Full wwPDB X-ray Structure Validation Report (i)

Feb 19, 2016 – 07:34 PM GMT

PDB ID	:	4TW0
Title	:	Crystal Structure of SCARB2 in Acidic Condition (pH4.8)
Authors	:	Dang, M.H.; Wang, X.X.; Rao, Z.H.
Deposited on	:	2014-06-29
Resolution	:	3.65 Å(reported)

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

The following versions of software and data (see references (1)) were used in the production of this report:

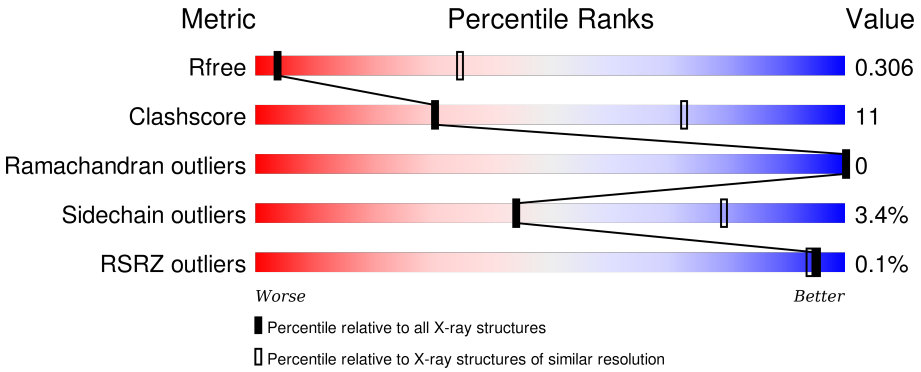
MolProbity	:	4.02b-467
Mogul	:	1.7.1 (RC1), CSD as537be (2016)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026982
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	rb-20026982

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 3.65 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	1014 (3.80-3.48)
Clashscore	102246	1130 (3.80-3.48)
Ramachandran outliers	100387	1084 (3.80-3.48)
Sidechain outliers	100360	1083 (3.80-3.48)
RSRZ outliers	91569	1021 (3.80-3.48)

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	393	72% 27% .
1	B	393	74% 25% .
1	C	393	73% 26% .
1	D	393	74% 25% .

2 Entry composition

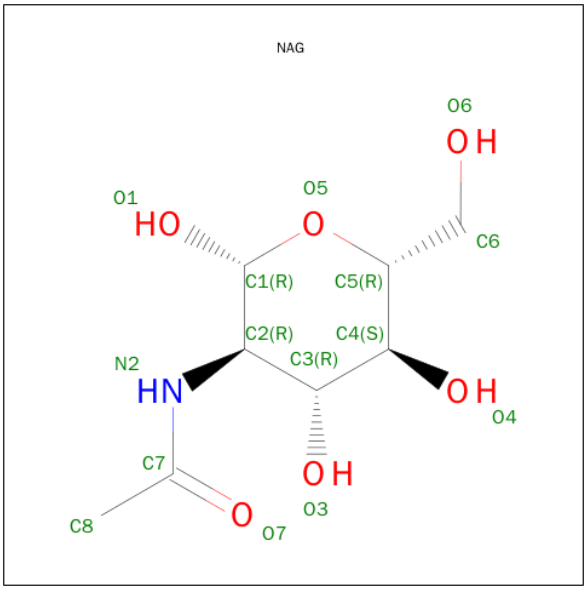
There are 4 unique types of molecules in this entry. The entry contains 13135 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 Scavenger receptor class B member 2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	393	Total	C	N	O	S	0	0	0
			3055	1980	494	570	11			
1	B	392	Total	C	N	O	S	0	0	0
			3024	1954	493	566	11			
1	C	393	Total	C	N	O	S	0	0	0
			3050	1971	496	572	11			
1	D	393	Total	C	N	O	S	0	0	0
			3058	1977	499	571	11			

- Molecule 2 is N-ACETYL-D-GLUCOSAMINE (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).



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

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

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

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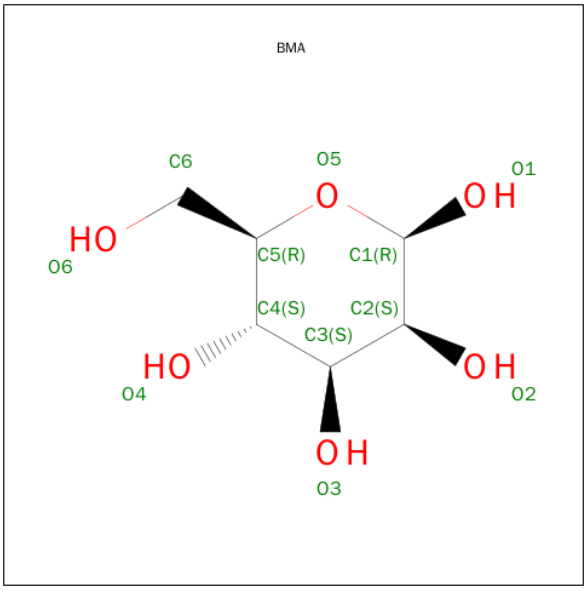
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	D	1	Total C N O 14 8 1 5	0	0
2	D	1	Total C N O 14 8 1 5	0	0
2	D	1	Total C N O 14 8 1 5	0	0
2	D	1	Total C N O 14 8 1 5	0	0
2	D	1	Total C N O 14 8 1 5	0	0
2	D	1	Total C N O 14 8 1 5	0	0
2	D	1	Total C N O 14 8 1 5	0	0
2	D	1	Total C N O 14 8 1 5	0	0

- Molecule 3 is BETA-D-MANNOSE (three-letter code: BMA) (formula: $C_6H_{12}O_6$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total C O 11 6 5	0	0
3	A	1	Total C O 11 6 5	0	0
3	A	1	Total C O 11 6 5	0	0

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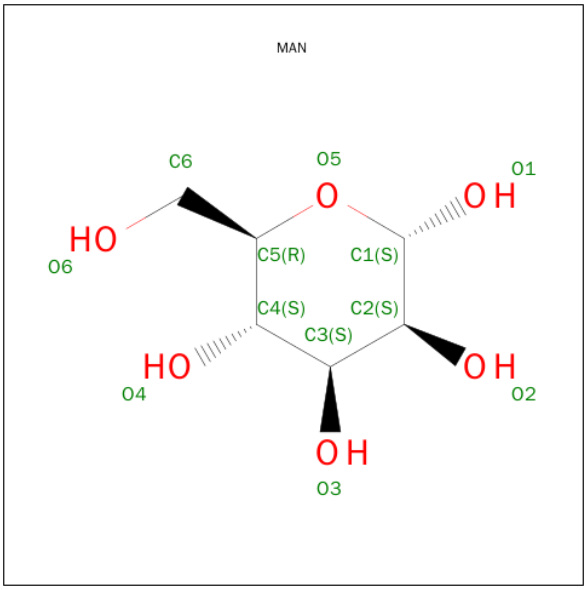
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	B	1	Total C O 11 6 5	0	0
3	B	1	Total C O 11 6 5	0	0
3	B	1	Total C O 11 6 5	0	0
3	C	1	Total C O 11 6 5	0	0
3	C	1	Total C O 11 6 5	0	0
3	C	1	Total C O 11 6 5	0	0
3	D	1	Total C O 11 6 5	0	0
3	D	1	Total C O 11 6 5	0	0
3	D	1	Total C O 11 6 5	0	0

- Molecule 4 is ALPHA-D-MANNOSE (three-letter code: MAN) (formula: $C_6H_{12}O_6$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total C O 11 6 5	0	0
4	A	1	Total C O 11 6 5	0	0

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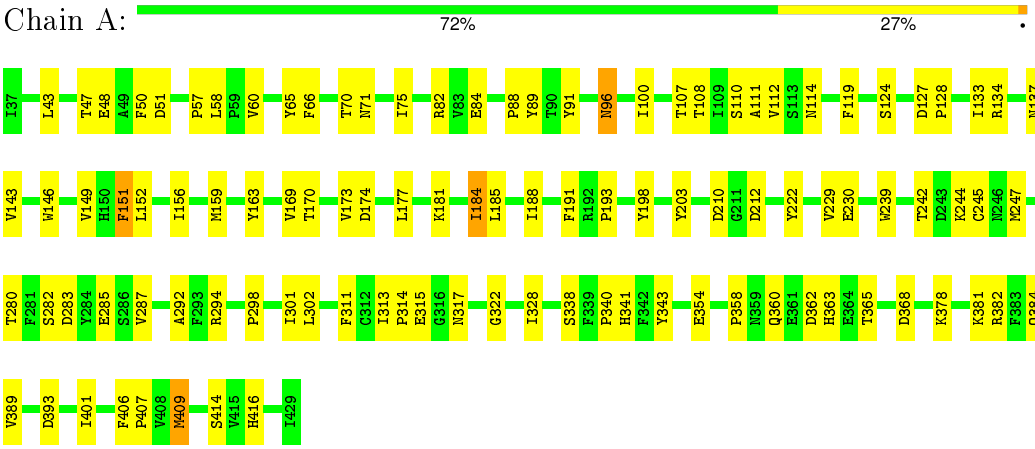
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	B	1	Total	C	O	0	0
			11	6	5		
4	B	1	Total	C	O	0	0
			11	6	5		
4	C	1	Total	C	O	0	0
			11	6	5		
4	C	1	Total	C	O	0	0
			11	6	5		
4	D	1	Total	C	O	0	0
			11	6	5		
4	D	1	Total	C	O	0	0
			11	6	5		

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.

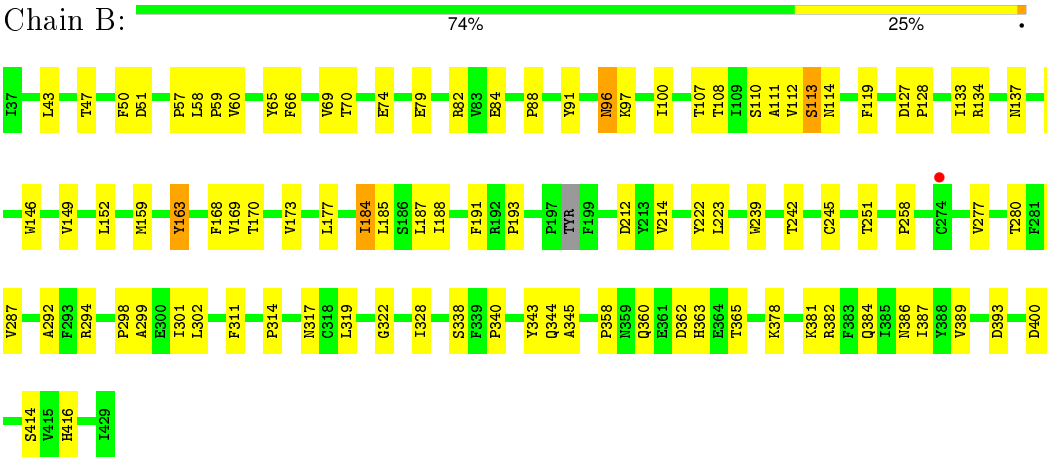
- Molecule 1: Scavenger receptor class B member 2

Chain A:



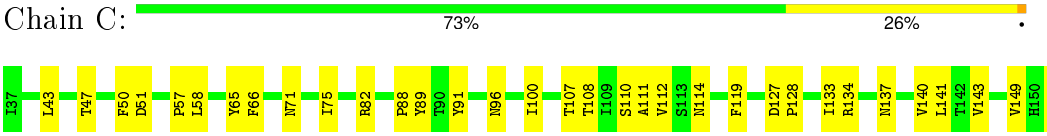
- Molecule 1: Scavenger receptor class B member 2

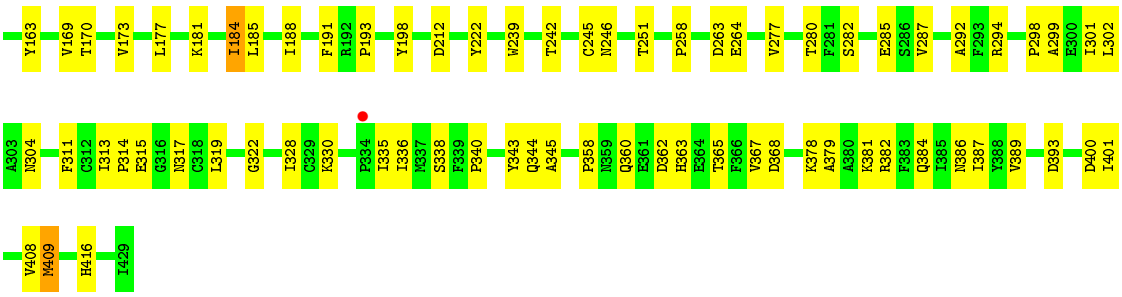
Chain B:



- Molecule 1: Scavenger receptor class B member 2

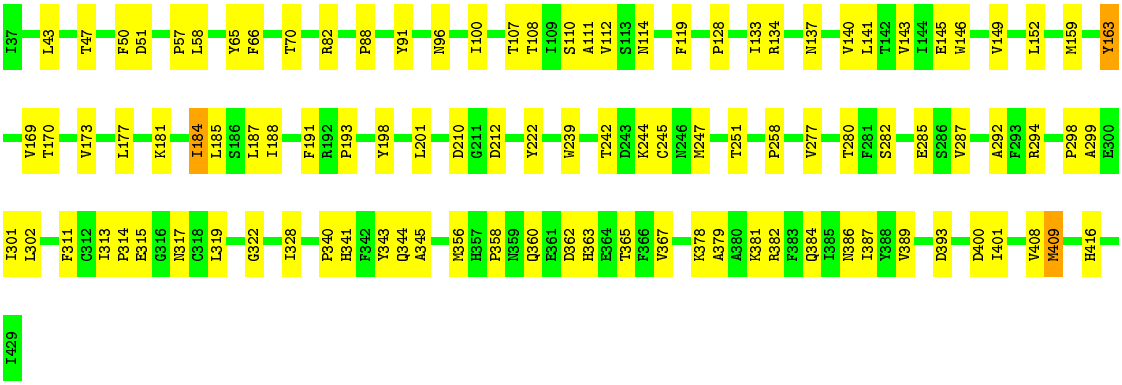
Chain C:





• Molecule 1: Scavenger receptor class B member 2

Chain D:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	103.99Å 99.64Å 125.85Å 90.00° 90.02° 90.00°	Depositor
Resolution (Å)	48.06 – 3.65 48.06 – 3.65	Depositor EDS
% Data completeness (in resolution range)	79.7 (48.06-3.65) 80.1 (48.06-3.65)	Depositor EDS
R_{merge}	0.14	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	3.00 (at 3.67Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.9_1692)	Depositor
R, R_{free}	0.249 , 0.303 0.253 , 0.306	Depositor DCC
R_{free} test set	1165 reflections (5.06%)	DCC
Wilson B-factor (Å^2)	62.6	Xtriage
Anisotropy	0.117	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.32 , 34.3	EDS
Estimated twinning fraction	0.000 for k,h,-l 0.000 for -k,-h,-l 0.358 for h,-k,-l	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.45$, $< L^2 > = 0.28$	Xtriage
Outliers	1 of 23164 reflections (0.004%)	Xtriage
F_o,F_c correlation	0.90	EDS
Total number of atoms	13135	wwPDB-VP
Average B, all atoms (Å^2)	60.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 54.19 % of the origin peak, indicating pseudo translational symmetry.The chance of finding a peak of this or larger height randomly in a structure without pseudo translational symmetry is equal to 3.7860e-05.The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

[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: BMA, NAG, MAN

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	0.31	0/3138	0.53	0/4287
1	B	0.30	0/3103	0.53	0/4238
1	C	0.30	0/3131	0.53	0/4278
1	D	0.30	0/3139	0.52	0/4285
All	All	0.30	0/12511	0.53	0/17088

There are no bond length outliers.

There are no bond angle outliers.

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	3055	0	2846	77	0
1	B	3024	0	2808	62	0
1	C	3050	0	2840	76	0
1	D	3058	0	2861	63	0
2	A	182	0	161	2	0
2	B	182	0	161	2	0
2	C	182	0	161	3	0
2	D	182	0	161	2	0
3	A	33	0	28	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	B	33	0	28	0	0
3	C	33	0	28	0	0
3	D	33	0	28	0	0
4	A	22	0	19	0	0
4	B	22	0	19	0	0
4	C	22	0	19	0	0
4	D	22	0	19	0	0
All	All	13135	0	12187	278	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 11.

All (278) 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:84:GLU:OE1	1:C:82:ARG:NH2	2.05	0.90
1:D:313:ILE:HG21	2:D:714:NAG:H61	1.63	0.81
1:C:313:ILE:HG21	2:C:714:NAG:H61	1.62	0.81
1:A:313:ILE:HG21	2:A:714:NAG:H61	1.64	0.80
1:C:133:ILE:HD12	1:C:173:VAL:HG22	1.70	0.72
1:A:242:THR:HG1	1:A:245:CYS:HG	1.38	0.71
1:A:133:ILE:HD12	1:A:173:VAL:HG22	1.71	0.71
1:A:128:PRO:HA	1:A:173:VAL:HB	1.74	0.69
1:A:365:THR:HG23	1:A:381:LYS:HA	1.75	0.69
1:A:242:THR:OG1	1:A:245:CYS:SG	2.48	0.68
1:A:143:VAL:HA	1:A:146:TRP:HB2	1.74	0.68
1:B:97:LYS:HG2	1:B:113:SER:HA	1.76	0.67
1:D:128:PRO:HA	1:D:173:VAL:HB	1.77	0.66
1:C:128:PRO:HA	1:C:173:VAL:HB	1.77	0.66
1:D:314:PRO:HB2	1:D:317:ASN:HB2	1.78	0.66
1:B:133:ILE:HD12	1:B:173:VAL:HG22	1.75	0.66
1:A:314:PRO:HB2	1:A:317:ASN:HB2	1.77	0.66
1:B:314:PRO:HB2	1:B:317:ASN:HB2	1.78	0.65
1:C:314:PRO:HB2	1:C:317:ASN:HB2	1.79	0.65
1:B:128:PRO:HA	1:B:173:VAL:HB	1.79	0.65
1:C:365:THR:HG23	1:C:381:LYS:HA	1.79	0.65
1:C:112:VAL:HG12	1:C:212:ASP:HA	1.79	0.65
1:B:242:THR:OG1	1:B:245:CYS:SG	2.52	0.64
1:D:313:ILE:HG13	1:D:328:ILE:HD11	1.79	0.63
1:D:133:ILE:HD12	1:D:173:VAL:HG22	1.79	0.63
1:C:134:ARG:HB2	1:C:170:THR:HG22	1.80	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:222:TYR:HD1	1:A:258:PRO:HG2	1.64	0.62
1:B:365:THR:HG23	1:B:381:LYS:HA	1.82	0.62
1:B:134:ARG:HB2	1:B:170:THR:HG22	1.82	0.62
1:A:185:LEU:HA	1:A:188:ILE:HD12	1.81	0.62
1:C:137:ASN:HD22	1:C:169:VAL:HG11	1.64	0.62
1:A:112:VAL:HG12	1:A:212:ASP:HA	1.82	0.61
1:C:222:TYR:HD1	1:C:258:PRO:HG2	1.64	0.61
1:C:242:THR:OG1	1:C:245:CYS:SG	2.56	0.61
1:D:365:THR:HG23	1:D:381:LYS:HA	1.83	0.61
1:D:222:TYR:HD1	1:D:258:PRO:HG2	1.65	0.60
1:D:185:LEU:HA	1:D:188:ILE:HD12	1.81	0.60
1:B:222:TYR:HD1	1:B:258:PRO:HG2	1.67	0.60
1:D:239:TRP:HB2	1:D:328:ILE:HG21	1.83	0.60
1:B:96:ASN:N	1:B:96:ASN:OD1	2.34	0.60
1:D:242:THR:OG1	1:D:245:CYS:SG	2.56	0.59
1:A:134:ARG:HB2	1:A:170:THR:HG22	1.85	0.59
1:B:242:THR:HG1	1:B:245:CYS:HG	1.47	0.59
1:B:185:LEU:HA	1:B:188:ILE:HD12	1.83	0.59
1:D:134:ARG:HB2	1:D:170:THR:HG22	1.83	0.59
1:C:159:MET:HE1	1:C:184:ILE:HG23	1.84	0.58
1:A:100:ILE:HG12	1:A:111:ALA:HB2	1.85	0.58
1:A:43:LEU:HA	1:A:50:PHE:HB2	1.86	0.58
1:A:239:TRP:HB2	1:A:328:ILE:HG21	1.84	0.58
1:A:298:PRO:O	1:A:301:ILE:HG22	2.03	0.58
1:C:239:TRP:HB2	1:C:328:ILE:HG21	1.86	0.57
1:C:263:ASP:OD1	1:C:264:GLU:N	2.37	0.57
1:C:185:LEU:HA	1:C:188:ILE:HD12	1.85	0.57
1:B:65:TYR:CZ	1:B:88:PRO:HB3	2.41	0.56
1:A:159:MET:HE1	1:A:184:ILE:HG23	1.85	0.56
1:B:100:ILE:HG12	1:B:111:ALA:HB2	1.85	0.56
1:B:239:TRP:HB2	1:B:328:ILE:HG21	1.86	0.56
1:A:82:ARG:HH11	1:C:82:ARG:NE	2.04	0.56
1:D:91:TYR:CE2	1:D:119:PHE:HB2	2.41	0.56
1:A:91:TYR:CE2	1:A:119:PHE:HB2	2.41	0.56
1:C:43:LEU:HA	1:C:50:PHE:HB2	1.88	0.56
1:D:100:ILE:HG12	1:D:111:ALA:HB2	1.88	0.55
1:B:223:LEU:HD12	2:B:718:NAG:H62	1.88	0.55
1:A:313:ILE:HG13	1:A:328:ILE:HD11	1.88	0.55
1:A:82:ARG:NH2	1:A:354:GLU:OE2	2.38	0.55
1:B:43:LEU:HA	1:B:50:PHE:HB2	1.89	0.55
1:A:137:ASN:HD22	1:A:169:VAL:HG11	1.72	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:91:TYR:CE2	1:C:119:PHE:HB2	2.42	0.55
1:A:287:VAL:HG11	1:A:378:LYS:HB2	1.89	0.55
1:B:285:GLU:O	1:B:292:ALA:N	2.39	0.55
1:D:287:VAL:HG11	1:D:378:LYS:HB2	1.88	0.55
1:D:362:ASP:O	1:D:382:ARG:NE	2.40	0.54
1:C:287:VAL:HG11	1:C:378:LYS:HB2	1.89	0.54
1:D:137:ASN:HD22	1:D:169:VAL:HG11	1.71	0.54
1:B:287:VAL:HG11	1:B:378:LYS:HB2	1.90	0.54
1:C:313:ILE:HG13	1:C:328:ILE:HD11	1.89	0.54
1:A:82:ARG:NH1	1:C:82:ARG:HE	2.06	0.54
1:D:159:MET:HE1	1:D:184:ILE:HG23	1.90	0.54
1:B:282:SER:HB2	1:B:294:ARG:HG3	1.90	0.53
1:D:43:LEU:HA	1:D:50:PHE:HB2	1.90	0.53
1:B:140:VAL:HA	1:B:143:VAL:HG22	1.90	0.53
1:A:82:ARG:HH11	1:C:82:ARG:HE	1.55	0.53
1:D:140:VAL:HA	1:D:143:VAL:HG22	1.90	0.53
1:B:322:GLY:HA3	1:B:345:ALA:HA	1.91	0.53
1:D:301:ILE:HG23	1:D:302:LEU:HG	1.91	0.53
1:A:140:VAL:HA	1:A:143:VAL:HG22	1.91	0.52
1:D:285:GLU:O	1:D:292:ALA:N	2.40	0.52
1:C:301:ILE:HG23	1:C:302:LEU:HG	1.92	0.52
1:D:277:VAL:HG13	1:D:301:ILE:HG12	1.92	0.52
1:A:362:ASP:O	1:A:382:ARG:NE	2.43	0.52
1:C:313:ILE:O	1:C:315:GLU:N	2.42	0.52
1:C:282:SER:HB2	1:C:294:ARG:HG3	1.92	0.52
1:A:65:TYR:CZ	1:A:88:PRO:HB3	2.45	0.52
1:D:282:SER:HB2	1:D:294:ARG:HG3	1.92	0.52
1:C:222:TYR:CD1	1:C:258:PRO:HG2	2.44	0.52
1:A:57:PRO:HG2	1:A:58:LEU:HG	1.92	0.52
1:C:100:ILE:HG12	1:C:111:ALA:HB2	1.91	0.52
1:A:152:LEU:O	1:A:156:ILE:HB	2.09	0.52
1:B:91:TYR:CE2	1:B:119:PHE:HB2	2.45	0.51
1:D:313:ILE:O	1:D:315:GLU:N	2.42	0.51
1:B:408:VAL:HG12	1:B:409:MET:HB3	1.92	0.51
1:A:282:SER:HB2	1:A:294:ARG:HG3	1.92	0.51
1:D:222:TYR:CD1	1:D:258:PRO:HG2	2.45	0.51
1:B:66:PHE:HZ	1:B:177:LEU:HG	1.75	0.51
1:A:222:TYR:CD1	1:A:258:PRO:HG2	2.45	0.51
1:A:141:LEU:HD13	1:A:387:ILE:HG21	1.93	0.51
1:C:141:LEU:HD13	1:C:387:ILE:HG21	1.93	0.51
1:C:66:PHE:HA	1:C:409:MET:HB2	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:242:THR:HG1	1:C:245:CYS:HG	1.52	0.51
1:C:277:VAL:HG13	1:C:301:ILE:HG12	1.93	0.51
1:C:140:VAL:HA	1:C:143:VAL:HG22	1.92	0.51
1:D:66:PHE:HZ	1:D:177:LEU:HG	1.76	0.50
1:A:313:ILE:CG1	1:A:328:ILE:HD11	2.42	0.50
1:B:343:TYR:CE1	1:B:360:GLN:HA	2.46	0.50
1:D:408:VAL:HG12	1:D:409:MET:HB3	1.94	0.50
1:D:65:TYR:CZ	1:D:88:PRO:HB3	2.46	0.50
1:C:57:PRO:HG2	1:C:58:LEU:HG	1.92	0.50
1:C:245:CYS:HB3	1:C:311:PHE:CE1	2.47	0.50
1:C:96:ASN:O	1:C:114:ASN:HB2	2.12	0.50
1:C:65:TYR:CZ	1:C:88:PRO:HB3	2.47	0.50
1:B:137:ASN:HD22	1:B:169:VAL:HG11	1.77	0.50
1:C:304:ASN:ND2	2:C:717:NAG:O7	2.44	0.50
1:D:191:PHE:O	1:D:193:PRO:HD3	2.11	0.49
1:D:313:ILE:CG1	1:D:328:ILE:HD11	2.41	0.49
1:A:245:CYS:HB3	1:A:311:PHE:CE1	2.47	0.49
1:D:389:VAL:HG11	1:D:401:ILE:HD13	1.93	0.49
1:A:313:ILE:O	1:A:315:GLU:N	2.42	0.49
1:B:222:TYR:CD1	1:B:258:PRO:HG2	2.47	0.49
1:B:362:ASP:O	1:B:382:ARG:NE	2.46	0.49
1:B:191:PHE:O	1:B:193:PRO:HD3	2.13	0.49
1:B:112:VAL:HG12	1:B:212:ASP:HA	1.95	0.48
1:A:389:VAL:HG11	1:A:401:ILE:HD13	1.96	0.48
1:C:362:ASP:O	1:C:382:ARG:NE	2.45	0.48
2:A:713:NAG:O3	2:A:713:NAG:H62	2.14	0.48
1:B:245:CYS:HB3	1:B:311:PHE:CE1	2.49	0.48
1:B:358:PRO:HA	1:B:363:HIS:ND1	2.28	0.48
1:A:65:TYR:O	1:A:409:MET:HB2	2.14	0.48
1:C:313:ILE:CG1	1:C:328:ILE:HD11	2.43	0.48
1:D:343:TYR:CE1	1:D:360:GLN:HA	2.49	0.48
1:B:57:PRO:HG2	1:B:58:LEU:HG	1.96	0.48
1:C:285:GLU:O	1:C:292:ALA:N	2.45	0.48
2:C:713:NAG:O3	2:C:713:NAG:H62	2.14	0.47
1:A:66:PHE:HZ	1:A:177:LEU:HG	1.78	0.47
1:B:163:TYR:HE1	1:B:187:LEU:HD22	1.79	0.47
1:D:358:PRO:HA	1:D:363:HIS:ND1	2.29	0.47
1:A:89:TYR:CZ	1:A:173:VAL:HG21	2.49	0.47
1:C:242:THR:O	1:C:246:ASN:ND2	2.34	0.47
1:B:100:ILE:HA	1:B:110:SER:O	2.14	0.47
1:C:389:VAL:HG11	1:C:401:ILE:HD13	1.95	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:112:VAL:HG12	1:D:212:ASP:HA	1.97	0.47
1:B:43:LEU:HB3	1:B:50:PHE:HD1	1.79	0.47
1:B:280:THR:HG23	1:B:298:PRO:HG3	1.97	0.47
1:A:71:ASN:O	1:A:75:ILE:HG13	2.15	0.47
1:C:191:PHE:O	1:C:193:PRO:HD3	2.14	0.47
1:B:159:MET:HE1	1:B:184:ILE:HG23	1.97	0.47
1:D:245:CYS:HB3	1:D:311:PHE:CE1	2.50	0.47
1:D:57:PRO:HG2	1:D:58:LEU:HG	1.96	0.47
1:B:239:TRP:CB	1:B:328:ILE:HG21	2.45	0.46
1:C:47:THR:O	1:C:51:ASP:HB2	2.15	0.46
1:A:96:ASN:O	1:A:114:ASN:HB2	2.15	0.46
2:D:713:NAG:O3	2:D:713:NAG:H62	2.15	0.46
1:C:408:VAL:HG12	1:C:409:MET:HB3	1.96	0.46
1:A:229:VAL:HG23	1:A:230:GLU:H	1.80	0.46
1:D:280:THR:HG23	1:D:298:PRO:HG3	1.97	0.46
1:C:71:ASN:O	1:C:75:ILE:HG13	2.15	0.46
1:B:96:ASN:O	1:B:114:ASN:HB2	2.16	0.46
1:D:299:ALA:HA	1:D:344:GLN:NE2	2.31	0.46
1:B:340:PRO:HA	1:B:384:GLN:OE1	2.15	0.46
2:B:713:NAG:O3	2:B:713:NAG:H62	2.16	0.46
1:A:340:PRO:HA	1:A:384:GLN:OE1	2.15	0.46
1:A:47:THR:O	1:A:51:ASP:HB2	2.16	0.46
1:C:358:PRO:HA	1:C:363:HIS:ND1	2.30	0.46
1:C:43:LEU:HB3	1:C:50:PHE:HD1	1.80	0.46
1:D:43:LEU:HB3	1:D:50:PHE:HD1	1.80	0.46
1:D:96:ASN:O	1:D:114:ASN:HB2	2.16	0.46
1:A:328:ILE:H	1:A:328:ILE:HD12	1.79	0.45
1:C:181:LYS:HD2	1:C:198:TYR:HE2	1.80	0.45
1:C:89:TYR:CZ	1:C:173:VAL:HG21	2.51	0.45
1:A:100:ILE:HA	1:A:110:SER:O	2.17	0.45
1:C:340:PRO:HA	1:C:384:GLN:OE1	2.17	0.45
1:D:340:PRO:HA	1:D:384:GLN:OE1	2.16	0.45
1:A:406:PHE:CD1	1:A:407:PRO:HD2	2.50	0.45
1:A:358:PRO:HA	1:A:363:HIS:ND1	2.31	0.45
1:B:389:VAL:HG11	1:B:401:ILE:HD13	1.99	0.45
1:C:280:THR:HG23	1:C:298:PRO:HG3	1.99	0.45
1:B:277:VAL:HG13	1:B:301:ILE:HG12	1.99	0.45
1:A:43:LEU:HB3	1:A:50:PHE:HD1	1.81	0.45
1:C:149:VAL:HB	1:C:152:LEU:HG	1.98	0.45
1:C:367:VAL:HG23	1:C:379:ALA:HB2	1.99	0.45
1:C:328:ILE:N	1:C:328:ILE:HD12	2.32	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:336:ILE:HB	1:C:386:ASN:HB2	1.99	0.45
1:A:181:LYS:HD2	1:A:198:TYR:HE2	1.82	0.44
1:C:328:ILE:H	1:C:328:ILE:HD12	1.82	0.44
1:B:43:LEU:HB3	1:B:50:PHE:CD1	2.53	0.44
1:A:302:LEU:HB3	1:A:322:GLY:HA2	1.99	0.44
1:A:343:TYR:CE1	1:A:360:GLN:HA	2.52	0.44
1:A:133:ILE:CD1	1:A:173:VAL:HG22	2.44	0.44
1:A:328:ILE:N	1:A:328:ILE:HD12	2.32	0.44
1:C:173:VAL:HG12	1:C:177:LEU:HD12	1.99	0.44
1:A:173:VAL:HG12	1:A:177:LEU:HD12	1.99	0.44
1:A:151:PHE:HD1	1:A:151:PHE:HA	1.70	0.44
1:C:66:PHE:HZ	1:C:177:LEU:HG	1.83	0.44
1:A:285:GLU:O	1:A:292:ALA:N	2.48	0.44
1:A:191:PHE:O	1:A:193:PRO:HD3	2.18	0.44
1:B:127:ASP:HA	1:B:128:PRO:HD2	1.83	0.44
1:C:299:ALA:HA	1:C:344:GLN:NE2	2.33	0.44
1:D:70:THR:HG22	1:D:82:ARG:O	2.17	0.44
1:B:47:THR:O	1:B:51:ASP:HB2	2.18	0.44
1:D:163:TYR:HE1	1:D:187:LEU:HD22	1.83	0.44
1:C:107:THR:HG23	1:C:108:THR:HG23	2.00	0.44
1:C:343:TYR:CE1	1:C:360:GLN:HA	2.53	0.43
1:B:74:GLU:HB3	1:B:79:GLU:CD	2.38	0.43
1:D:328:ILE:HD12	1:D:328:ILE:N	2.33	0.43
1:D:173:VAL:HG12	1:D:177:LEU:HD12	1.99	0.43
1:D:341:HIS:HA	1:D:356:MET:SD	2.58	0.43
1:B:299:ALA:HA	1:B:344:GLN:NE2	2.33	0.43
1:B:149:VAL:HB	1:B:152:LEU:HG	1.99	0.43
1:C:133:ILE:CD1	1:C:173:VAL:HG22	2.43	0.43
1:D:141:LEU:HD13	1:D:387:ILE:HG21	2.01	0.43
1:A:340:PRO:HG2	1:A:382:ARG:HB3	2.00	0.43
1:C:340:PRO:HG2	1:C:382:ARG:HB3	2.01	0.43
1:B:141:LEU:HD13	1:B:387:ILE:HG21	1.99	0.43
1:A:107:THR:HG23	1:A:108:THR:HG23	2.00	0.43
1:D:47:THR:O	1:D:51:ASP:HB2	2.18	0.43
1:A:280:THR:HG23	1:A:298:PRO:HG3	2.01	0.42
1:B:110:SER:CB	1:B:214:VAL:HG12	2.48	0.42
1:D:100:ILE:HA	1:D:110:SER:O	2.19	0.42
1:C:338:SER:OG	1:C:386:ASN:ND2	2.50	0.42
1:C:408:VAL:HG12	1:C:409:MET:N	2.33	0.42
1:D:66:PHE:HA	1:D:409:MET:HB2	2.00	0.42
1:B:133:ILE:CD1	1:B:173:VAL:HG22	2.45	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:60:VAL:HG13	1:B:414:SER:O	2.19	0.42
1:D:149:VAL:HB	1:D:152:LEU:HG	2.01	0.42
1:B:340:PRO:HG2	1:B:382:ARG:HB3	2.01	0.42
1:A:368:ASP:OD2	1:A:378:LYS:HE2	2.20	0.42
1:D:107:THR:HG23	1:D:108:THR:HG23	2.02	0.42
1:D:43:LEU:HB3	1:D:50:PHE:CD1	2.54	0.42
1:B:159:MET:HE3	1:B:159:MET:HB3	1.84	0.42
1:B:69:VAL:HG11	1:B:168:PHE:CE1	2.55	0.42
1:D:367:VAL:HG23	1:D:379:ALA:HB2	2.01	0.42
1:A:313:ILE:HD13	1:A:313:ILE:HA	1.72	0.42
1:A:198:TYR:HB2	1:A:203:TYR:CZ	2.55	0.42
1:C:313:ILE:HD13	1:C:313:ILE:HA	1.73	0.42
1:D:201:LEU:HA	1:D:201:LEU:HD23	1.87	0.42
1:B:107:THR:HG23	1:B:108:THR:HG23	2.02	0.42
1:A:43:LEU:HB3	1:A:50:PHE:CD1	2.55	0.41
1:D:141:LEU:O	1:D:145:GLU:HG2	2.21	0.41
1:A:60:VAL:HG13	1:A:414:SER:O	2.21	0.41
1:A:70:THR:HG21	1:A:84:GLU:HG3	2.02	0.41
1:C:330:LYS:HG3	1:C:335:ILE:HG21	2.02	0.41
1:A:244:LYS:HA	1:A:247:MET:HE3	2.02	0.41
1:D:128:PRO:CA	1:D:173:VAL:HB	2.49	0.41
1:C:302:LEU:HA	1:C:302:LEU:HD23	1.61	0.41
1:D:341:HIS:N	1:D:384:GLN:OE1	2.52	0.41
1:C:43:LEU:HB3	1:C:50:PHE:CD1	2.55	0.41
1:D:181:LYS:HD2	1:D:198:TYR:HE2	1.85	0.41
1:C:313:ILE:C	1:C:315:GLU:H	2.24	0.41
1:A:127:ASP:HA	1:A:128:PRO:HD2	1.84	0.41
1:A:149:VAL:HB	1:A:152:LEU:HG	2.00	0.41
1:B:70:THR:HG21	1:B:84:GLU:HG3	2.03	0.41
1:A:89:TYR:HA	1:A:124:SER:HB3	2.01	0.41
1:A:341:HIS:N	1:A:384:GLN:OE1	2.54	0.41
1:C:100:ILE:HA	1:C:110:SER:O	2.20	0.41
1:A:338:SER:OG	1:A:386:ASN:ND2	2.49	0.41
1:D:313:ILE:C	1:D:315:GLU:H	2.25	0.41
1:B:66:PHE:HA	1:B:409:MET:HB2	2.03	0.41
1:D:408:VAL:HG12	1:D:409:MET:N	2.36	0.40
1:B:173:VAL:HG12	1:B:177:LEU:HD12	2.03	0.40
1:C:134:ARG:HA	1:C:170:THR:HA	2.03	0.40
1:D:322:GLY:HA3	1:D:345:ALA:HA	2.02	0.40
1:A:128:PRO:O	1:A:174:ASP:N	2.40	0.40
1:C:322:GLY:HA3	1:C:345:ALA:HA	2.02	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:338:SER:OG	1:B:386:ASN:ND2	2.50	0.40
1:C:127:ASP:HA	1:C:128:PRO:HD2	1.84	0.40
1:C:368:ASP:OD2	1:C:378:LYS:HE2	2.21	0.40
1:A:283:ASP:N	1:A:283:ASP:OD2	2.54	0.40
1:B:58:LEU:HA	1:B:59:PRO:HD2	1.93	0.40
1:D:244:LYS:HA	1:D:247:MET:HE3	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	391/393 (100%)	370 (95%)	21 (5%)	0	100	100
1	B	388/393 (99%)	367 (95%)	21 (5%)	0	100	100
1	C	391/393 (100%)	370 (95%)	21 (5%)	0	100	100
1	D	391/393 (100%)	368 (94%)	23 (6%)	0	100	100
All	All	1561/1572 (99%)	1475 (94%)	86 (6%)	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	317/354 (90%)	307 (97%)	10 (3%)	46 80
1	B	312/354 (88%)	299 (96%)	13 (4%)	36 75
1	C	317/354 (90%)	308 (97%)	9 (3%)	51 82
1	D	318/354 (90%)	307 (96%)	11 (4%)	43 79
All	All	1264/1416 (89%)	1221 (97%)	43 (3%)	44 79

All (43) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	48	GLU
1	A	96	ASN
1	A	151	PHE
1	A	163	TYR
1	A	184	ILE
1	A	210	ASP
1	A	251	THR
1	A	393	ASP
1	A	409	MET
1	A	416	HIS
1	B	82	ARG
1	B	96	ASN
1	B	113	SER
1	B	146	TRP
1	B	163	TYR
1	B	184	ILE
1	B	251	THR
1	B	302	LEU
1	B	319	LEU
1	B	393	ASP
1	B	400	ASP
1	B	409	MET
1	B	416	HIS
1	C	151	PHE
1	C	163	TYR
1	C	184	ILE
1	C	251	THR
1	C	319	LEU
1	C	393	ASP
1	C	400	ASP
1	C	409	MET
1	C	416	HIS
1	D	146	TRP

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Mol	Chain	Res	Type
1	D	163	TYR
1	D	184	ILE
1	D	210	ASP
1	D	251	THR
1	D	319	LEU
1	D	386	ASN
1	D	393	ASP
1	D	400	ASP
1	D	409	MET
1	D	416	HIS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	344	GLN
1	B	344	GLN
1	D	344	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

There are no carbohydrates in this entry.

5.6 Ligand geometry

72 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	NAG	A	701	1,2	14,14,15	0.64	1 (7%)	15,19,21	0.42	0
2	NAG	A	702	3,2	14,14,15	0.27	0	15,19,21	0.59	0
3	BMA	A	703	2,4	11,11,12	0.75	0	15,15,17	1.34	3 (20%)
4	MAN	A	704	3	11,11,12	0.77	0	15,15,17	1.53	2 (13%)
2	NAG	A	705	1,2	14,14,15	0.96	1 (7%)	15,19,21	1.72	3 (20%)
2	NAG	A	706	3,2	14,14,15	0.51	0	15,19,21	0.52	0
3	BMA	A	707	2,4	11,11,12	0.56	0	15,15,17	1.11	1 (6%)
4	MAN	A	708	3,2	11,11,12	0.88	0	15,15,17	1.43	2 (13%)
2	NAG	A	709	4	14,14,15	0.39	0	15,19,21	1.15	2 (13%)
2	NAG	A	710	1,2	14,14,15	0.48	0	15,19,21	1.50	2 (13%)
2	NAG	A	711	2	14,14,15	0.67	1 (7%)	15,19,21	0.50	0
2	NAG	A	712	1,2	14,14,15	0.41	0	15,19,21	0.67	1 (6%)
2	NAG	A	713	2	14,14,15	1.48	1 (7%)	15,19,21	1.64	1 (6%)
2	NAG	A	714	1,2	14,14,15	0.77	1 (7%)	15,19,21	0.77	0
2	NAG	A	715	3,2	14,14,15	0.68	0	15,19,21	0.50	0
3	BMA	A	716	2	11,11,12	0.76	0	15,15,17	0.93	1 (6%)
2	NAG	A	717	1	14,14,15	0.31	0	15,19,21	0.79	1 (6%)
2	NAG	A	718	1	14,14,15	0.31	0	15,19,21	0.66	0
2	NAG	B	701	1,2	14,14,15	0.58	1 (7%)	15,19,21	0.41	0
2	NAG	B	702	3,2	14,14,15	0.18	0	15,19,21	0.63	0
3	BMA	B	703	2,4	11,11,12	0.70	0	15,15,17	1.32	3 (20%)
4	MAN	B	704	3	11,11,12	0.81	0	15,15,17	1.52	2 (13%)
2	NAG	B	705	1,2	14,14,15	0.87	1 (7%)	15,19,21	1.64	3 (20%)
2	NAG	B	706	3,2	14,14,15	0.59	0	15,19,21	0.56	0
3	BMA	B	707	2,4	11,11,12	0.56	0	15,15,17	1.09	1 (6%)
4	MAN	B	708	3,2	11,11,12	0.89	0	15,15,17	1.40	1 (6%)
2	NAG	B	709	4	14,14,15	0.39	0	15,19,21	1.16	2 (13%)
2	NAG	B	710	1,2	14,14,15	0.49	0	15,19,21	1.42	2 (13%)
2	NAG	B	711	2	14,14,15	0.57	0	15,19,21	0.48	0
2	NAG	B	712	1,2	14,14,15	0.35	0	15,19,21	0.75	1 (6%)
2	NAG	B	713	2	14,14,15	1.39	1 (7%)	15,19,21	1.63	1 (6%)
2	NAG	B	714	1,2	14,14,15	0.76	1 (7%)	15,19,21	0.74	0
2	NAG	B	715	3,2	14,14,15	0.72	0	15,19,21	0.53	0
3	BMA	B	716	2	11,11,12	0.81	0	15,15,17	0.94	0
2	NAG	B	717	1	14,14,15	0.40	0	15,19,21	0.68	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
2	NAG	B	718	1	14,14,15	0.79	1 (7%)	15,19,21	1.09	2 (13%)
2	NAG	C	701	1,2	14,14,15	0.65	1 (7%)	15,19,21	0.40	0
2	NAG	C	702	3,2	14,14,15	0.23	0	15,19,21	0.59	0
3	BMA	C	703	2,4	11,11,12	0.73	0	15,15,17	1.39	3 (20%)
4	MAN	C	704	3	11,11,12	0.81	0	15,15,17	1.53	1 (6%)
2	NAG	C	705	1,2	14,14,15	0.93	1 (7%)	15,19,21	1.71	3 (20%)
2	NAG	C	706	3,2	14,14,15	0.53	0	15,19,21	0.44	0
3	BMA	C	707	2,4	11,11,12	0.72	0	15,15,17	1.18	1 (6%)
4	MAN	C	708	3,2	11,11,12	0.92	0	15,15,17	1.42	2 (13%)
2	NAG	C	709	4	14,14,15	0.40	0	15,19,21	1.15	2 (13%)
2	NAG	C	710	1,2	14,14,15	0.49	0	15,19,21	1.47	2 (13%)
2	NAG	C	711	2	14,14,15	0.67	1 (7%)	15,19,21	0.49	0
2	NAG	C	712	1,2	14,14,15	0.37	0	15,19,21	0.73	1 (6%)
2	NAG	C	713	2	14,14,15	1.42	1 (7%)	15,19,21	1.64	1 (6%)
2	NAG	C	714	1,2	14,14,15	0.79	1 (7%)	15,19,21	0.74	0
2	NAG	C	715	3,2	14,14,15	0.70	1 (7%)	15,19,21	0.53	0
3	BMA	C	716	2	11,11,12	0.73	0	15,15,17	0.90	0
2	NAG	C	717	1	14,14,15	0.62	0	15,19,21	0.58	0
2	NAG	C	718	1	14,14,15	0.59	0	15,19,21	0.65	0
2	NAG	D	701	1,2	14,14,15	0.57	0	15,19,21	0.41	0
2	NAG	D	702	3,2	14,14,15	0.22	0	15,19,21	0.60	0
3	BMA	D	703	2,4	11,11,12	0.82	0	15,15,17	1.34	3 (20%)
4	MAN	D	704	3	11,11,12	0.74	0	15,15,17	1.49	2 (13%)
2	NAG	D	705	1,2	14,14,15	0.89	1 (7%)	15,19,21	1.66	3 (20%)
2	NAG	D	706	3,2	14,14,15	0.60	0	15,19,21	0.54	0
3	BMA	D	707	2,4	11,11,12	0.62	0	15,15,17	1.15	1 (6%)
4	MAN	D	708	3,2	11,11,12	0.93	0	15,15,17	1.38	2 (13%)
2	NAG	D	709	4	14,14,15	0.40	0	15,19,21	1.16	2 (13%)
2	NAG	D	710	1,2	14,14,15	0.53	0	15,19,21	1.47	2 (13%)
2	NAG	D	711	2	14,14,15	0.57	0	15,19,21	0.47	0
2	NAG	D	712	1,2	14,14,15	0.30	0	15,19,21	0.71	1 (6%)
2	NAG	D	713	2	14,14,15	1.43	1 (7%)	15,19,21	1.64	1 (6%)
2	NAG	D	714	1,2	14,14,15	0.78	1 (7%)	15,19,21	0.72	0
2	NAG	D	715	3,2	14,14,15	0.68	0	15,19,21	0.56	0
3	BMA	D	716	2	11,11,12	0.80	0	15,15,17	0.90	0
2	NAG	D	717	1	14,14,15	1.56	1 (7%)	15,19,21	1.35	2 (13%)
2	NAG	D	718	1	14,14,15	0.68	1 (7%)	15,19,21	1.39	2 (13%)

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	NAG	A	701	1,2	-	0/6/23/26	0/1/1/1
2	NAG	A	702	3,2	-	0/6/23/26	0/1/1/1
3	BMA	A	703	2,4	-	0/2/19/22	0/1/1/1
4	MAN	A	704	3	-	0/2/19/22	1/1/1/1
2	NAG	A	705	1,2	-	0/6/23/26	0/1/1/1
2	NAG	A	706	3,2	-	0/6/23/26	0/1/1/1
3	BMA	A	707	2,4	-	0/2/19/22	0/1/1/1
4	MAN	A	708	3,2	-	0/2/19/22	0/1/1/1
2	NAG	A	709	4	-	0/6/23/26	0/1/1/1
2	NAG	A	710	1,2	-	0/6/23/26	0/1/1/1
2	NAG	A	711	2	-	0/6/23/26	0/1/1/1
2	NAG	A	712	1,2	-	0/6/23/26	0/1/1/1
2	NAG	A	713	2	-	0/6/23/26	0/1/1/1
2	NAG	A	714	1,2	-	0/6/23/26	0/1/1/1
2	NAG	A	715	3,2	-	0/6/23/26	0/1/1/1
3	BMA	A	716	2	-	0/2/19/22	0/1/1/1
2	NAG	A	717	1	-	0/6/23/26	0/1/1/1
2	NAG	A	718	1	-	0/6/23/26	0/1/1/1
2	NAG	B	701	1,2	-	0/6/23/26	0/1/1/1
2	NAG	B	702	3,2	-	0/6/23/26	0/1/1/1
3	BMA	B	703	2,4	-	0/2/19/22	0/1/1/1
4	MAN	B	704	3	-	0/2/19/22	1/1/1/1
2	NAG	B	705	1,2	-	0/6/23/26	0/1/1/1
2	NAG	B	706	3,2	-	0/6/23/26	0/1/1/1
3	BMA	B	707	2,4	-	0/2/19/22	0/1/1/1
4	MAN	B	708	3,2	-	0/2/19/22	0/1/1/1
2	NAG	B	709	4	-	0/6/23/26	0/1/1/1
2	NAG	B	710	1,2	-	0/6/23/26	0/1/1/1
2	NAG	B	711	2	-	0/6/23/26	0/1/1/1
2	NAG	B	712	1,2	-	0/6/23/26	0/1/1/1
2	NAG	B	713	2	-	0/6/23/26	0/1/1/1
2	NAG	B	714	1,2	-	0/6/23/26	0/1/1/1
2	NAG	B	715	3,2	-	0/6/23/26	0/1/1/1
3	BMA	B	716	2	-	0/2/19/22	0/1/1/1
2	NAG	B	717	1	-	0/6/23/26	0/1/1/1
2	NAG	B	718	1	-	0/6/23/26	0/1/1/1
2	NAG	C	701	1,2	-	0/6/23/26	0/1/1/1
2	NAG	C	702	3,2	-	0/6/23/26	0/1/1/1
3	BMA	C	703	2,4	-	0/2/19/22	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	MAN	C	704	3	-	0/2/19/22	1/1/1/1
2	NAG	C	705	1,2	-	0/6/23/26	0/1/1/1
2	NAG	C	706	3,2	-	0/6/23/26	0/1/1/1
3	BMA	C	707	2,4	-	0/2/19/22	0/1/1/1
4	MAN	C	708	3,2	-	0/2/19/22	0/1/1/1
2	NAG	C	709	4	-	0/6/23/26	0/1/1/1
2	NAG	C	710	1,2	-	0/6/23/26	0/1/1/1
2	NAG	C	711	2	-	0/6/23/26	0/1/1/1
2	NAG	C	712	1,2	-	0/6/23/26	0/1/1/1
2	NAG	C	713	2	-	0/6/23/26	0/1/1/1
2	NAG	C	714	1,2	-	0/6/23/26	0/1/1/1
2	NAG	C	715	3,2	-	0/6/23/26	0/1/1/1
3	BMA	C	716	2	-	0/2/19/22	0/1/1/1
2	NAG	C	717	1	-	0/6/23/26	0/1/1/1
2	NAG	C	718	1	-	0/6/23/26	0/1/1/1
2	NAG	D	701	1,2	-	0/6/23/26	0/1/1/1
2	NAG	D	702	3,2	-	0/6/23/26	0/1/1/1
3	BMA	D	703	2,4	-	0/2/19/22	0/1/1/1
4	MAN	D	704	3	-	0/2/19/22	1/1/1/1
2	NAG	D	705	1,2	-	0/6/23/26	0/1/1/1
2	NAG	D	706	3,2	-	0/6/23/26	0/1/1/1
3	BMA	D	707	2,4	-	0/2/19/22	0/1/1/1
4	MAN	D	708	3,2	-	0/2/19/22	0/1/1/1
2	NAG	D	709	4	-	0/6/23/26	0/1/1/1
2	NAG	D	710	1,2	-	0/6/23/26	0/1/1/1
2	NAG	D	711	2	-	0/6/23/26	0/1/1/1
2	NAG	D	712	1,2	-	0/6/23/26	0/1/1/1
2	NAG	D	713	2	-	0/6/23/26	0/1/1/1
2	NAG	D	714	1,2	-	0/6/23/26	0/1/1/1
2	NAG	D	715	3,2	-	0/6/23/26	0/1/1/1
3	BMA	D	716	2	-	0/2/19/22	0/1/1/1
2	NAG	D	717	1	-	0/6/23/26	0/1/1/1
2	NAG	D	718	1	-	0/6/23/26	0/1/1/1

All (21) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	717	NAG	O5-C1	-5.68	1.34	1.43
2	A	705	NAG	C1-C2	-3.13	1.48	1.52
2	C	705	NAG	C1-C2	-2.99	1.48	1.52
2	D	705	NAG	C1-C2	-2.82	1.48	1.52
2	B	705	NAG	C1-C2	-2.77	1.48	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	701	NAG	O5-C1	-2.34	1.39	1.43
2	A	701	NAG	O5-C1	-2.31	1.40	1.43
2	A	711	NAG	O5-C1	-2.16	1.40	1.43
2	C	711	NAG	O5-C1	-2.10	1.40	1.43
2	B	701	NAG	O5-C1	-2.07	1.40	1.43
2	C	715	NAG	O5-C1	-2.03	1.40	1.43
2	D	718	NAG	O5-C1	2.01	1.47	1.43
2	B	718	NAG	C1-C2	2.40	1.55	1.52
2	A	714	NAG	C1-C2	2.53	1.56	1.52
2	B	714	NAG	C1-C2	2.53	1.56	1.52
2	C	714	NAG	C1-C2	2.55	1.56	1.52
2	D	714	NAG	C1-C2	2.62	1.56	1.52
2	B	713	NAG	O5-C1	4.94	1.51	1.43
2	C	713	NAG	O5-C1	4.95	1.51	1.43
2	D	713	NAG	O5-C1	5.05	1.51	1.43
2	A	713	NAG	O5-C1	5.17	1.52	1.43

All (74) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	C	708	MAN	O2-C2-C1	-3.41	102.41	109.23
4	A	708	MAN	O2-C2-C1	-3.36	102.52	109.23
4	D	708	MAN	O2-C2-C1	-3.27	102.68	109.23
4	B	708	MAN	O2-C2-C1	-3.26	102.71	109.23
3	C	707	BMA	O2-C2-C3	-3.10	103.94	110.19
3	D	707	BMA	O2-C2-C3	-2.82	104.51	110.19
3	A	707	BMA	O2-C2-C3	-2.75	104.65	110.19
2	B	712	NAG	O4-C4-C3	-2.69	104.29	110.36
2	C	712	NAG	O4-C4-C3	-2.53	104.66	110.36
2	D	712	NAG	O4-C4-C3	-2.52	104.67	110.36
2	C	710	NAG	O3-C3-C2	-2.52	103.98	109.37
2	D	710	NAG	O3-C3-C2	-2.50	104.02	109.37
3	B	707	BMA	O2-C2-C3	-2.50	105.15	110.19
3	C	703	BMA	O2-C2-C3	-2.46	105.24	110.19
2	B	709	NAG	C2-N2-C7	-2.42	119.96	123.11
2	D	709	NAG	C2-N2-C7	-2.41	119.97	123.11
2	A	709	NAG	C2-N2-C7	-2.38	120.01	123.11
2	C	709	NAG	C2-N2-C7	-2.37	120.02	123.11
2	A	712	NAG	O4-C4-C3	-2.37	105.01	110.36
2	B	710	NAG	O3-C3-C2	-2.36	104.33	109.37
2	A	710	NAG	O3-C3-C2	-2.29	104.47	109.37
3	B	703	BMA	O2-C2-C3	-2.27	105.61	110.19

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	A	703	BMA	O2-C2-C3	-2.27	105.61	110.19
4	B	704	MAN	O2-C2-C3	-2.24	105.67	110.19
3	D	703	BMA	O2-C2-C3	-2.19	105.77	110.19
4	D	704	MAN	O2-C2-C3	-2.18	105.79	110.19
2	B	718	NAG	O3-C3-C4	-2.13	105.56	110.36
3	A	716	BMA	O2-C2-C3	-2.11	105.93	110.19
4	A	704	MAN	O2-C2-C3	-2.06	106.03	110.19
2	D	718	NAG	C4-C3-C2	-2.01	108.22	111.34
2	B	709	NAG	C8-C7-N2	2.03	119.99	116.10
2	D	709	NAG	C8-C7-N2	2.04	120.00	116.10
2	A	709	NAG	C8-C7-N2	2.04	120.01	116.10
2	C	709	NAG	C8-C7-N2	2.05	120.02	116.10
4	C	708	MAN	O3-C3-C2	2.06	113.79	110.01
2	A	717	NAG	O3-C3-C2	2.10	113.87	109.37
4	A	708	MAN	O3-C3-C2	2.12	113.90	110.01
4	D	708	MAN	O3-C3-C2	2.14	113.94	110.01
3	B	703	BMA	C1-C2-C3	2.48	112.56	109.55
2	B	718	NAG	O3-C3-C2	2.49	114.70	109.37
3	D	703	BMA	C1-C2-C3	2.51	112.59	109.55
3	A	703	BMA	C1-C2-C3	2.55	112.64	109.55
2	B	705	NAG	O5-C5-C4	2.55	114.36	110.13
3	B	703	BMA	C1-O5-C5	2.59	115.95	112.14
2	D	705	NAG	O5-C5-C4	2.60	114.45	110.13
3	C	703	BMA	C1-C2-C3	2.66	112.77	109.55
3	D	703	BMA	C1-O5-C5	2.68	116.07	112.14
2	A	705	NAG	O5-C5-C4	2.68	114.57	110.13
3	A	703	BMA	C1-O5-C5	2.69	116.09	112.14
3	C	703	BMA	C1-O5-C5	2.74	116.17	112.14
2	C	705	NAG	O5-C5-C4	2.75	114.68	110.13
2	D	717	NAG	C4-C3-C2	3.01	116.02	111.34
2	B	705	NAG	C1-O5-C5	3.26	116.93	112.14
2	D	718	NAG	O3-C3-C2	3.27	116.38	109.37
2	D	705	NAG	C1-O5-C5	3.28	116.97	112.14
2	A	705	NAG	C1-O5-C5	3.62	117.47	112.14
2	D	717	NAG	C3-C4-C5	3.70	116.82	110.23
2	C	705	NAG	C1-O5-C5	3.74	117.64	112.14
2	C	705	NAG	C2-N2-C7	3.96	128.25	123.11
2	A	705	NAG	C2-N2-C7	4.02	128.33	123.11
2	B	705	NAG	C2-N2-C7	4.05	128.37	123.11
2	D	705	NAG	C2-N2-C7	4.11	128.46	123.11
2	B	710	NAG	C1-O5-C5	4.20	118.31	112.14
2	C	710	NAG	C1-O5-C5	4.35	118.53	112.14

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	D	710	NAG	C1-O5-C5	4.39	118.60	112.14
2	A	710	NAG	C1-O5-C5	4.50	118.75	112.14
4	D	704	MAN	C1-O5-C5	4.53	118.80	112.14
4	B	704	MAN	C1-O5-C5	4.53	118.80	112.14
4	A	704	MAN	C1-O5-C5	4.67	119.01	112.14
4	C	704	MAN	C1-O5-C5	4.74	119.11	112.14
2	B	713	NAG	C1-O5-C5	5.94	120.88	112.14
2	D	713	NAG	C1-O5-C5	6.00	120.97	112.14
2	C	713	NAG	C1-O5-C5	6.03	121.00	112.14
2	A	713	NAG	C1-O5-C5	6.06	121.05	112.14

There are no chirality outliers.

There are no torsion outliers.

All (4) ring outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	C	704	MAN	C1-C2-C3-C4-C5-O5
4	A	704	MAN	C1-C2-C3-C4-C5-O5
4	B	704	MAN	C1-C2-C3-C4-C5-O5
4	D	704	MAN	C1-C2-C3-C4-C5-O5

9 monomers are involved in 9 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	713	NAG	1	0
2	A	714	NAG	1	0
2	B	713	NAG	1	0
2	B	718	NAG	1	0
2	C	713	NAG	1	0
2	C	714	NAG	1	0
2	C	717	NAG	1	0
2	D	713	NAG	1	0
2	D	714	NAG	1	0

5.7 Other polymers

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	393/393 (100%)	-0.08	0 100 100	18, 58, 102, 135	0
1	B	392/393 (99%)	-0.13	1 (0%) 94 90	21, 56, 101, 122	0
1	C	393/393 (100%)	-0.09	1 (0%) 94 90	20, 57, 101, 124	0
1	D	393/393 (100%)	-0.16	0 100 100	20, 57, 101, 124	0
All	All	1571/1572 (99%)	-0.12	2 (0%) 95 94	18, 57, 101, 135	0

All (2) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	274	CYS	2.4
1	C	334	PRO	2.1

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

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

6.3 Carbohydrates

There are no carbohydrates in this entry.

6.4 Ligands

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
2	NAG	C	714	14/15	0.89	0.30	1.05	72,85,96,99	0
2	NAG	B	714	14/15	0.92	0.29	0.88	72,85,90,96	0
2	NAG	A	710	14/15	0.87	0.33	0.83	69,80,97,101	0
2	NAG	C	710	14/15	0.87	0.29	0.60	72,81,98,98	0
2	NAG	B	710	14/15	0.86	0.29	0.08	69,80,92,95	0
2	NAG	A	714	14/15	0.92	0.26	-0.19	72,84,96,98	0
2	NAG	D	706	14/15	0.91	0.25	-0.19	41,59,68,74	0
2	NAG	D	714	14/15	0.92	0.23	-0.26	72,84,90,108	0
2	NAG	D	705	14/15	0.94	0.22	-0.38	37,48,59,60	0
2	NAG	A	705	14/15	0.92	0.24	-0.42	37,44,54,68	0
2	NAG	D	710	14/15	0.85	0.24	-0.44	69,81,88,94	0
2	NAG	C	705	14/15	0.94	0.25	-0.49	37,48,61,69	0
2	NAG	C	706	14/15	0.95	0.23	-0.63	41,49,62,63	0
2	NAG	B	701	14/15	0.93	0.21	-0.72	37,40,46,60	0
2	NAG	A	706	14/15	0.94	0.20	-0.88	38,45,66,67	0
2	NAG	B	706	14/15	0.93	0.23	-0.88	41,53,67,73	0
2	NAG	A	701	14/15	0.95	0.20	-0.96	37,40,52,55	0
2	NAG	D	701	14/15	0.94	0.21	-1.08	38,40,46,58	0
2	NAG	C	701	14/15	0.96	0.20	-1.13	37,40,50,54	0
2	NAG	C	712	14/15	0.91	0.18	-1.14	53,69,81,84	0
2	NAG	B	705	14/15	0.92	0.21	-1.39	36,48,58,59	0
2	NAG	A	712	14/15	0.85	0.20	-1.49	53,70,81,82	0
2	NAG	D	712	14/15	0.92	0.17	-1.50	55,63,81,81	0
2	NAG	B	712	14/15	0.89	0.19	-2.32	53,63,81,83	0
2	NAG	D	709	14/15	0.79	0.29	-	100,117,123,124	0
3	BMA	C	716	11/12	0.63	0.36	-	100,116,122,124	0
2	NAG	B	715	14/15	0.85	0.39	-	82,105,121,122	0
2	NAG	A	713	14/15	0.85	0.18	-	86,97,112,112	0
4	MAN	B	704	11/12	0.76	0.30	-	117,127,134,134	0
2	NAG	B	709	14/15	0.80	0.35	-	102,117,123,127	0
2	NAG	B	702	14/15	0.94	0.17	-	45,57,69,73	0
2	NAG	D	718	14/15	0.79	0.25	-	81,101,118,123	0
4	MAN	C	704	11/12	0.71	0.34	-	121,127,137,137	0
2	NAG	C	715	14/15	0.89	0.33	-	96,107,119,123	0
2	NAG	B	713	14/15	0.83	0.20	-	85,100,114,116	0
4	MAN	B	708	11/12	0.93	0.16	-	96,102,107,107	0
2	NAG	D	717	14/15	0.77	0.19	-	72,107,140,144	0
3	BMA	A	707	11/12	0.90	0.15	-	68,76,102,107	0
3	BMA	D	716	11/12	0.66	0.35	-	110,118,127,133	0
3	BMA	B	716	11/12	0.61	0.30	-	113,117,124,131	0
4	MAN	D	704	11/12	0.79	0.25	-	117,125,131,137	0
2	NAG	C	711	14/15	0.76	0.40	-	84,101,106,109	0
2	NAG	C	717	14/15	0.70	0.21	-	68,104,124,129	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
3	BMA	A	716	11/12	0.66	0.27	-	103,115,123,123	0
4	MAN	A	704	11/12	0.70	0.45	-	118,124,141,147	0
2	NAG	C	713	14/15	0.88	0.20	-	85,98,108,108	0
2	NAG	B	711	14/15	0.78	0.32	-	92,98,110,112	0
2	NAG	C	718	14/15	0.86	0.20	-	86,103,114,122	0
2	NAG	D	702	14/15	0.96	0.19	-	47,61,73,78	0
3	BMA	B	703	11/12	0.89	0.14	-	82,92,105,113	0
2	NAG	D	711	14/15	0.77	0.35	-	92,100,109,115	0
3	BMA	A	703	11/12	0.91	0.12	-	82,94,104,115	0
4	MAN	D	708	11/12	0.89	0.20	-	94,103,108,110	0
3	BMA	B	707	11/12	0.89	0.22	-	69,82,102,108	0
2	NAG	B	718	14/15	0.75	0.26	-	93,112,139,139	0
2	NAG	A	711	14/15	0.76	0.37	-	87,101,107,108	0
2	NAG	A	715	14/15	0.82	0.34	-	95,107,119,127	0
2	NAG	D	713	14/15	0.84	0.23	-	85,97,109,113	0
2	NAG	C	702	14/15	0.95	0.19	-	49,56,73,83	0
3	BMA	C	707	11/12	0.90	0.16	-	68,76,95,108	0
2	NAG	A	702	14/15	0.96	0.15	-	45,52,82,85	0
4	MAN	C	708	11/12	0.85	0.21	-	94,104,111,112	0
2	NAG	D	715	14/15	0.86	0.32	-	82,103,116,125	0
2	NAG	A	709	14/15	0.71	0.38	-	96,117,128,131	0
4	MAN	A	708	11/12	0.85	0.19	-	95,101,107,107	0
3	BMA	D	707	11/12	0.90	0.19	-	70,85,101,105	0
3	BMA	C	703	11/12	0.90	0.15	-	84,94,106,113	0
3	BMA	D	703	11/12	0.90	0.16	-	82,99,111,114	0
2	NAG	A	717	14/15	0.74	0.23	-	52,93,123,128	0
2	NAG	B	717	14/15	0.74	0.27	-	87,114,143,161	0
2	NAG	A	718	14/15	0.83	0.20	-	85,105,131,134	0
2	NAG	C	709	14/15	0.80	0.32	-	95,113,122,124	0

6.5 Other polymers

There are no such residues in this entry.