Full wwPDB X-ray Structure Validation Report (i)

Aug 29, 2023 – 02:35 PM EDT

PDB ID	:	3MN8
Title	:	Structure of Drosophila melanogaster carboxypeptidase D isoform 1B short
Authors	:	Tanco, S.; Arolas, J.L.; Guevara, T.; Lorenzo, J.; Aviles, F.X.; Gomis-Ruth, F.X.
Deposited on	:	2010-04-21
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
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

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

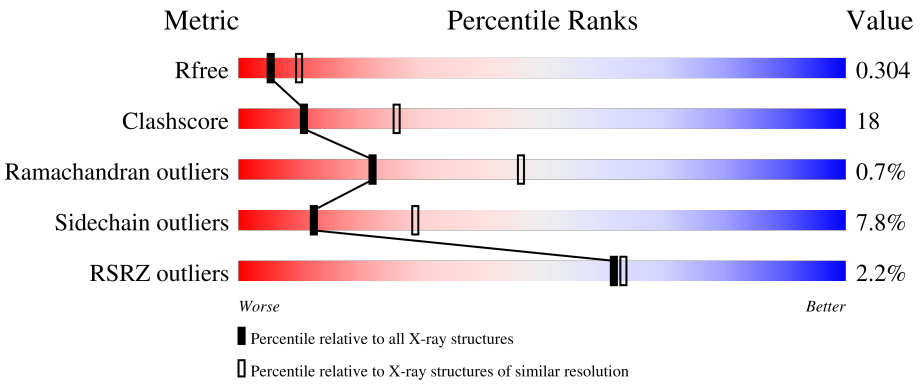
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.35
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35

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}	130704	2808 (2.70-2.70)
Clashscore	141614	3122 (2.70-2.70)
Ramachandran outliers	138981	3069 (2.70-2.70)
Sidechain outliers	138945	3069 (2.70-2.70)
RSRZ outliers	127900	2737 (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 of the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. 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	435	% 55% 29% • 12%
1	B	435	% 58% 27% • 11%
1	C	435	3% 56% 27% 6% 11%
1	D	435	3% 58% 26% 5% 11%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard

residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
4	GEM	A	601	-	-	X	-
4	GEM	B	601	-	-	X	-

2 Entry composition (i)

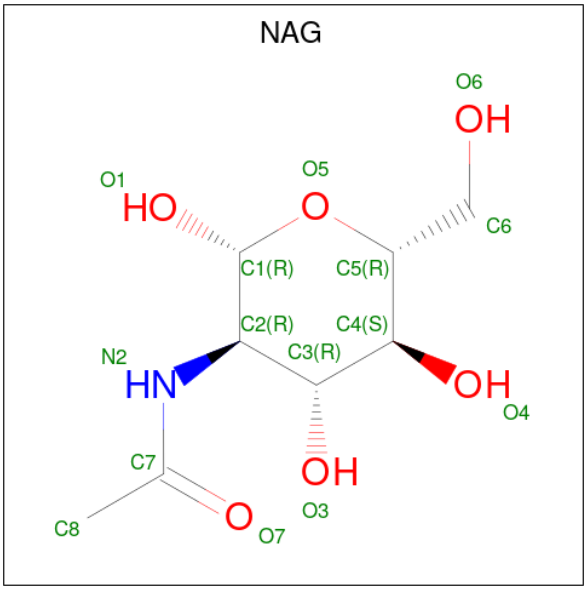
There are 6 unique types of molecules in this entry. The entry contains 12468 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 LP15968p.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	383	3013	1889	532	579	13	0	0	0
1	B	386	3040	1905	536	586	13	0	0	0
1	C	385	3032	1900	537	582	13	0	0	0
1	D	385	3028	1899	534	582	13	0	0	0

- Molecule 2 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).



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

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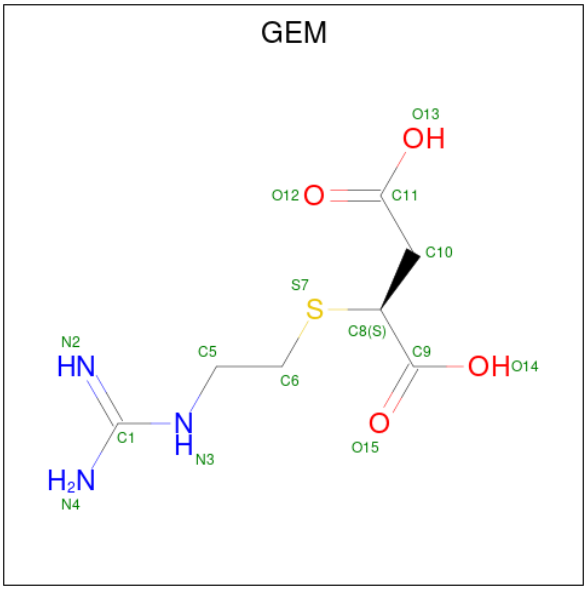
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	N	O		
2	C	1	14	8	1	5	0	0
			Total	C	N	O		
2	D	1	14	8	1	5	0	0

- Molecule 3 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Zn		
3	A	1	1	1	0	0
			Total	Zn		
3	B	1	1	1	0	0
			Total	Zn		
3	C	1	1	1	0	0
			Total	Zn		
3	D	1	1	1	0	0

- Molecule 4 is (2-GUANIDINOETHYLMERCAPTO)SUCCINIC ACID (three-letter code: GEM) (formula: $C_7H_{13}N_3O_4S$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	N	O	S		
4	A	1	15	7	3	4	1	0	0
			Total	C	N	O	S		
4	B	1	15	7	3	4	1	0	0
			Total	C	N	O	S		
4	C	1	15	7	3	4	1	0	0

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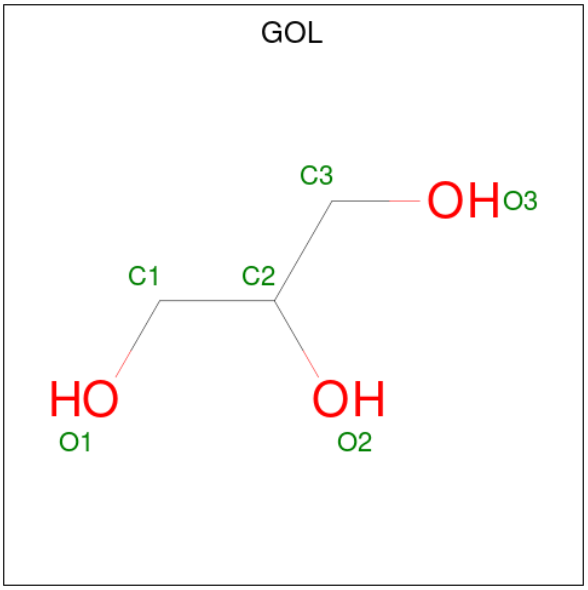
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	N	O	S		
4	D	1	15	7	3	4	1	0	0

- Molecule 5 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).



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

- Molecule 6 is water.

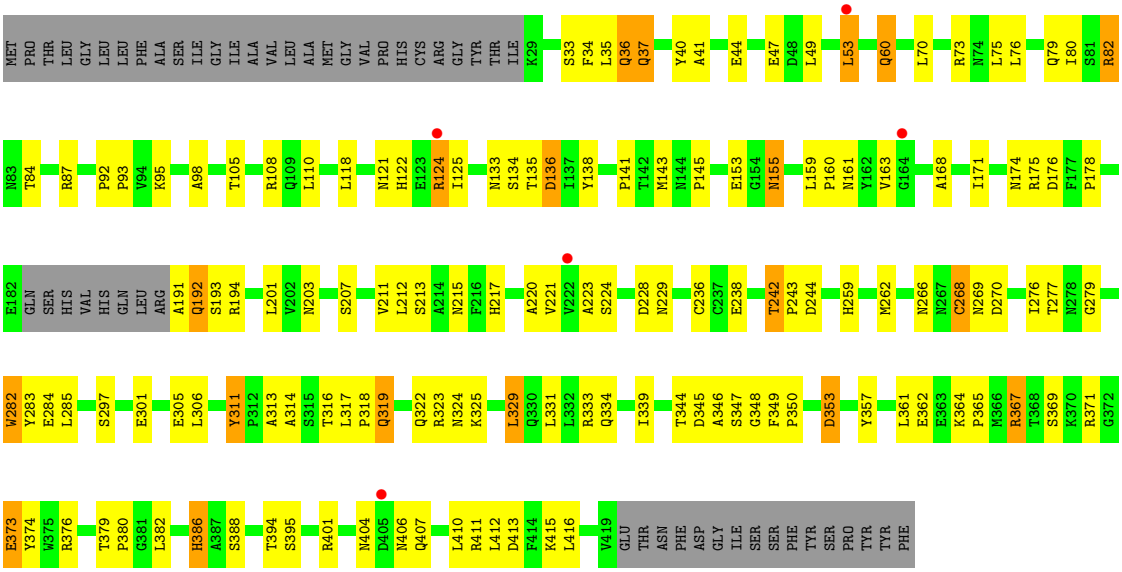
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
6	A	50	50	50	0	0
			Total	O		
6	B	54	54	54	0	0
			Total	O		
6	C	51	51	51	0	0
			Total	O		
6	D	56	56	56	0	0

3 Residue-property plots (i)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes 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.

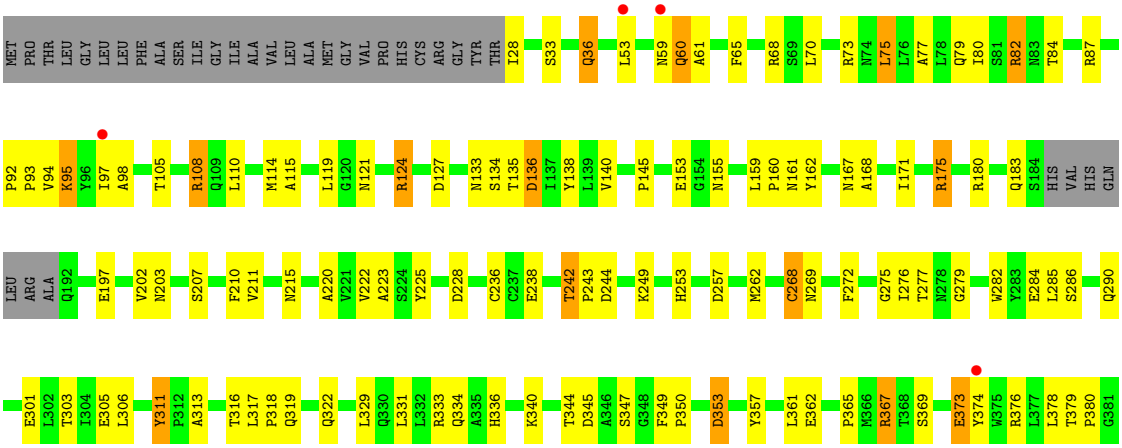
• Molecule 1: LP15968p

Chain A:



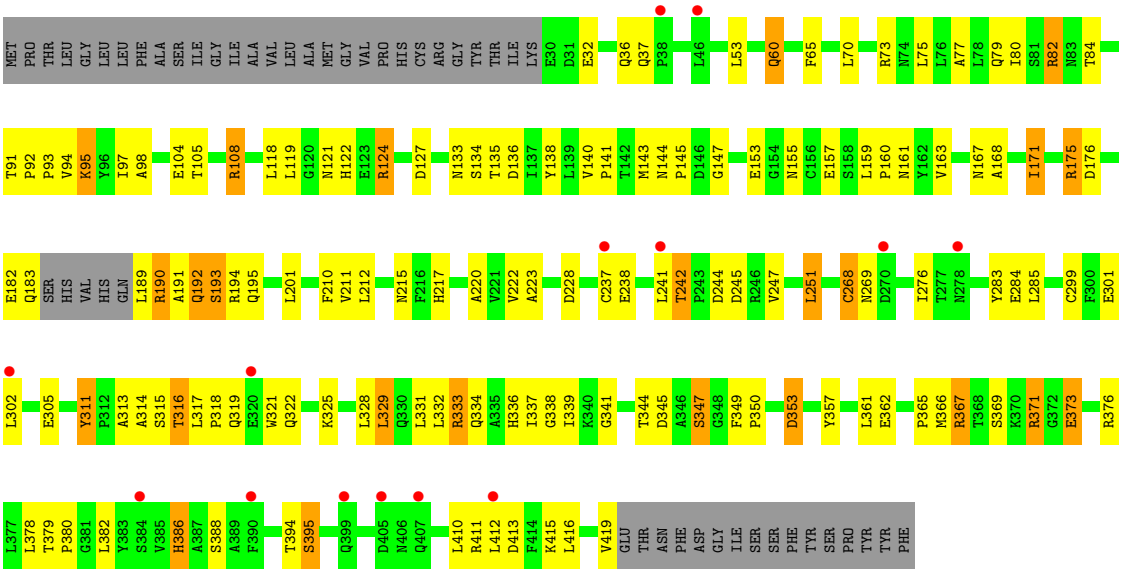
• Molecule 1: LP15968p

Chain B:



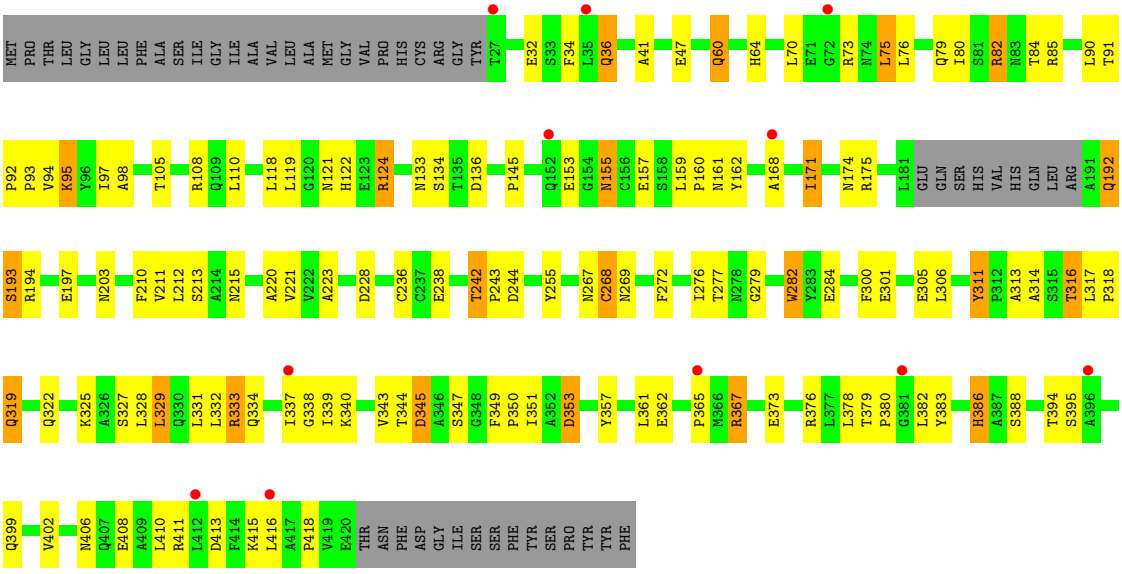
• Molecule 1: LP15968p

Chain C:



• Molecule 1: LP15968p

Chain D:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	97.02Å 135.70Å 141.71Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.00 – 2.70 49.01 – 2.70	Depositor EDS
% Data completeness (in resolution range)	100.0 (49.00-2.70) 88.3 (49.01-2.70)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	3.36 (at 2.69Å)	Xtriage
Refinement program	PHENIX (phenix.refine)	Depositor
R, R_{free}	0.211 , 0.282 0.225 , 0.304	Depositor DCC
R_{free} test set	749 reflections (1.44%)	wwPDB-VP
Wilson B-factor (Å^2)	43.4	Xtriage
Anisotropy	0.458	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.32 , 41.0	EDS
L-test for twinning[2]	$< \|L\| > = 0.39$, $< L^2 > = 0.22$	Xtriage
Estimated twinning fraction	0.076 for -h,l,k	Xtriage
F_o,F_c correlation	0.90	EDS
Total number of atoms	12468	wwPDB-VP
Average B, all atoms (Å^2)	45.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.45% 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, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: NAG, GOL, ZN, GEM

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	0.38	0/3082	0.63	6/4185 (0.1%)
1	B	0.40	0/3109	0.62	4/4221 (0.1%)
1	C	0.40	0/3101	0.64	10/4211 (0.2%)
1	D	0.40	0/3097	0.61	2/4206 (0.0%)
All	All	0.40	0/12389	0.62	22/16823 (0.1%)

There are no bond length outliers.

All (22) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	175	ARG	NE-CZ-NH2	-6.88	116.86	120.30
1	A	401	ARG	NE-CZ-NH2	-6.09	117.25	120.30
1	B	175	ARG	NE-CZ-NH1	6.06	123.33	120.30
1	B	367	ARG	NE-CZ-NH1	-5.80	117.40	120.30
1	A	371	ARG	NE-CZ-NH1	-5.68	117.46	120.30
1	C	333	ARG	NE-CZ-NH2	-5.58	117.51	120.30
1	C	371	ARG	NE-CZ-NH2	5.52	123.06	120.30
1	A	371	ARG	NE-CZ-NH2	5.45	123.02	120.30
1	C	108	ARG	NE-CZ-NH1	-5.41	117.59	120.30
1	C	333	ARG	NE-CZ-NH1	5.34	122.97	120.30
1	C	371	ARG	NE-CZ-NH1	-5.33	117.63	120.30
1	C	175	ARG	NE-CZ-NH1	5.31	122.96	120.30
1	A	401	ARG	NE-CZ-NH1	5.30	122.95	120.30
1	C	82	ARG	NE-CZ-NH2	-5.21	117.69	120.30
1	D	333	ARG	NE-CZ-NH2	5.12	122.86	120.30
1	C	367	ARG	NE-CZ-NH2	5.09	122.85	120.30
1	C	82	ARG	NE-CZ-NH1	5.07	122.83	120.30
1	B	108	ARG	NE-CZ-NH1	-5.06	117.77	120.30
1	D	333	ARG	NE-CZ-NH1	-5.06	117.77	120.30
1	A	333	ARG	NE-CZ-NH2	5.02	122.81	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	108	ARG	NE-CZ-NH2	5.01	122.81	120.30
1	A	333	ARG	NE-CZ-NH1	-5.01	117.80	120.30

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3013	0	2892	116	0
1	B	3040	0	2917	103	0
1	C	3032	0	2911	112	0
1	D	3028	0	2910	111	0
2	A	14	0	13	1	0
2	B	14	0	13	0	0
2	C	14	0	13	1	0
2	D	14	0	13	2	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
3	C	1	0	0	0	0
3	D	1	0	0	0	0
4	A	15	0	10	6	0
4	B	15	0	10	6	0
4	C	15	0	10	3	0
4	D	15	0	10	0	0
5	A	18	0	24	0	0
5	C	6	0	8	0	0
6	A	50	0	0	3	0
6	B	54	0	0	5	0
6	C	51	0	0	5	0
6	D	56	0	0	5	0
All	All	12468	0	11754	439	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 18.

All (439) 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:345:ASP:HB2	1:A:349:PHE:H	1.19	1.05
1:A:357:TYR:HB2	1:A:386:HIS:CE1	2.01	0.95
1:B:345:ASP:HB2	1:B:349:PHE:H	1.31	0.95
1:C:357:TYR:HB2	1:C:386:HIS:CE1	2.10	0.86
1:C:73:ARG:HD2	1:C:145:PRO:HB2	1.58	0.85
1:B:73:ARG:HD2	1:B:145:PRO:HB2	1.56	0.85
1:B:357:TYR:HB2	1:B:386:HIS:CE1	2.12	0.85
1:D:73:ARG:HD2	1:D:145:PRO:HB2	1.58	0.85
1:C:345:ASP:HB2	1:C:349:PHE:H	1.43	0.84
1:A:73:ARG:HD2	1:A:145:PRO:HB2	1.61	0.81
1:D:357:TYR:HB2	1:D:386:HIS:CE1	2.16	0.81
1:A:345:ASP:HB2	1:A:349:PHE:N	1.97	0.80
1:A:193:SER:HA	1:B:68:ARG:NH2	1.96	0.80
1:D:192:GLN:HG2	1:D:193:SER:H	1.47	0.78
1:B:242:THR:HG22	1:B:244:ASP:H	1.49	0.76
1:B:407:GLN:HG2	6:B:1022:HOH:O	1.85	0.76
1:C:65:PHE:HD1	1:D:203:ASN:HD21	1.35	0.75
1:B:242:THR:CG2	1:B:244:ASP:H	2.00	0.73
2:D:501:NAG:H3	2:D:501:NAG:H83	1.69	0.73
1:B:223:ALA:HB3	1:B:276:ILE:HG22	1.71	0.72
1:D:242:THR:HG22	1:D:244:ASP:H	1.55	0.72
1:B:242:THR:HG22	1:B:244:ASP:N	2.04	0.71
1:D:388:SER:HB3	1:D:394:THR:HG23	1.73	0.71
1:C:353:ASP:CG	1:C:367:ARG:HD3	2.10	0.71
1:C:242:THR:CG2	1:C:244:ASP:H	2.04	0.71
1:C:189:LEU:HD23	1:C:190:ARG:HH21	1.55	0.70
1:A:242:THR:CG2	1:A:244:ASP:H	2.04	0.70
1:D:223:ALA:HB3	1:D:276:ILE:HG22	1.72	0.69
1:C:65:PHE:HD1	1:D:203:ASN:ND2	1.89	0.69
1:A:193:SER:HA	1:B:68:ARG:HH22	1.56	0.68
1:C:217:HIS:HA	6:C:1003:HOH:O	1.93	0.68
1:A:178:PRO:HG3	1:A:194:ARG:NH2	2.09	0.68
1:A:242:THR:HG22	1:A:244:ASP:H	1.58	0.68
1:D:415:LYS:HB2	6:D:1047:HOH:O	1.94	0.68
1:D:242:THR:CG2	1:D:244:ASP:H	2.07	0.68
2:C:501:NAG:H83	2:C:501:NAG:H3	1.76	0.68
1:B:361:LEU:HD13	1:B:376:ARG:HH21	1.59	0.67
1:B:353:ASP:CG	1:B:367:ARG:HD3	2.14	0.67
1:A:242:THR:HG22	1:A:244:ASP:N	2.10	0.67
1:C:357:TYR:CE2	1:C:365:PRO:HG3	2.30	0.67
1:D:361:LEU:HD13	1:D:376:ARG:HH21	1.59	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:223:ALA:HB3	1:A:276:ILE:HG22	1.76	0.66
1:B:28:ILE:HD12	1:B:28:ILE:N	2.11	0.66
1:D:32:GLU:HA	1:D:34:PHE:CE2	2.30	0.66
1:C:251:LEU:HB3	1:C:302:LEU:HD11	1.77	0.66
1:B:60:GLN:O	1:B:80:ILE:HA	1.96	0.66
1:D:242:THR:HG22	1:D:244:ASP:N	2.10	0.66
1:D:406:ASN:HD22	1:D:408:GLU:H	1.44	0.66
1:C:70:LEU:HD12	1:C:168:ALA:HB3	1.77	0.65
1:C:349:PHE:CG	1:C:350:PRO:HD2	2.31	0.65
1:B:345:ASP:HB2	1:B:349:PHE:N	2.08	0.65
1:A:374:TYR:HA	6:A:1039:HOH:O	1.96	0.65
1:C:220:ALA:O	1:C:305:GLU:HB3	1.96	0.64
1:B:395:SER:HB3	1:B:416:LEU:CD2	2.28	0.64
1:A:361:LEU:HD13	1:A:376:ARG:HH21	1.61	0.64
1:A:357:TYR:HB2	1:A:386:HIS:HE1	1.59	0.64
1:C:357:TYR:HB2	1:C:386:HIS:HE1	1.62	0.64
1:D:349:PHE:CG	1:D:350:PRO:HD2	2.33	0.64
1:A:174:ASN:O	1:A:175:ARG:HD3	1.98	0.64
1:C:388:SER:HB3	1:C:394:THR:HG23	1.79	0.64
1:A:44:GLU:HB2	6:A:1001:HOH:O	1.97	0.63
1:C:316:THR:HG21	6:C:1031:HOH:O	1.99	0.63
1:D:70:LEU:HD12	1:D:168:ALA:HB3	1.81	0.63
1:A:344:THR:CG2	1:A:415:LYS:HG2	2.28	0.63
1:B:290:GLN:HB2	6:B:1015:HOH:O	1.97	0.63
1:A:161:ASN:HB2	1:A:163:VAL:HG23	1.78	0.63
1:B:282:TRP:CZ3	4:B:601:GEM:HC52	2.33	0.63
1:A:105:THR:O	1:A:108:ARG:HB3	1.98	0.63
1:C:105:THR:O	1:C:108:ARG:HB3	1.99	0.63
1:B:175:ARG:HH22	4:B:601:GEM:C9	2.11	0.63
1:D:345:ASP:HB2	1:D:349:PHE:H	1.63	0.62
1:A:388:SER:HB3	1:A:394:THR:HG23	1.81	0.62
1:A:357:TYR:HB2	1:A:386:HIS:ND1	2.14	0.62
1:D:331:LEU:HD23	1:D:331:LEU:O	1.99	0.62
1:B:105:THR:O	1:B:108:ARG:HB3	1.99	0.62
1:C:242:THR:HG22	1:C:244:ASP:H	1.65	0.62
1:B:82:ARG:HH21	1:B:133:ASN:ND2	1.98	0.61
1:C:345:ASP:HB3	1:C:347:SER:N	2.15	0.61
1:A:176:ASP:O	1:A:194:ARG:HD2	2.01	0.61
1:B:374:TYR:HA	6:B:1020:HOH:O	1.99	0.61
1:A:203:ASN:HD21	1:B:65:PHE:HD1	1.47	0.61
1:A:212:LEU:HD12	1:A:213:SER:H	1.66	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:282:TRP:CE3	4:A:601:GEM:HC52	2.36	0.60
1:C:93:PRO:HD2	1:C:211:VAL:HG23	1.83	0.60
1:A:203:ASN:ND2	1:B:65:PHE:HD1	2.00	0.60
1:B:79:GLN:HB2	1:B:138:TYR:CE2	2.36	0.60
1:B:160:PRO:O	1:B:161:ASN:HB2	2.02	0.59
1:A:345:ASP:HB3	1:A:347:SER:N	2.18	0.59
1:A:345:ASP:CB	1:A:349:PHE:H	2.05	0.59
1:B:357:TYR:CE2	1:B:365:PRO:HG3	2.37	0.59
1:B:349:PHE:CG	1:B:350:PRO:HD2	2.37	0.59
1:C:143:MET:SD	1:C:201:LEU:HD22	2.43	0.59
1:C:313:ALA:O	1:C:316:THR:HB	2.02	0.59
1:C:242:THR:HG22	1:C:244:ASP:N	2.18	0.58
1:D:82:ARG:HH21	1:D:133:ASN:ND2	2.01	0.58
1:B:388:SER:HB3	1:B:394:THR:HG23	1.85	0.58
1:D:395:SER:HB3	1:D:416:LEU:CD2	2.33	0.58
1:B:345:ASP:HB3	1:B:347:SER:N	2.19	0.58
1:A:331:LEU:HD23	1:A:331:LEU:O	2.03	0.58
1:C:223:ALA:HB3	1:C:276:ILE:HG22	1.86	0.58
1:C:345:ASP:HB3	1:C:347:SER:H	1.70	0.57
1:C:175:ARG:NH2	1:C:285:LEU:HD22	2.19	0.57
1:B:344:THR:CG2	1:B:415:LYS:HG2	2.34	0.57
1:C:379:THR:HG23	1:C:380:PRO:HD2	1.85	0.57
1:C:53:LEU:HD13	1:C:119:LEU:HD12	1.86	0.57
1:D:192:GLN:CG	1:D:193:SER:H	2.17	0.57
1:D:94:VAL:HG13	1:D:212:LEU:O	2.05	0.57
1:C:283:TYR:O	4:C:601:GEM:N4	2.29	0.56
1:C:361:LEU:HD13	1:C:376:ARG:HH21	1.70	0.56
1:D:93:PRO:HD2	1:D:211:VAL:HG23	1.87	0.56
1:D:316:THR:HG21	6:D:1045:HOH:O	2.05	0.56
1:D:357:TYR:CE2	1:D:365:PRO:HG3	2.41	0.56
1:A:236:CYS:HB2	1:A:282:TRP:O	2.06	0.56
1:D:353:ASP:HA	1:D:367:ARG:HG2	1.88	0.56
1:B:357:TYR:HB2	1:B:386:HIS:ND1	2.21	0.56
1:C:369:SER:OG	1:C:373:GLU:HG3	2.05	0.56
1:C:411:ARG:NH1	1:C:413:ASP:OD2	2.39	0.55
1:D:242:THR:HG23	1:D:243:PRO:HD2	1.87	0.55
1:B:411:ARG:HD2	1:B:413:ASP:OD1	2.05	0.55
1:C:182:GLU:HG3	1:C:183:GLN:H	1.72	0.55
1:D:174:ASN:O	1:D:175:ARG:HD3	2.07	0.55
1:D:331:LEU:HD23	1:D:331:LEU:C	2.27	0.55
1:D:345:ASP:CB	1:D:349:PHE:H	2.20	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:60:GLN:O	1:D:80:ILE:HA	2.07	0.55
1:A:47:GLU:HG2	1:A:76:LEU:HD11	1.89	0.54
1:C:189:LEU:HD23	1:C:190:ARG:NH2	2.23	0.54
1:C:77:ALA:HB2	1:C:140:VAL:HG22	1.89	0.54
1:B:61:ALA:HB2	1:B:119:LEU:HD11	1.89	0.54
1:D:313:ALA:O	1:D:316:THR:HB	2.08	0.54
1:A:331:LEU:HD23	1:A:331:LEU:C	2.28	0.54
1:C:161:ASN:HB2	1:C:163:VAL:HG23	1.90	0.54
1:D:345:ASP:HB3	1:D:347:SER:HB2	1.90	0.54
1:C:325:LYS:O	1:C:329:LEU:HD22	2.07	0.54
1:D:338:GLY:HA2	1:D:378:LEU:HB2	1.90	0.54
1:A:153:GLU:HA	1:A:311:TYR:CD2	2.43	0.54
1:A:369:SER:OG	1:A:373:GLU:HG3	2.07	0.54
1:A:357:TYR:CB	1:A:386:HIS:CE1	2.85	0.53
1:C:192:GLN:HA	1:C:192:GLN:HE21	1.72	0.53
1:A:313:ALA:O	1:A:316:THR:HB	2.07	0.53
1:C:299:CYS:HB2	6:C:1037:HOH:O	2.07	0.53
1:C:339:ILE:HG22	1:C:410:LEU:HB2	1.89	0.53
1:D:353:ASP:CG	1:D:367:ARG:HE	2.11	0.53
1:C:220:ALA:HA	1:C:268:CYS:SG	2.47	0.53
1:C:344:THR:CG2	1:C:415:LYS:HG2	2.39	0.53
1:A:325:LYS:O	1:A:329:LEU:HD22	2.09	0.53
1:C:155:ASN:HA	6:C:1030:HOH:O	2.08	0.53
1:B:175:ARG:NH2	1:B:285:LEU:HD22	2.24	0.53
1:C:212:LEU:HD21	1:C:331:LEU:HD23	1.90	0.53
1:C:411:ARG:HD2	1:C:413:ASP:OD1	2.09	0.53
1:D:212:LEU:HD21	1:D:331:LEU:HD23	1.90	0.53
1:A:82:ARG:HH21	1:A:133:ASN:ND2	2.07	0.53
1:A:193:SER:CA	1:B:68:ARG:HH22	2.22	0.53
1:B:159:LEU:O	1:B:162:TYR:N	2.40	0.53
1:D:331:LEU:O	1:D:334:GLN:HB2	2.09	0.53
1:D:161:ASN:O	1:D:162:TYR:HB2	2.07	0.53
1:A:382:LEU:HD12	1:A:382:LEU:O	2.08	0.52
1:C:94:VAL:HG13	1:C:212:LEU:O	2.09	0.52
1:D:85:ARG:HD3	6:D:1004:HOH:O	2.09	0.52
1:D:192:GLN:HG2	1:D:193:SER:N	2.21	0.52
1:D:344:THR:CG2	1:D:415:LYS:HG2	2.39	0.52
1:C:242:THR:HG23	1:C:244:ASP:H	1.73	0.52
1:D:314:ALA:O	1:D:317:LEU:HG	2.10	0.52
1:B:175:ARG:NH2	4:B:601:GEM:C9	2.73	0.52
1:B:382:LEU:HD12	1:B:382:LEU:O	2.10	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:357:TYR:HB2	1:C:386:HIS:ND1	2.25	0.52
1:D:220:ALA:HA	1:D:268:CYS:SG	2.50	0.51
1:B:160:PRO:O	1:B:161:ASN:CB	2.58	0.51
1:A:220:ALA:HA	1:A:268:CYS:SG	2.51	0.51
1:B:382:LEU:HD12	1:B:382:LEU:C	2.31	0.51
1:C:153:GLU:HA	1:C:311:TYR:CD2	2.46	0.51
1:D:228:ASP:OD1	1:D:279:GLY:HA3	2.10	0.51
1:A:49:LEU:HD23	1:A:53:LEU:HD22	1.91	0.51
1:D:345:ASP:HB3	1:D:347:SER:N	2.25	0.51
1:D:418:PRO:HD3	6:D:1048:HOH:O	2.09	0.51
1:A:395:SER:HB3	1:A:416:LEU:CD2	2.41	0.51
1:B:340:LYS:O	1:B:411:ARG:HA	2.10	0.51
1:C:97:ILE:N	1:C:97:ILE:HD12	2.26	0.51
1:A:143:MET:SD	1:A:201:LEU:HD22	2.51	0.51
1:A:406:ASN:CG	1:A:407:GLN:N	2.64	0.51
1:A:60:GLN:O	1:A:80:ILE:HA	2.11	0.50
1:A:228:ASP:OD1	1:A:279:GLY:HA3	2.11	0.50
1:D:95:LYS:HD3	1:D:210:PHE:CG	2.46	0.50
1:A:345:ASP:OD1	1:A:349:PHE:HB3	2.11	0.50
1:C:317:LEU:HB2	1:C:318:PRO:HD3	1.93	0.50
1:A:344:THR:HG23	1:A:345:ASP:O	2.12	0.50
1:B:220:ALA:HA	1:B:268:CYS:SG	2.52	0.50
1:C:215:ASN:ND2	1:C:301:GLU:OE2	2.44	0.50
1:A:93:PRO:HD2	1:A:211:VAL:HG23	1.93	0.50
1:C:36:GLN:HA	1:C:36:GLN:NE2	2.27	0.50
1:A:406:ASN:CG	1:A:407:GLN:H	2.14	0.49
1:B:331:LEU:O	1:B:334:GLN:HB2	2.11	0.49
1:C:382:LEU:O	1:C:382:LEU:HD12	2.12	0.49
1:A:317:LEU:HB2	1:A:318:PRO:HD3	1.93	0.49
1:A:121:ASN:HA	1:A:124:ARG:HG3	1.93	0.49
1:C:95:LYS:HD3	1:C:210:PHE:CG	2.46	0.49
1:D:220:ALA:O	1:D:305:GLU:HB3	2.13	0.49
1:C:36:GLN:HG3	1:C:37:GLN:HG3	1.94	0.49
1:B:225:TYR:OH	1:B:249:LYS:HE3	2.13	0.49
1:C:104:GLU:HB2	6:C:1003:HOH:O	2.11	0.49
1:D:159:LEU:O	1:D:162:TYR:N	2.36	0.49
1:B:127:ASP:O	1:B:333:ARG:NH2	2.46	0.49
1:C:97:ILE:O	1:C:215:ASN:HA	2.13	0.49
1:C:176:ASP:O	1:C:194:ARG:HD2	2.13	0.49
1:B:95:LYS:HD3	1:B:210:PHE:CG	2.47	0.49
1:D:105:THR:O	1:D:108:ARG:HB3	2.12	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:98:ALA:HB3	1:C:141:PRO:O	2.13	0.49
1:A:217:HIS:HB3	4:A:601:GEM:O12	2.12	0.49
1:A:353:ASP:CG	1:A:367:ARG:HE	2.17	0.48
1:D:411:ARG:NH1	1:D:413:ASP:OD2	2.46	0.48
1:C:334:GLN:O	1:C:337:ILE:HG12	2.13	0.48
1:A:36:GLN:O	1:A:36:GLN:HG3	2.13	0.48
1:B:303:THR:HG21	4:B:601:GEM:HC62	1.95	0.48
1:C:121:ASN:HA	1:C:124:ARG:HG3	1.94	0.48
1:D:268:CYS:O	1:D:269:ASN:HB2	2.14	0.48
1:A:357:TYR:CB	1:A:386:HIS:HE1	2.23	0.48
1:B:87:ARG:HG3	1:B:136:ASP:CG	2.33	0.48
1:A:411:ARG:NH1	1:A:413:ASP:OD2	2.47	0.48
1:B:349:PHE:CD2	1:B:350:PRO:HD2	2.48	0.48
1:B:153:GLU:HA	1:B:311:TYR:CD2	2.49	0.48
1:B:215:ASN:ND2	1:B:301:GLU:OE2	2.47	0.48
1:B:272:PHE:CD2	1:B:277:THR:HB	2.49	0.48
1:B:331:LEU:C	1:B:331:LEU:HD23	2.33	0.48
1:C:341:GLY:HA3	1:C:412:LEU:O	2.14	0.48
1:B:70:LEU:HD12	1:B:168:ALA:HB3	1.96	0.47
1:D:339:ILE:HG22	1:D:410:LEU:HB2	1.95	0.47
1:B:180:ARG:HD2	6:B:1007:HOH:O	2.13	0.47
1:B:313:ALA:O	1:B:316:THR:HB	2.13	0.47
1:C:349:PHE:CD2	1:C:350:PRO:HD2	2.49	0.47
1:B:262:MET:O	1:B:275:GLY:HA3	2.15	0.47
1:B:344:THR:HG23	1:B:415:LYS:HG2	1.97	0.47
1:C:159:LEU:HB3	1:C:160:PRO:HD2	1.96	0.47
1:D:345:ASP:HB2	1:D:349:PHE:N	2.28	0.47
1:D:95:LYS:HD3	1:D:210:PHE:CD2	2.49	0.47
1:D:328:LEU:O	1:D:332:LEU:HG	2.14	0.47
1:B:222:VAL:HG22	1:B:223:ALA:N	2.30	0.47
1:B:406:ASN:HD22	1:B:408:GLU:H	1.63	0.47
1:D:41:ALA:O	1:D:108:ARG:NH1	2.48	0.47
1:B:228:ASP:O	1:B:284:GLU:HA	2.15	0.47
1:A:228:ASP:O	1:A:284:GLU:HA	2.15	0.47
1:B:92:PRO:HD2	1:B:134:SER:O	2.15	0.47
1:B:228:ASP:CG	4:B:601:GEM:HN41	2.18	0.47
1:B:411:ARG:NH1	1:B:413:ASP:OD2	2.48	0.47
1:A:124:ARG:HB2	1:A:125:ILE:HD12	1.96	0.46
1:C:105:THR:HG21	1:C:311:TYR:CE1	2.49	0.46
1:A:203:ASN:O	1:A:207:SER:HB3	2.16	0.46
1:D:379:THR:HG23	1:D:380:PRO:HD2	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:37:GLN:O	1:A:37:GLN:OE1	2.34	0.46
1:A:159:LEU:HB3	1:A:160:PRO:HD2	1.97	0.46
1:A:357:TYR:CE2	1:A:365:PRO:HG3	2.50	0.46
1:A:382:LEU:HD12	1:A:382:LEU:C	2.35	0.46
1:D:236:CYS:HB2	1:D:282:TRP:O	2.15	0.46
1:D:411:ARG:HD2	1:D:413:ASP:OD1	2.15	0.46
1:C:36:GLN:CA	1:C:36:GLN:HE21	2.29	0.46
1:C:60:GLN:O	1:C:80:ILE:HA	2.14	0.46
1:A:213:SER:O	1:A:301:GLU:HA	2.16	0.46
1:B:407:GLN:CG	6:B:1022:HOH:O	2.54	0.46
1:B:242:THR:HG23	1:B:243:PRO:HD2	1.97	0.45
1:B:334:GLN:C	1:B:336:HIS:H	2.18	0.45
1:B:357:TYR:HB2	1:B:386:HIS:HE1	1.71	0.45
1:D:267:ASN:ND2	6:D:1020:HOH:O	2.48	0.45
1:C:153:GLU:HA	1:C:311:TYR:CE2	2.51	0.45
1:D:91:THR:HA	1:D:92:PRO:HD3	1.82	0.45
1:C:331:LEU:HD23	1:C:331:LEU:C	2.36	0.45
1:C:334:GLN:C	1:C:336:HIS:H	2.19	0.45
1:D:244:ASP:OD1	1:D:376:ARG:NH2	2.49	0.45
1:A:41:ALA:O	1:A:108:ARG:NH1	2.49	0.45
1:A:346:ALA:C	1:A:348:GLY:H	2.20	0.45
1:D:349:PHE:CD2	1:D:350:PRO:HD2	2.52	0.45
1:A:47:GLU:HG2	1:A:76:LEU:CD1	2.46	0.45
1:A:191:ALA:O	1:A:192:GLN:O	2.34	0.45
1:A:192:GLN:HB3	1:A:193:SER:H	1.48	0.45
1:A:33:SER:C	1:A:35:LEU:H	2.20	0.45
1:C:345:ASP:HB2	1:C:349:PHE:N	2.21	0.45
1:A:98:ALA:HB3	1:A:141:PRO:O	2.16	0.45
1:C:268:CYS:O	1:C:269:ASN:HB2	2.17	0.45
1:A:259:HIS:HB3	1:A:262:MET:HB3	1.99	0.45
1:B:77:ALA:HB2	1:B:140:VAL:HG22	1.99	0.45
1:C:175:ARG:HH22	4:C:601:GEM:C9	2.30	0.45
1:D:357:TYR:HB2	1:D:386:HIS:ND1	2.30	0.45
1:B:53:LEU:HD13	1:B:119:LEU:HD12	1.99	0.45
1:C:395:SER:HB3	1:C:416:LEU:CD2	2.47	0.45
1:A:33:SER:O	1:A:35:LEU:N	2.50	0.44
1:A:331:LEU:O	1:A:334:GLN:HB2	2.17	0.44
1:B:282:TRP:CE3	4:B:601:GEM:HC52	2.51	0.44
1:C:228:ASP:O	1:C:284:GLU:HA	2.16	0.44
1:D:97:ILE:HG22	1:D:98:ALA:N	2.31	0.44
1:A:70:LEU:HD12	1:A:168:ALA:HB3	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:349:PHE:CG	1:A:350:PRO:HD2	2.52	0.44
1:A:411:ARG:HD2	1:A:413:ASP:OD1	2.17	0.44
1:B:380:PRO:HA	1:B:402:VAL:O	2.18	0.44
1:C:32:GLU:OE1	1:C:321:TRP:NE1	2.46	0.44
1:A:224:SER:HA	1:A:277:THR:O	2.18	0.44
1:A:386:HIS:HD2	6:A:1047:HOH:O	1.99	0.44
1:D:110:LEU:HD12	1:D:306:LEU:HD13	2.00	0.44
1:D:75:LEU:HD21	1:D:197:GLU:HG3	2.00	0.44
1:A:353:ASP:HA	1:A:367:ARG:HG2	1.98	0.44
1:D:314:ALA:HA	1:D:317:LEU:HG	2.00	0.44
1:A:212:LEU:HD21	1:A:331:LEU:HD23	1.98	0.44
1:A:282:TRP:CZ3	4:A:601:GEM:HC52	2.52	0.44
1:A:339:ILE:HG22	1:A:410:LEU:HB2	1.99	0.44
1:B:93:PRO:HD2	1:B:211:VAL:HG23	2.00	0.44
1:C:217:HIS:HB3	4:C:601:GEM:O12	2.17	0.44
1:A:229:ASN:HB3	1:A:285:LEU:O	2.18	0.44
1:D:386:HIS:HD1	1:D:386:HIS:C	2.19	0.44
1:A:221:VAL:HG23	1:A:268:CYS:SG	2.58	0.43
1:D:272:PHE:CD2	1:D:277:THR:HB	2.53	0.43
1:B:121:ASN:HA	1:B:124:ARG:HG3	1.99	0.43
1:D:343:VAL:HG12	1:D:351:ILE:HD12	2.00	0.43
1:A:228:ASP:CG	4:A:601:GEM:HN41	2.21	0.43
2:A:501:NAG:H3	2:A:501:NAG:H83	2.00	0.43
1:C:79:GLN:HB2	1:C:138:TYR:CE2	2.53	0.43
1:A:118:LEU:O	1:A:122:HIS:HB3	2.17	0.43
1:A:380:PRO:HD3	1:A:404:ASN:HD22	1.83	0.43
1:B:75:LEU:HD21	1:B:197:GLU:HG3	2.00	0.43
1:B:253:HIS:O	1:B:257:ASP:HB2	2.17	0.43
1:C:192:GLN:HB3	1:C:193:SER:H	1.60	0.43
1:C:382:LEU:HD12	1:C:382:LEU:C	2.39	0.43
1:D:121:ASN:HA	1:D:124:ARG:HG3	2.01	0.43
1:D:357:TYR:HB2	1:D:386:HIS:HE1	1.75	0.43
1:B:87:ARG:HH22	1:B:373:GLU:CD	2.21	0.43
1:B:228:ASP:OD1	1:B:279:GLY:HA3	2.18	0.43
1:B:379:THR:HG23	1:B:380:PRO:HD2	1.99	0.43
1:C:328:LEU:O	1:C:332:LEU:HG	2.18	0.43
1:C:366:MET:CE	1:C:376:ARG:HH11	2.32	0.43
1:A:242:THR:HG23	1:A:244:ASP:H	1.79	0.43
1:A:305:GLU:OE1	4:A:601:GEM:O12	2.36	0.43
1:B:395:SER:HB3	1:B:416:LEU:HD21	2.00	0.43
1:C:97:ILE:HG22	1:C:98:ALA:N	2.33	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:369:SER:HG	1:C:373:GLU:HG3	1.83	0.43
1:C:92:PRO:HD2	1:C:134:SER:O	2.19	0.43
1:C:353:ASP:HA	1:C:367:ARG:CD	2.48	0.43
1:A:153:GLU:HA	1:A:311:TYR:CE2	2.54	0.43
1:C:144:ASN:ND2	1:C:147:GLY:HA3	2.33	0.43
1:D:340:LYS:O	1:D:411:ARG:HA	2.18	0.43
1:A:87:ARG:HH22	1:A:373:GLU:CD	2.22	0.43
1:B:331:LEU:O	1:B:331:LEU:HD23	2.18	0.43
1:C:315:SER:O	1:C:318:PRO:HD2	2.19	0.43
1:A:110:LEU:HD12	1:A:306:LEU:HD13	2.00	0.42
1:B:317:LEU:HB2	1:B:318:PRO:HD3	2.00	0.42
1:D:47:GLU:HG2	1:D:76:LEU:HD11	2.01	0.42
1:A:242:THR:HG23	1:A:243:PRO:HD2	2.00	0.42
1:A:306:LEU:HD22	1:A:324:ASN:OD1	2.17	0.42
1:B:153:GLU:HA	1:B:311:TYR:CE2	2.53	0.42
1:C:95:LYS:HD3	1:C:210:PHE:CD2	2.54	0.42
1:C:241:LEU:HD22	1:C:245:ASP:OD1	2.19	0.42
1:D:153:GLU:HA	1:D:311:TYR:CD2	2.54	0.42
1:C:171:ILE:HD12	1:C:171:ILE:C	2.39	0.42
1:C:357:TYR:CB	1:C:386:HIS:HE1	2.30	0.42
1:A:160:PRO:O	1:A:161:ASN:HB2	2.19	0.42
1:B:33:SER:O	1:B:36:GLN:HB2	2.20	0.42
1:C:91:THR:HG23	1:C:134:SER:O	2.19	0.42
1:D:155:ASN:HB3	1:D:157:GLU:O	2.20	0.42
1:D:383:TYR:O	1:D:399:GLN:HA	2.20	0.42
1:B:94:VAL:HG12	1:B:95:LYS:N	2.34	0.42
1:B:114:MET:O	1:B:115:ALA:C	2.58	0.42
1:B:242:THR:HG23	1:B:244:ASP:H	1.82	0.42
1:C:127:ASP:O	1:C:333:ARG:NH2	2.53	0.42
1:C:247:VAL:HG12	1:C:251:LEU:HD22	2.02	0.42
1:D:155:ASN:HD22	1:D:155:ASN:HA	1.71	0.42
1:D:345:ASP:CB	1:D:347:SER:HB2	2.49	0.42
1:C:244:ASP:OD1	1:C:376:ARG:NH2	2.53	0.42
1:C:353:ASP:OD2	1:C:367:ARG:HD3	2.20	0.42
1:D:192:GLN:C	1:D:194:ARG:H	2.23	0.42
1:D:300:PHE:N	1:D:300:PHE:CD2	2.88	0.42
1:A:283:TYR:O	4:A:601:GEM:N2	2.52	0.42
1:B:220:ALA:O	1:B:305:GLU:HB3	2.20	0.42
1:B:268:CYS:O	1:B:269:ASN:HB2	2.20	0.42
1:C:314:ALA:HA	1:C:317:LEU:HG	2.01	0.42
1:C:345:ASP:OD1	1:C:349:PHE:HB3	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:47:GLU:HG2	1:D:76:LEU:CD1	2.49	0.42
1:D:60:GLN:HE21	1:D:60:GLN:HB3	1.61	0.42
1:D:94:VAL:HG12	1:D:95:LYS:N	2.35	0.42
1:D:325:LYS:O	1:D:329:LEU:HD22	2.19	0.42
1:A:92:PRO:HD2	1:A:134:SER:O	2.19	0.42
1:C:189:LEU:HD23	1:C:189:LEU:N	2.34	0.42
1:D:300:PHE:N	1:D:300:PHE:HD2	2.18	0.42
1:D:36:GLN:HE21	1:D:36:GLN:HB2	1.59	0.41
1:D:329:LEU:O	1:D:333:ARG:HG3	2.20	0.41
1:B:175:ARG:HA	1:B:286:SER:O	2.20	0.41
1:C:36:GLN:HA	1:C:36:GLN:HE21	1.85	0.41
1:C:176:ASP:OD2	1:C:195:GLN:HG2	2.20	0.41
1:D:92:PRO:HD2	1:D:134:SER:O	2.21	0.41
1:D:345:ASP:HB2	1:D:349:PHE:O	2.20	0.41
1:D:382:LEU:HD12	1:D:382:LEU:C	2.41	0.41
2:D:501:NAG:H3	2:D:501:NAG:C8	2.44	0.41
1:A:266:ASN:HA	1:A:270:ASP:O	2.20	0.41
1:A:411:ARG:HG3	1:A:412:LEU:N	2.35	0.41
1:B:357:TYR:CB	1:B:386:HIS:HE1	2.33	0.41
1:A:40:TYR:CZ	1:A:317:LEU:HD21	2.55	0.41
1:C:338:GLY:HA2	1:C:378:LEU:HB2	2.03	0.41
1:D:221:VAL:HG23	1:D:268:CYS:SG	2.60	0.41
1:A:79:GLN:HB2	1:A:138:TYR:CE2	2.55	0.41
1:B:60:GLN:HE21	1:B:60:GLN:HB3	1.68	0.41
1:B:110:LEU:HD12	1:B:306:LEU:HD13	2.02	0.41
1:B:369:SER:OG	1:B:373:GLU:HG3	2.21	0.41
1:D:118:LEU:O	1:D:122:HIS:HB3	2.21	0.41
1:D:213:SER:O	1:D:301:GLU:HA	2.21	0.41
1:A:60:GLN:HE21	1:A:60:GLN:HB3	1.60	0.41
1:A:121:ASN:O	1:A:124:ARG:HG3	2.21	0.41
1:C:36:GLN:NE2	1:C:36:GLN:CA	2.84	0.41
1:D:119:LEU:HD23	1:D:119:LEU:HA	1.89	0.41
1:D:64:HIS:NE2	1:D:79:GLN:OE1	2.52	0.41
1:D:171:ILE:HD12	1:D:171:ILE:C	2.41	0.41
1:A:87:ARG:HG3	1:A:136:ASP:CG	2.42	0.41
1:A:118:LEU:HD23	1:A:118:LEU:HA	1.93	0.41
1:A:319:GLN:O	1:A:323:ARG:HG3	2.21	0.41
1:A:344:THR:HG23	1:A:415:LYS:HG2	2.02	0.41
1:B:236:CYS:HB2	1:B:282:TRP:O	2.21	0.41
1:C:155:ASN:HB3	1:C:157:GLU:O	2.21	0.41
1:C:331:LEU:O	1:C:334:GLN:HB2	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:97:ILE:O	1:D:215:ASN:HA	2.20	0.41
1:D:255:TYR:CG	1:D:327:SER:HB3	2.55	0.41
1:D:380:PRO:HA	1:D:402:VAL:O	2.20	0.41
1:B:353:ASP:HA	1:B:367:ARG:CD	2.51	0.41
1:D:90:LEU:HD23	1:D:90:LEU:HA	1.94	0.41
1:D:228:ASP:O	1:D:284:GLU:HA	2.21	0.41
1:A:379:THR:HG23	1:A:380:PRO:HD2	2.03	0.40
1:C:82:ARG:HH21	1:C:133:ASN:ND2	2.19	0.40
1:D:242:THR:HG23	1:D:243:PRO:CD	2.51	0.40
1:A:155:ASN:HD22	1:A:155:ASN:HA	1.71	0.40
1:A:220:ALA:O	1:A:305:GLU:HB3	2.21	0.40
1:A:268:CYS:O	1:A:269:ASN:HB2	2.20	0.40
1:B:97:ILE:O	1:B:215:ASN:HA	2.21	0.40
1:B:345:ASP:HB3	1:B:347:SER:H	1.84	0.40
1:D:192:GLN:HB3	1:D:194:ARG:HG3	2.03	0.40
1:A:314:ALA:HA	1:A:317:LEU:HG	2.02	0.40
1:B:203:ASN:O	1:B:207:SER:HB3	2.21	0.40
1:B:357:TYR:CB	1:B:386:HIS:CE1	2.94	0.40
1:C:350:PRO:HB3	1:C:371:ARG:O	2.20	0.40
1:D:334:GLN:O	1:D:337:ILE:HG12	2.21	0.40
1:A:297:SER:O	1:A:364:LYS:NZ	2.50	0.40
1:B:378:LEU:HD22	1:B:383:TYR:CE2	2.57	0.40
1:C:118:LEU:O	1:C:122:HIS:HB3	2.21	0.40
1:C:222:VAL:HG22	1:C:223:ALA:N	2.36	0.40
1:D:317:LEU:HB2	1:D:318:PRO:HD3	2.03	0.40
1:D:331:LEU:C	1:D:331:LEU:CD2	2.89	0.40
1:B:97:ILE:HG22	1:B:98:ALA:N	2.37	0.40
1:D:319:GLN:HE21	1:D:319:GLN:H	1.69	0.40
1:D:332:LEU:HD23	1:D:332:LEU:HA	1.89	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	379/435 (87%)	353 (93%)	23 (6%)	3 (1%)	19	43
1	B	382/435 (88%)	357 (94%)	23 (6%)	2 (0%)	29	54
1	C	381/435 (88%)	355 (93%)	23 (6%)	3 (1%)	19	43
1	D	381/435 (88%)	359 (94%)	19 (5%)	3 (1%)	19	43
All	All	1523/1740 (88%)	1424 (94%)	88 (6%)	11 (1%)	22	46

All (11) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	192	GLN
1	D	192	GLN
1	A	34	PHE
1	D	160	PRO
1	B	167	ASN
1	C	395	SER
1	D	282	TRP
1	A	282	TRP
1	C	167	ASN
1	C	191	ALA
1	B	202	VAL

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	324/368 (88%)	298 (92%)	26 (8%)	12	27
1	B	328/368 (89%)	304 (93%)	24 (7%)	14	33
1	C	326/368 (89%)	299 (92%)	27 (8%)	11	25
1	D	326/368 (89%)	301 (92%)	25 (8%)	13	30
All	All	1304/1472 (89%)	1202 (92%)	102 (8%)	12	29

All (102) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	36	GLN
1	A	37	GLN
1	A	53	LEU
1	A	60	GLN
1	A	75	LEU
1	A	82	ARG
1	A	84	THR
1	A	95	LYS
1	A	124	ARG
1	A	135	THR
1	A	136	ASP
1	A	155	ASN
1	A	171	ILE
1	A	215	ASN
1	A	238	GLU
1	A	242	THR
1	A	268	CYS
1	A	311	TYR
1	A	319	GLN
1	A	322	GLN
1	A	329	LEU
1	A	353	ASP
1	A	362	GLU
1	A	367	ARG
1	A	373	GLU
1	A	386	HIS
1	B	36	GLN
1	B	59	ASN
1	B	60	GLN
1	B	75	LEU
1	B	82	ARG
1	B	84	THR
1	B	95	LYS
1	B	124	ARG
1	B	135	THR
1	B	136	ASP
1	B	155	ASN
1	B	171	ILE
1	B	183	GLN
1	B	238	GLU
1	B	242	THR
1	B	268	CYS
1	B	311	TYR

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Mol	Chain	Res	Type
1	B	319	GLN
1	B	322	GLN
1	B	329	LEU
1	B	353	ASP
1	B	362	GLU
1	B	373	GLU
1	B	386	HIS
1	C	60	GLN
1	C	75	LEU
1	C	84	THR
1	C	95	LYS
1	C	124	ARG
1	C	135	THR
1	C	136	ASP
1	C	171	ILE
1	C	190	ARG
1	C	192	GLN
1	C	193	SER
1	C	237	CYS
1	C	238	GLU
1	C	242	THR
1	C	251	LEU
1	C	268	CYS
1	C	311	TYR
1	C	316	THR
1	C	319	GLN
1	C	322	GLN
1	C	329	LEU
1	C	347	SER
1	C	353	ASP
1	C	362	GLU
1	C	373	GLU
1	C	386	HIS
1	C	419	VAL
1	D	36	GLN
1	D	60	GLN
1	D	75	LEU
1	D	82	ARG
1	D	84	THR
1	D	95	LYS
1	D	124	ARG
1	D	136	ASP

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Mol	Chain	Res	Type
1	D	155	ASN
1	D	171	ILE
1	D	193	SER
1	D	238	GLU
1	D	242	THR
1	D	268	CYS
1	D	311	TYR
1	D	316	THR
1	D	319	GLN
1	D	322	GLN
1	D	329	LEU
1	D	345	ASP
1	D	353	ASP
1	D	362	GLU
1	D	367	ARG
1	D	373	GLU
1	D	386	HIS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (38) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	36	GLN
1	A	60	GLN
1	A	152	GLN
1	A	155	ASN
1	A	267	ASN
1	A	269	ASN
1	A	281	HIS
1	A	319	GLN
1	A	322	GLN
1	B	36	GLN
1	B	60	GLN
1	B	152	GLN
1	B	155	ASN
1	B	192	GLN
1	B	267	ASN
1	B	269	ASN
1	B	281	HIS
1	B	319	GLN
1	B	406	ASN
1	C	36	GLN
1	C	37	GLN

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Mol	Chain	Res	Type
1	C	60	GLN
1	C	152	GLN
1	C	155	ASN
1	C	192	GLN
1	C	234	ASN
1	C	253	HIS
1	C	267	ASN
1	C	269	ASN
1	C	281	HIS
1	C	319	GLN
1	D	36	GLN
1	D	60	GLN
1	D	152	GLN
1	D	269	ASN
1	D	281	HIS
1	D	319	GLN
1	D	406	ASN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains (i)

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

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 16 ligands modelled in this entry, 4 are monoatomic - leaving 12 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	$\#\|Z\| > 2$
5	GOL	A	801	-	5,5,5	0.29	0	5,5,5	0.35	0
2	NAG	B	501	1	14,14,15	0.69	0	17,19,21	1.04	0
4	GEM	C	601	3	14,14,14	1.93	2 (14%)	11,17,17	1.93	1 (9%)
5	GOL	A	802	-	5,5,5	0.34	0	5,5,5	0.27	0
4	GEM	A	601	3	14,14,14	1.79	2 (14%)	11,17,17	1.19	1 (9%)
5	GOL	C	804	-	5,5,5	0.29	0	5,5,5	0.63	0
5	GOL	A	803	-	5,5,5	0.34	0	5,5,5	0.24	0
2	NAG	A	501	1	14,14,15	0.70	0	17,19,21	1.09	2 (11%)
4	GEM	B	601	3	14,14,14	2.09	2 (14%)	11,17,17	1.17	1 (9%)
2	NAG	C	501	1	14,14,15	0.56	0	17,19,21	2.04	8 (47%)
2	NAG	D	501	1	14,14,15	0.49	0	17,19,21	1.18	3 (17%)
4	GEM	D	601	3	14,14,14	1.73	2 (14%)	11,17,17	2.47	4 (36%)

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
5	GOL	A	801	-	-	0/4/4/4	-
2	NAG	B	501	1	-	5/6/23/26	0/1/1/1
4	GEM	C	601	3	-	6/15/15/15	-
5	GOL	A	802	-	-	2/4/4/4	-
4	GEM	A	601	3	-	3/15/15/15	-
5	GOL	C	804	-	-	3/4/4/4	-
5	GOL	A	803	-	-	2/4/4/4	-
2	NAG	A	501	1	-	3/6/23/26	0/1/1/1
4	GEM	B	601	3	-	8/15/15/15	-
2	NAG	C	501	1	-	3/6/23/26	0/1/1/1
2	NAG	D	501	1	-	3/6/23/26	0/1/1/1
4	GEM	D	601	3	-	5/15/15/15	-

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	601	GEM	C8-S7	-6.48	1.76	1.83
4	C	601	GEM	C8-S7	-5.91	1.76	1.83
4	A	601	GEM	C8-S7	-5.23	1.77	1.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	D	601	GEM	C8-S7	-4.49	1.78	1.83
4	D	601	GEM	C6-S7	-3.75	1.76	1.81
4	B	601	GEM	C6-S7	-3.42	1.77	1.81
4	A	601	GEM	C6-S7	-3.11	1.77	1.81
4	C	601	GEM	C6-S7	-3.10	1.77	1.81

All (20) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	D	601	GEM	C6-C5-N3	-6.59	98.58	112.42
4	C	601	GEM	C6-C5-N3	-5.25	101.38	112.42
2	C	501	NAG	C1-O5-C5	4.06	117.69	112.19
2	C	501	NAG	O5-C1-C2	3.22	116.37	111.29
2	A	501	NAG	C2-N2-C7	3.13	127.36	122.90
2	C	501	NAG	C3-C4-C5	-2.98	104.93	110.24
2	C	501	NAG	C2-N2-C7	2.38	126.30	122.90
4	D	601	GEM	O12-C11-C10	-2.38	115.17	122.80
2	C	501	NAG	C4-C3-C2	-2.36	107.56	111.02
4	D	601	GEM	O14-C9-C8	2.33	120.69	114.05
4	A	601	GEM	C6-C5-N3	-2.32	107.54	112.42
2	D	501	NAG	C1-O5-C5	2.29	115.29	112.19
2	C	501	NAG	O5-C5-C6	2.27	110.76	107.20
2	C	501	NAG	O3-C3-C2	2.26	114.15	109.47
4	D	601	GEM	O13-C11-C10	2.25	121.30	114.07
2	D	501	NAG	C2-N2-C7	2.22	126.06	122.90
2	A	501	NAG	C8-C7-N2	2.17	119.78	116.10
4	B	601	GEM	O12-C11-C10	-2.08	116.12	122.80
2	D	501	NAG	C8-C7-N2	2.06	119.59	116.10
2	C	501	NAG	C8-C7-N2	2.01	119.50	116.10

There are no chirality outliers.

All (43) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	501	NAG	C8-C7-N2-C2
2	A	501	NAG	O7-C7-N2-C2
2	B	501	NAG	C3-C2-N2-C7
2	B	501	NAG	C8-C7-N2-C2
2	B	501	NAG	O7-C7-N2-C2
2	C	501	NAG	C8-C7-N2-C2
2	C	501	NAG	O7-C7-N2-C2
2	D	501	NAG	C8-C7-N2-C2

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Mol	Chain	Res	Type	Atoms
4	D	601	GEM	N3-C5-C6-S7
5	A	802	GOL	O1-C1-C2-C3
5	C	804	GOL	O1-C1-C2-O2
5	C	804	GOL	O1-C1-C2-C3
2	D	501	NAG	O7-C7-N2-C2
2	B	501	NAG	O5-C5-C6-O6
2	B	501	NAG	C4-C5-C6-O6
4	C	601	GEM	N3-C5-C6-S7
5	A	802	GOL	O1-C1-C2-O2
4	B	601	GEM	C8-C10-C11-O12
4	B	601	GEM	C8-C10-C11-O13
2	C	501	NAG	C3-C2-N2-C7
5	A	803	GOL	O1-C1-C2-O2
4	C	601	GEM	C10-C8-C9-O15
4	A	601	GEM	S7-C8-C9-O15
4	B	601	GEM	S7-C8-C9-O15
4	C	601	GEM	S7-C8-C9-O15
4	D	601	GEM	S7-C8-C9-O15
5	A	803	GOL	O1-C1-C2-C3
4	B	601	GEM	C10-C8-S7-C6
4	B	601	GEM	C11-C10-C8-S7
4	C	601	GEM	C5-C6-S7-C8
4	D	601	GEM	C5-C6-S7-C8
2	A	501	NAG	C3-C2-N2-C7
2	D	501	NAG	C3-C2-N2-C7
4	A	601	GEM	S7-C8-C9-O14
4	B	601	GEM	S7-C8-C9-O14
4	D	601	GEM	S7-C8-C9-O14
4	C	601	GEM	C10-C8-C9-O14
4	A	601	GEM	C9-C8-S7-C6
4	B	601	GEM	C9-C8-S7-C6
4	C	601	GEM	C9-C8-S7-C6
4	D	601	GEM	C9-C8-S7-C6
5	C	804	GOL	C1-C2-C3-O3
4	B	601	GEM	C10-C8-C9-O14

There are no ring outliers.

6 monomers are involved in 19 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	C	601	GEM	3	0
4	A	601	GEM	6	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	501	NAG	1	0
4	B	601	GEM	6	0
2	C	501	NAG	1	0
2	D	501	NAG	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 (i)

6.1 Protein, DNA and RNA chains (i)

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, 95th 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	383/435 (88%)	-0.00	5 (1%)	77	78	21, 43, 71, 98	0
1	B	386/435 (88%)	-0.05	4 (1%)	82	83	23, 42, 70, 94	0
1	C	385/435 (88%)	0.08	14 (3%)	42	42	21, 43, 71, 100	0
1	D	385/435 (88%)	0.03	11 (2%)	51	52	23, 43, 71, 120	0
All	All	1539/1740 (88%)	0.02	34 (2%)	62	63	21, 43, 71, 120	0

All (34) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	38	PRO	7.1
1	C	399	GLN	5.0
1	C	407	GLN	4.3
1	C	302	LEU	4.2
1	D	337	ILE	3.5
1	A	222	VAL	3.3
1	C	390	PHE	3.3
1	C	412	LEU	3.3
1	A	164	GLY	2.8
1	C	270	ASP	2.7
1	C	241	LEU	2.6
1	D	35	LEU	2.6
1	D	396	ALA	2.6
1	B	53	LEU	2.6
1	C	405	ASP	2.6
1	A	405	ASP	2.5
1	A	124	ARG	2.5
1	D	27	THR	2.5
1	D	365	PRO	2.4
1	D	381	GLY	2.4
1	B	374	TYR	2.3

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Mol	Chain	Res	Type	RSRZ
1	C	46	LEU	2.3
1	C	384	SER	2.3
1	C	237	CYS	2.3
1	D	168	ALA	2.2
1	D	152	GLN	2.2
1	C	320	GLU	2.2
1	C	278	ASN	2.2
1	B	97	ILE	2.2
1	D	412	LEU	2.1
1	B	59	ASN	2.1
1	A	53	LEU	2.1
1	D	72	GLY	2.1
1	D	416	LEU	2.0

6.2 Non-standard residues in protein, DNA, RNA chains (i)

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

6.3 Carbohydrates (i)

There are no monosaccharides in this entry.

6.4 Ligands (i)

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. The B-factors column lists the minimum, median, 95th 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	B-factors(Å^2)	Q<0.9
2	NAG	D	501	14/15	0.75	0.23	78,107,121,125	0
5	GOL	A	803	6/6	0.80	0.13	40,56,59,61	0
5	GOL	C	804	6/6	0.81	0.16	44,63,65,69	0
5	GOL	A	801	6/6	0.82	0.24	30,36,40,40	0
2	NAG	C	501	14/15	0.84	0.22	58,69,104,105	0
5	GOL	A	802	6/6	0.88	0.15	53,54,64,67	0
2	NAG	A	501	14/15	0.89	0.18	39,71,79,89	0
2	NAG	B	501	14/15	0.90	0.14	44,65,83,97	0
4	GEM	A	601	15/15	0.95	0.14	32,43,64,65	0
4	GEM	C	601	15/15	0.96	0.15	35,44,58,59	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
4	GEM	D	601	15/15	0.96	0.15	27,38,55,68	0
4	GEM	B	601	15/15	0.96	0.15	22,31,47,57	0
3	ZN	A	999	1/1	0.98	0.12	42,42,42,42	0
3	ZN	D	999	1/1	0.99	0.12	33,33,33,33	0
3	ZN	B	999	1/1	0.99	0.09	38,38,38,38	0
3	ZN	C	999	1/1	0.99	0.10	42,42,42,42	0

6.5 Other polymers (i)

There are no such residues in this entry.