	B	874	ASN
1	B	900	ILE
1	B	944	LYS
1	B	948	ASN
1	B	949	LEU
1	B	971	ASN

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Mol	Chain	Res	Type
1	B	974	VAL
1	B	1067	ARG
1	B	1088	LEU
1	B	1117	ASN
1	B	1150	ARG
1	B	1170	ILE
1	B	1175	TYR
1	B	1184	ARG
1	B	1255	GLU
1	B	1263	ILE
1	B	1264	GLU
1	B	1276	HIS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (49) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	873	GLN
1	A	874	ASN
1	A	894	ASN
1	A	898	ASN
1	A	921	GLN
1	A	922	ASN
1	A	928	ASN
1	A	948	ASN
1	A	960	ASN
1	A	971	ASN
1	A	979	GLN
1	A	982	ASN
1	A	988	ASN
1	A	1015	ASN
1	A	1045	GLN
1	A	1061	ASN
1	A	1114	ASN
1	A	1117	ASN
1	A	1136	ASN
1	A	1154	ASN
1	A	1167	ASN
1	A	1174	GLN
1	A	1198	GLN
1	A	1215	ASN
1	A	1229	ASN
1	A	1276	HIS

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Mol	Chain	Res	Type
1	B	873	GLN
1	B	874	ASN
1	B	921	GLN
1	B	928	ASN
1	B	948	ASN
1	B	971	ASN
1	B	982	ASN
1	B	988	ASN
1	B	1047	ASN
1	B	1061	ASN
1	B	1063	ASN
1	B	1114	ASN
1	B	1117	ASN
1	B	1125	ASN
1	B	1152	ASN
1	B	1154	ASN
1	B	1162	ASN
1	B	1167	ASN
1	B	1185	ASN
1	B	1198	GLN
1	B	1215	ASN
1	B	1223	GLN
1	B	1276	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

7 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
2	SO4	A	1301	-	4,4,4	0.19	0	6,6,6	0.07	0
2	SO4	A	1302	-	4,4,4	0.02	0	6,6,6	0.12	0
2	SO4	A	1303	-	4,4,4	0.26	0	6,6,6	0.09	0
3	GOL	A	1304	-	5,5,5	0.58	0	5,5,5	0.67	0
3	GOL	B	1401	-	5,5,5	0.59	0	5,5,5	0.57	0
3	GOL	B	1402	-	5,5,5	0.67	0	5,5,5	0.66	0
4	SIA	B	1403	-	17,21,21	3.61	6 (35%)	19,31,31	0.95	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
2	SO4	A	1301	-	-	0/0/0/0	0/0/0/0
2	SO4	A	1302	-	-	0/0/0/0	0/0/0/0
2	SO4	A	1303	-	-	0/0/0/0	0/0/0/0
3	GOL	A	1304	-	-	0/4/4/4	0/0/0/0
3	GOL	B	1401	-	-	0/4/4/4	0/0/0/0
3	GOL	B	1402	-	-	0/4/4/4	0/0/0/0
4	SIA	B	1403	-	-	0/14/38/38	0/1/1/1

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	1403	SIA	C3-C4	2.20	1.56	1.53
4	B	1403	SIA	C7-C6	3.23	1.57	1.52
4	B	1403	SIA	O6-C6	3.51	1.50	1.44
4	B	1403	SIA	C6-C5	4.04	1.59	1.53
4	B	1403	SIA	O2-C2	8.40	1.48	1.40
4	B	1403	SIA	O6-C2	9.85	1.52	1.42

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

3 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	1303	SO4	1	0
3	A	1304	GOL	1	0
4	B	1403	SIA	2	0

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
1	A	412/423 (97%)	-0.20	8 (1%)	70	70	13, 32, 65, 86	0
1	B	415/423 (98%)	-0.26	6 (1%)	78	77	19, 33, 54, 68	0
All	All	827/846 (97%)	-0.23	14 (1%)	73	74	13, 33, 59, 86	0

All (14) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	1033	LEU	3.7
1	B	1053	GLY	3.3
1	A	925	ILE	3.3
1	A	1013	MET	2.7
1	B	1059	SER	2.7
1	B	1150	ARG	2.7
1	A	1034	THR	2.7
1	A	926	VAL	2.4
1	A	1031	LYS	2.3
1	A	1029	LYS	2.2
1	B	864	ILE	2.1
1	A	1050	PRO	2.1
1	B	1263	ILE	2.1
1	B	1264	GLU	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
3	GOL	A	1304	6/6	0.85	0.25	5.97	61,61,62,64	0
3	GOL	B	1401	6/6	0.90	0.20	2.14	38,40,42,44	0
3	GOL	B	1402	6/6	0.96	0.28	1.37	34,38,38,39	0
4	SIA	B	1403	21/21	0.92	0.16	1.20	53,58,60,61	0
2	SO4	A	1301	5/5	0.99	0.13	-0.09	33,35,36,36	0
2	SO4	A	1302	5/5	0.82	0.22	-	69,69,69,69	5
2	SO4	A	1303	5/5	0.97	0.20	-	64,64,65,67	0

6.5 Other polymers

There are no such residues in this entry.