W O R L D W I D E

wwPDB

P R O T E I N   D A T A   B A N K

Full wwPDB X-ray Structure Validation Report (i)

Jan 31, 2016 – 08:49 PM GMT

PDB ID	:	1M6B
Title	:	Structure of the HER3 (ERBB3) Extracellular Domain
Authors	:	Leahy, D.J.; Cho, H.-S.
Deposited on	:	2002-07-15
Resolution	:	2.60 Å(reported)

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

|		
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	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
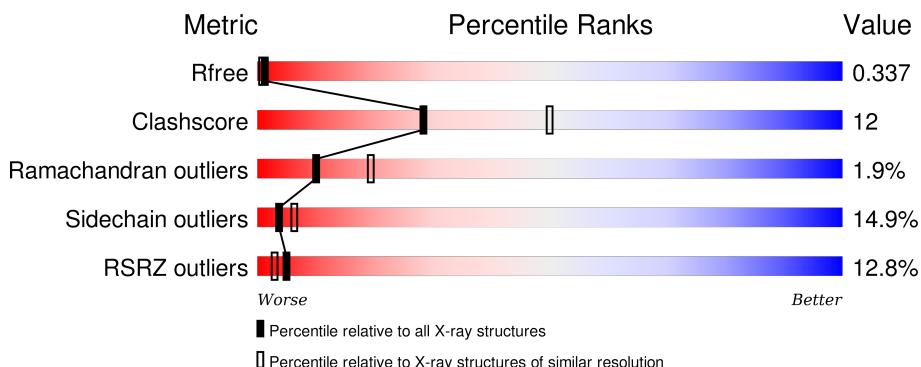
1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION
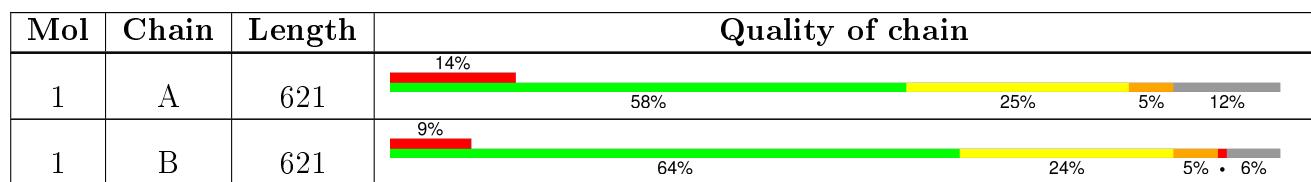
The reported resolution of this entry is 2.60 Å.

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	Percentile Ranks	Value
Rfree		0.337
Clashscore		12
Ramachandran outliers		1.9%
Sidechain outliers		14.9%
RSRZ outliers		12.8%

Worse　　　　*Better*

■ Percentile relative to all X-ray structures
▯ Percentile relative to X-ray structures of similar resolution

Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	91344	2328 (2.60-2.60)
Clashscore	102246	2679 (2.60-2.60)
Ramachandran outliers	100387	2635 (2.60-2.60)
Sidechain outliers	100360	2635 (2.60-2.60)
RSRZ outliers	91569	2334 (2.60-2.60)

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	621	14%　58%　25%　5%　12%
1	B	621	9%　64%　24%　5% · 6%

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
2	NAG	A	626	X	-	-	-
2	NAG	A	627	-	-	-	X
2	NAG	A	628	X	-	-	-
2	NAG	B	622	-	-	-	X
2	NAG	B	627	X	-	-	-
2	NAG	B	628	X	-	-	-
5	SO4	B	5001	-	-	X	X

2 Entry composition (i)

There are 6 unique types of molecules in this entry. The entry contains 9012 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.
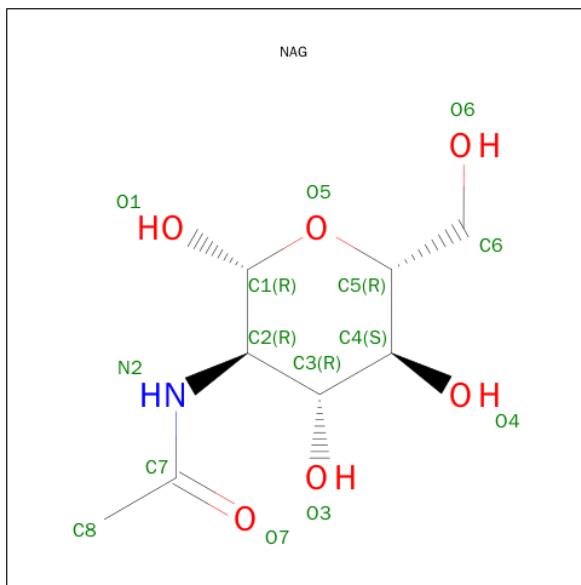
- Molecule 1 is a protein called Receptor protein-tyrosine kinase erbB-3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	549	Total	C	N	O	S	0	0	0
			4206	2603	765	784	54			
1	B	584	Total	C	N	O	S	0	0	0
			4478	2766	813	840	59			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	61	VAL	ILE	ENGINEERED	UNP P21860
B	61	VAL	ILE	ENGINEERED	UNP P21860

- Molecule 2 is SUGAR (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		

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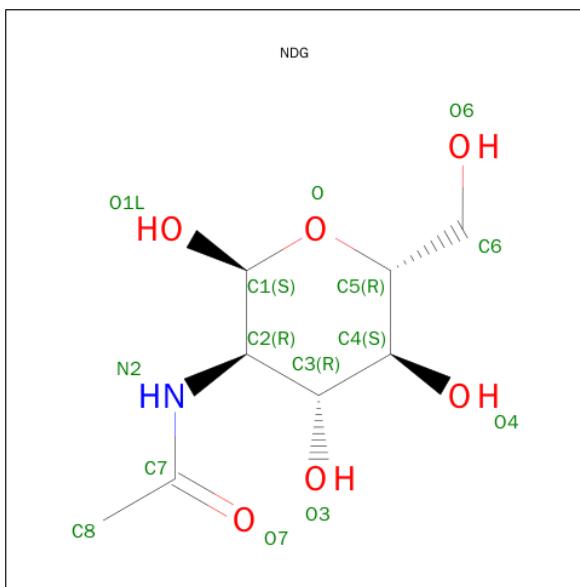
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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	N	O	0	0
			14	8	1	5		
2	A	1	Total	C	N	O	0	0
			14	8	1	5		
2	A	1	Total	C	N	O	0	0
			14	8	1	5		
2	A	1	Total	C	N	O	0	0
			14	8	1	5		
2	A	1	Total	C	N	O	0	0
			14	8	1	5		
2	A	1	Total	C	N	O	0	0
	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

- Molecule 3 is a polymer of unknown type called SUGAR (2-MER).
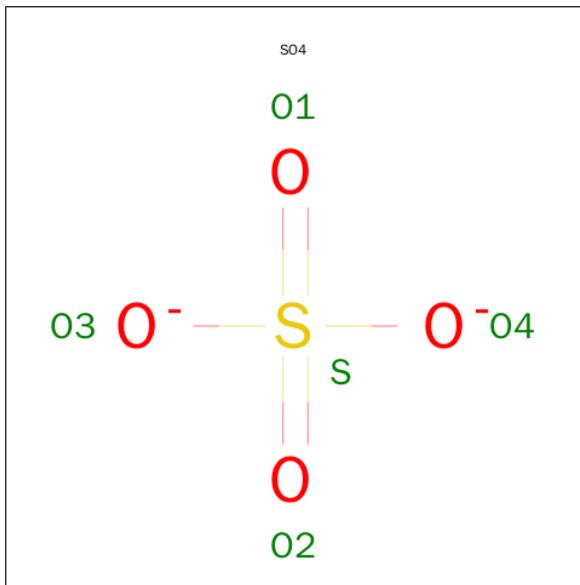
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	2	Total	C	N	O	0	0
			28	16	2	10		
3	B	2	Total	C	N	O	0	0
			28	16	2	10		

- Molecule 4 is SUGAR (2-(ACETYLAMINO)-2-DEOXY-A-D-GLUCOPYRANOSE) (three-letter code: NDG) (formula: $C_8H_{15}NO_6$).

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

• Molecule 5 is SULFATE ION (three-letter code: SO4) (formula: O_4S).

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	O	S		
5	B	1	5	4	1	0	0
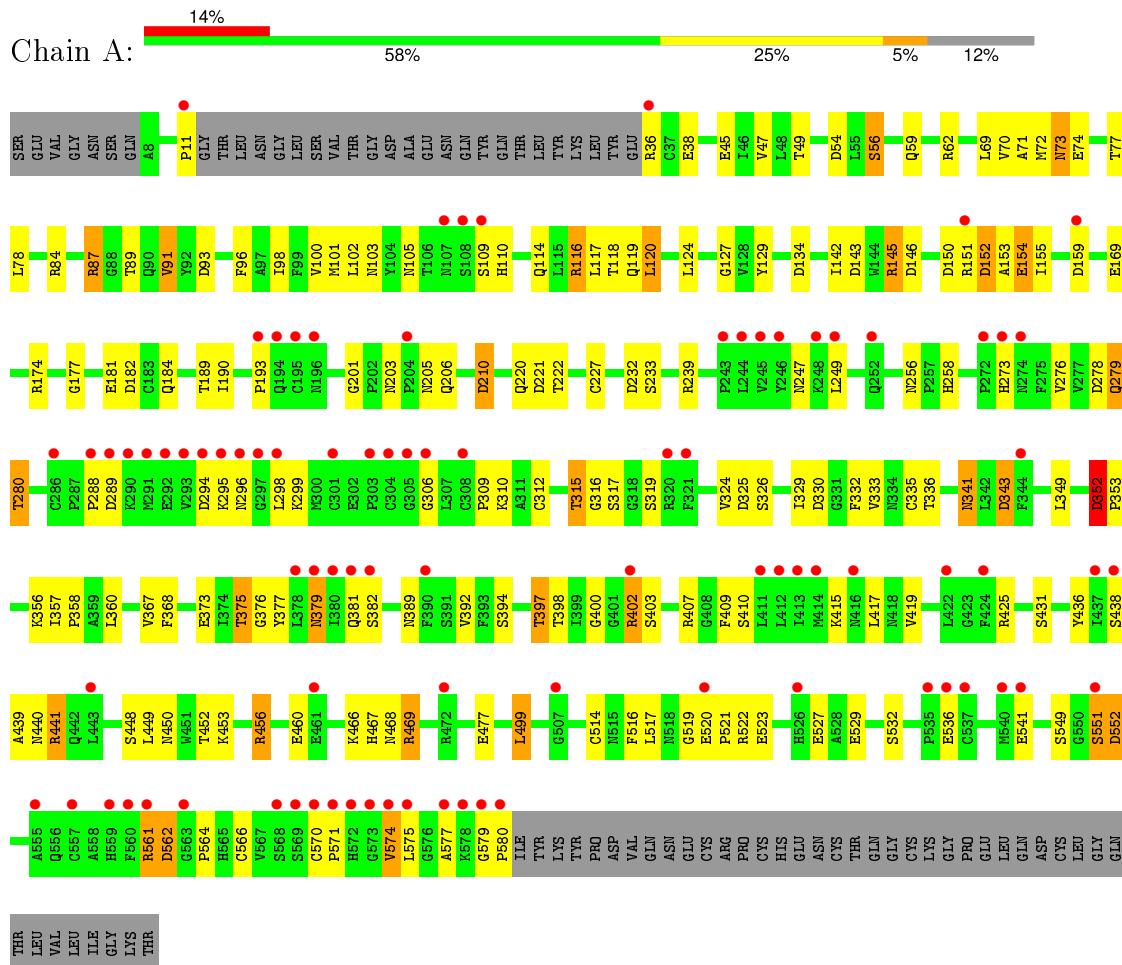
• Molecule 6 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	20	Total　O 20　　20	0	0
6	B	65	Total　O 65　　65	0	0
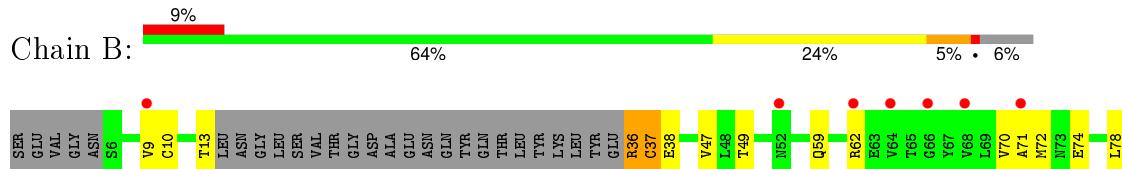
3 Residue-property plots ⓘ
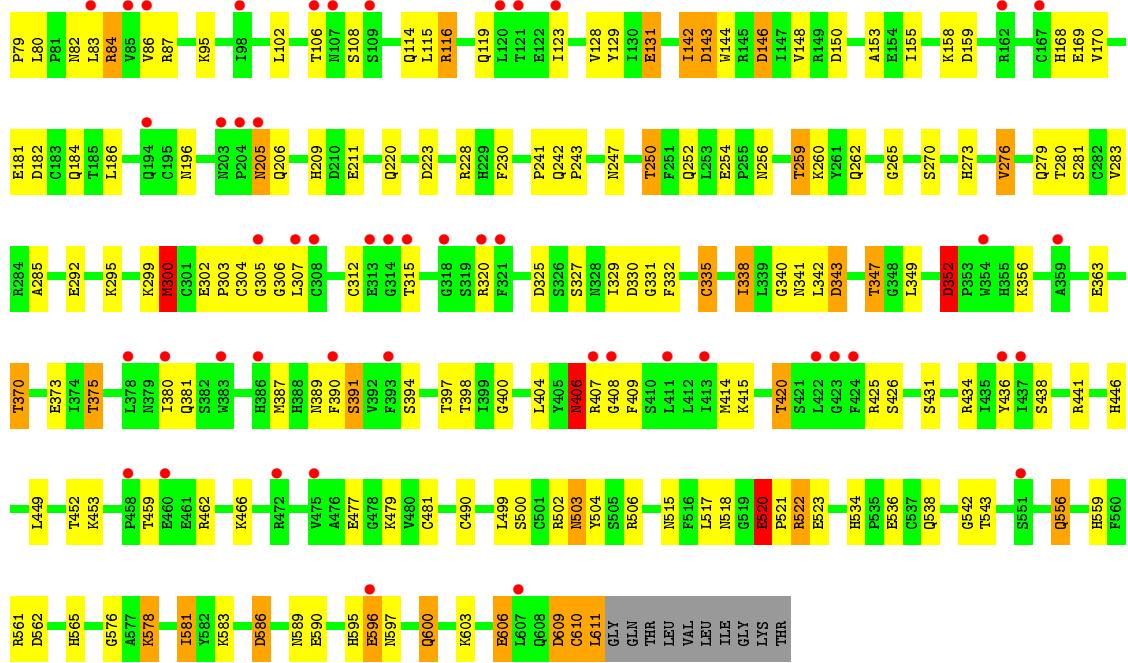
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according 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: Receptor protein-tyrosine kinase erbB-3

- Molecule 1: Receptor protein-tyrosine kinase erbB-3

4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α, β, γ	236.26Å 49.62Å 190.86Å 90.00° 125.56° 90.00°	Depositor
Resolution (Å)	20.00 – 2.60 28.74 – 2.60	Depositor EDS
% Data completeness (in resolution range)	94.5 (20.00-2.60) 90.7 (28.74-2.60)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.97 (at 2.61Å)	Xtriage
Refinement program	REFMAC 5.1.19	Depositor
R, R_{free}	0.235 , 0.294 0.299 , 0.337	Depositor DCC
R_{free} test set	2619 reflections (5.09%)	DCC
Wilson B-factor (Å^2)	48.1	Xtriage
Anisotropy	0.756	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.35 , 30.4	EDS
Estimated twinning fraction	0.000 for h,-k,-h-l	Xtriage
L-test for twinning[2]	$< |L| > = 0.50$, $< L^2 > = 0.33$	Xtriage
Outliers	1 of 54360 reflections (0.002%)	Xtriage
F_o,F_c correlation	0.87	EDS
Total number of atoms	9012	wwPDB-VP
Average B, all atoms (Å^2)	17.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.52% of the height of the origin peak. No significant pseudotranslation is detected.*

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[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 (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: NAG, NDG, 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	0.56	0/4308	0.84	15/5845 (0.3%)
1	B	0.62	1/4586 (0.0%)	0.86	8/6222 (0.1%)
All	All	0.59	1/8894 (0.0%)	0.85	23/12067 (0.2%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	300	MET	SD-CE	5.39	2.08	1.77

All (23) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	352	ASP	CB-CG-OD2	8.78	126.20	118.30
1	A	221	ASP	CB-CG-OD2	6.58	124.22	118.30
1	B	146	ASP	CB-CG-OD2	6.36	124.02	118.30
1	B	143	ASP	CB-CG-OD2	6.24	123.91	118.30
1	B	325	ASP	CB-CG-OD2	6.20	123.88	118.30
1	A	232	ASP	CB-CG-OD2	6.14	123.83	118.30
1	B	609	ASP	CB-CG-OD2	6.14	123.83	118.30
1	A	143	ASP	CB-CG-OD2	6.07	123.77	118.30
1	A	325	ASP	CB-CG-OD2	6.06	123.75	118.30
1	A	146	ASP	CB-CG-OD2	6.00	123.70	118.30
1	A	352	ASP	CB-CG-OD2	5.82	123.54	118.30
1	B	343	ASP	CB-CG-OD2	5.76	123.49	118.30
1	A	93	ASP	CB-CG-OD2	5.74	123.47	118.30
1	A	134	ASP	CB-CG-OD2	5.38	123.15	118.30
1	A	210	ASP	CB-CG-OD2	5.36	123.12	118.30
1	A	289	ASP	CB-CG-OD2	5.34	123.10	118.30
1	B	159	ASP	CB-CG-OD2	5.33	123.10	118.30
1	A	152	ASP	CB-CG-OD2	5.31	123.08	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	552	ASP	CB-CG-OD2	5.20	122.98	118.30
1	A	343	ASP	CB-CG-OD2	5.13	122.92	118.30
1	A	159	ASP	CB-CG-OD2	5.12	122.90	118.30
1	A	278	ASP	CB-CG-OD2	5.04	122.83	118.30
1	B	562	ASP	CB-CG-OD2	5.03	122.83	118.30

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	4206	0	3996	79	0
1	B	4478	0	4242	123	0
2	A	98	0	91	0	0
2	B	70	0	65	2	0
3	A	28	0	25	1	0
3	B	28	0	25	1	0
4	B	14	0	13	0	0
5	B	5	0	0	4	0
6	A	20	0	0	3	0
6	B	65	0	0	7	0
All	All	9012	0	8457	202	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 12.

All (202) 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:300:MET:SD	1:B:300:MET:CE	2.08	1.42
1:B:116:ARG:HG3	1:B:116:ARG:HH11	1.11	1.11
1:B:335:CYS:O	1:B:370:THR:HG22	1.56	1.03
1:B:452:THR:HG22	1:B:459:THR:HG21	1.42	1.00
1:B:578:LYS:H	1:B:578:LYS:HE2	1.31	0.96

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:247:ASN:ND2	6:B:1072:HOH:O	2.01	0.91
1:B:520:GLU:HB2	1:B:521:PRO:CD	2.00	0.90
1:B:452:THR:CG2	1:B:459:THR:HG21	2.03	0.87
1:B:168:HIS:HD2	1:B:170:VAL:HB	1.41	0.86
1:B:250:THR:HG21	1:B:254:GLU:OE2	1.75	0.86
1:B:534:HIS:HD2	1:B:536:GLU:H	1.26	0.84
1:A:330:ASP:O	1:A:333:VAL:HG23	1.77	0.83
1:A:145:ARG:HE	1:A:155:ILE:HD13	1.44	0.83
1:B:335:CYS:O	1:B:370:THR:CG2	2.28	0.82
1:B:436:TYR:CE2	1:B:438:SER:HB2	2.18	0.79
1:A:315:THR:HG21	1:A:343:ASP:HB2	1.65	0.79
1:B:452:THR:HG22	1:B:459:THR:CG2	2.12	0.78
1:A:469:ARG:NH2	1:A:477:GLU:OE2	2.16	0.76
1:A:551:SER:HB2	1:A:566:CYS:H	1.51	0.75
1:B:36:ARG:HD3	1:B:37:CYS:H	1.50	0.75
1:B:520:GLU:HB2	1:B:521:PRO:HD3	1.68	0.75
1:B:434:ARG:HG2	1:B:462:ARG:HB2	1.69	0.75
1:B:116:ARG:NH1	1:B:116:ARG:HG3	1.92	0.75
1:B:559:HIS:NE2	5:B:5001:SO4:O2	2.21	0.74
1:B:565:HIS:HD2	6:B:1058:HOH:O	1.72	0.73
1:A:87:ARG:HG2	1:A:124:LEU:HD12	1.69	0.73
1:A:456:ARG:HH11	1:A:456:ARG:HB2	1.54	0.72
1:B:534:HIS:CD2	1:B:536:GLU:H	2.08	0.72
1:B:420:THR:HG22	1:B:479:LYS:NZ	2.04	0.72
1:B:559:HIS:NE2	5:B:5001:SO4:O4	2.25	0.70
1:B:247:ASN:CG	6:B:1072:HOH:O	2.27	0.69
1:A:73:ASN:ND2	1:A:103:ASN:OD1	2.25	0.69
1:B:414:MET:O	1:B:415:LYS:HG2	1.92	0.68
1:B:243:PRO:HA	1:B:259:THR:HG23	1.77	0.67
1:B:315:THR:HG22	1:B:343:ASP:OD2	1.94	0.67
1:A:150:ASP:HB3	1:A:153:ALA:HB2	1.77	0.67
1:B:381:GLN:HG2	1:B:415:LYS:HE2	1.77	0.67
1:B:116:ARG:HH11	1:B:116:ARG:CG	1.97	0.66
1:B:586:ASP:HB2	1:B:590:GLU:H	1.60	0.66
1:B:534:HIS:CD2	1:B:536:GLU:HB2	2.32	0.65
1:B:209:HIS:HD2	1:B:211:GLU:H	1.41	0.65
1:A:375:THR:HA	1:A:402:ARG:HH11	1.61	0.65
1:B:520:GLU:CB	1:B:521:PRO:CD	2.74	0.64
1:B:520:GLU:HB2	1:B:521:PRO:HD2	1.77	0.64
1:B:150:ASP:HB3	1:B:153:ALA:HB2	1.80	0.64
1:B:420:THR:HG22	1:B:479:LYS:HZ3	1.63	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:552:ASP:HA	1:A:564:PRO:O	1.99	0.63
1:B:36:ARG:CB	1:B:36:ARG:HH11	2.12	0.62
1:B:559:HIS:NE2	5:B:5001:SO4:S	2.69	0.62
1:B:220:GLN:HB2	1:B:223:ASP:OD2	2.00	0.62
1:A:551:SER:HB2	1:A:566:CYS:N	2.15	0.61
1:A:70:VAL:HB	1:A:100:VAL:HG22	1.83	0.60
3:A:624:NAG:H81	6:A:1045:HOH:O	2.00	0.60
1:A:117:LEU:HD13	1:A:120:LEU:HD22	1.83	0.60
1:A:440:ASN:HD22	1:A:468:ASN:ND2	1.99	0.60
1:B:243:PRO:HA	1:B:259:THR:CG2	2.33	0.59
1:B:302:GLU:HG3	1:B:303:PRO:HD2	1.84	0.58
1:A:315:THR:CG2	1:A:343:ASP:HB2	2.34	0.58
1:A:440:ASN:H	1:A:468:ASN:HD22	1.52	0.58
1:B:578:LYS:N	1:B:578:LYS:HE2	2.11	0.58
1:A:436:TYR:CE2	1:A:438:SER:HB2	2.40	0.57
1:B:586:ASP:HB2	1:B:590:GLU:N	2.19	0.57
1:A:341:ASN:HD22	1:A:377:TYR:H	1.52	0.57
1:B:283:VAL:HG12	1:B:285:ALA:H	1.69	0.56
1:B:36:ARG:HD3	1:B:37:CYS:HB2	1.87	0.56
1:A:332:PHE:O	1:A:335:CYS:HB2	2.06	0.56
1:B:373:GLU:HG3	1:B:398:THR:HB	1.87	0.56
1:B:304:CYS:O	1:B:306:GLY:N	2.38	0.56
1:B:129:TYR:CE2	1:B:131:GLU:HB2	2.41	0.55
1:A:72:MET:HE1	1:A:102:LEU:HB2	1.87	0.55
1:B:114:GLN:OE1	1:B:116:ARG:HD3	2.07	0.55
1:B:606:GLU:HB2	1:B:609:ASP:OD2	2.06	0.55
1:B:241:PRO:HG2	1:B:260:LYS:HG3	1.89	0.55
1:A:256:ASN:HD21	1:A:258:HIS:HB2	1.72	0.55
1:B:565:HIS:CD2	6:B:1058:HOH:O	2.55	0.55
1:A:84:ARG:HD3	1:A:119:GLN:HG3	1.88	0.54
1:A:574:VAL:O	1:A:580:PRO:HA	2.07	0.54
1:A:466:LYS:HG3	1:A:467:HIS:CD2	2.42	0.54
1:B:520:GLU:CB	1:B:521:PRO:HD3	2.34	0.54
1:B:610:CYS:O	1:B:611:LEU:O	2.25	0.54
1:A:456:ARG:HB2	1:A:456:ARG:NH1	2.20	0.54
1:B:534:HIS:HD2	1:B:536:GLU:HB2	1.73	0.54
1:B:438:SER:OG	1:B:466:LYS:HG3	2.08	0.54
1:B:36:ARG:CD	1:B:37:CYS:H	2.19	0.53
1:B:36:ARG:HH11	1:B:36:ARG:HB2	1.73	0.53
1:A:397:THR:HG22	1:A:398:THR:OG1	2.09	0.53
1:A:87:ARG:NH2	1:A:227:CYS:O	2.27	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:425:ARG:NH1	6:A:1025:HOH:O	2.41	0.52
1:B:228:ARG:HG2	1:B:228:ARG:HH11	1.75	0.52
1:A:415:LYS:HA	1:A:439:ALA:O	2.10	0.52
1:B:262:GLN:HB2	1:B:281:SER:CB	2.40	0.52
1:B:400:GLY:O	1:B:431:SER:HB2	2.09	0.52
1:A:449:LEU:HD12	1:A:499:LEU:HD12	1.92	0.51
1:A:349:LEU:HD12	1:A:382:SER:OG	2.10	0.51
1:A:341:ASN:HD22	1:A:376:GLY:HA3	1.75	0.51
1:A:201:GLY:HA3	1:A:206:GLN:OE1	2.11	0.51
1:B:80:LEU:HD13	1:B:83:LEU:HD22	1.92	0.50
1:B:518:ASN:HA	1:B:522:ARG:CZ	2.40	0.50
1:B:146:ASP:OD1	1:B:186:LEU:HA	2.11	0.50
1:B:209:HIS:CD2	1:B:211:GLU:H	2.25	0.50
1:A:440:ASN:H	1:A:468:ASN:ND2	2.09	0.50
1:B:47:VAL:HA	1:B:71:ALA:O	2.12	0.50
1:A:519:GLY:O	1:A:522:ARG:HD3	2.12	0.50
1:A:222:THR:HG22	1:A:222:THR:O	2.12	0.50
1:B:168:HIS:CD2	1:B:170:VAL:HB	2.32	0.50
1:B:609:ASP:O	1:B:610:CYS:SG	2.70	0.50
1:A:54:ASP:OD1	1:A:56:SER:HB3	2.12	0.49
1:B:247:ASN:OD1	1:B:247:ASN:C	2.50	0.49
1:A:469:ARG:HD3	6:A:1022:HOH:O	2.11	0.49
1:B:330:ASP:C	1:B:332:PHE:H	2.16	0.49
1:B:243:PRO:HD2	6:B:1065:HOH:O	2.13	0.48
1:B:446:HIS:HA	6:B:1042:HOH:O	2.14	0.48
1:A:520:GLU:HB2	1:A:521:PRO:HD3	1.96	0.48
1:A:279:GLN:CG	1:A:280:THR:H	2.25	0.48
1:A:127:GLY:HA3	1:A:154:GLU:O	2.14	0.48
1:B:143:ASP:H	1:B:184:GLN:HE22	1.61	0.48
1:B:409:PHE:CE2	1:B:436:TYR:HB2	2.49	0.48
1:A:341:ASN:ND2	1:A:376:GLY:HA3	2.28	0.48
1:A:409:PHE:CD2	1:A:436:TYR:HB2	2.49	0.47
1:A:174:ARG:HB3	1:A:184:GLN:HB3	1.96	0.47
1:A:38:GLU:OE1	1:A:62:ARG:NH1	2.47	0.47
1:B:404:LEU:HD13	1:B:408:GLY:HA2	1.96	0.47
1:B:515:ASN:HB3	1:B:518:ASN:O	2.14	0.47
1:B:583:LYS:NZ	6:B:1069:HOH:O	2.47	0.47
1:A:450:ASN:ND2	1:A:453:LYS:HD2	2.29	0.47
1:B:409:PHE:CD2	1:B:436:TYR:HB2	2.49	0.47
1:B:397:THR:HA	1:B:426:SER:O	2.13	0.47
1:B:205:ASN:ND2	1:B:206:GLN:HG3	2.29	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:499:LEU:HA	1:B:499:LEU:HD23	1.78	0.46
1:B:78:LEU:HD23	1:B:115:LEU:HD22	1.98	0.46
1:A:373:GLU:HG3	1:A:398:THR:HB	1.97	0.46
1:A:379:ASN:HD21	1:A:381:GLN:HG3	1.81	0.46
1:A:394:SER:HB2	1:A:425:ARG:HD3	1.97	0.46
1:B:453:LYS:HE2	2:B:627:NAG:O6	2.15	0.46
1:A:72:MET:CE	1:A:102:LEU:HB2	2.46	0.46
1:B:406:ASN:HB3	1:B:407:ARG:H	1.49	0.46
1:A:449:LEU:CD1	1:A:499:LEU:HD12	2.46	0.45
1:B:506:ARG:HD3	1:B:523:GLU:OE1	2.16	0.45
1:A:368:PHE:HB2	1:A:392:VAL:CG1	2.46	0.45
1:B:595:HIS:C	1:B:597:ASN:H	2.19	0.45
1:A:376:GLY:HA2	1:A:403:SER:H	1.81	0.45
1:B:576:GLY:HA3	1:B:581:ILE:CD1	2.47	0.45
1:B:262:GLN:HB2	1:B:281:SER:HB3	1.99	0.45
1:B:205:ASN:HD22	1:B:206:GLN:HG3	1.81	0.45
1:B:380:ILE:HG21	1:B:390:PHE:CE2	2.51	0.45
1:B:420:THR:HG22	1:B:479:LYS:HZ1	1.81	0.45
1:A:309:PRO:HA	1:A:336:THR:OG1	2.17	0.45
1:B:230:PHE:HA	1:B:265:GLY:O	2.17	0.45
1:B:559:HIS:CD2	5:B:5001:SO4:O2	2.70	0.45
1:B:243:PRO:CA	1:B:259:THR:HG23	2.46	0.45
1:A:514:CYS:HB2	1:A:516:PHE:CE1	2.52	0.45
1:A:417:LEU:HD22	1:A:441:ARG:HG3	1.98	0.44
1:B:72:MET:CE	1:B:102:LEU:HB2	2.47	0.44
1:A:356:LYS:O	1:A:358:PRO:HD3	2.17	0.44
1:A:375:THR:HA	1:A:402:ARG:NH1	2.27	0.44
1:A:222:THR:CG2	1:A:222:THR:O	2.65	0.44
1:A:349:LEU:HD23	1:A:360:LEU:HD12	1.99	0.44
1:A:96:PHE:CD2	1:A:129:TYR:HB2	2.52	0.44
1:A:352:ASP:HA	1:A:353:PRO:HD3	1.76	0.44
1:A:74:GLU:HB3	1:A:110:HIS:HB3	2.00	0.44
1:B:59:GLN:O	1:B:82:ASN:ND2	2.39	0.44
1:B:116:ARG:NH1	1:B:116:ARG:CG	2.65	0.43
1:A:440:ASN:HD22	1:A:468:ASN:HD21	1.62	0.43
1:B:340:GLY:H	1:B:375:THR:HB	1.83	0.43
1:B:242:GLN:O	1:B:259:THR:HG23	2.17	0.43
1:B:128:VAL:HG21	1:B:144:TRP:CE3	2.54	0.43
1:A:400:GLY:HA3	1:A:402:ARG:CZ	2.48	0.43
1:B:589:ASN:HA	1:B:589:ASN:HD22	1.62	0.43
1:B:148:VAL:HG21	1:B:155:ILE:HD11	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:315:THR:CG2	1:A:316:GLY:N	2.82	0.43
1:A:71:ALA:C	1:A:72:MET:HG2	2.39	0.43
1:A:91:VAL:O	1:A:91:VAL:CG1	2.66	0.43
1:B:503:ASN:HB2	1:B:504:TYR:H	1.62	0.43
1:B:452:THR:OG1	2:B:627:NAG:H5	2.19	0.43
1:B:347:THR:HG22	1:B:352:ASP:HB2	2.00	0.43
1:A:45:GLU:HG2	1:A:69:LEU:HD23	2.00	0.42
1:A:169:GLU:OE2	1:B:62:ARG:NH2	2.53	0.42
1:A:47:VAL:HA	1:A:71:ALA:O	2.18	0.42
1:B:70:VAL:HG21	1:B:78:LEU:HD22	2.01	0.42
1:B:115:LEU:HA	1:B:115:LEU:HD23	1.81	0.42
1:A:579:GLY:HA2	1:A:580:PRO:HD2	1.87	0.42
1:B:262:GLN:HB2	1:B:281:SER:HB2	2.02	0.42
1:B:506:ARG:NH1	1:B:523:GLU:OE2	2.53	0.42
1:B:338:ILE:HD13	1:B:342:LEU:HD11	2.00	0.42
1:B:375:THR:O	1:B:400:GLY:HA3	2.20	0.42
1:B:143:ASP:N	1:B:184:GLN:HE22	2.17	0.41
1:B:538:GLN:HB3	1:B:556:GLN:HB3	2.01	0.41
1:B:256:ASN:O	1:B:259:THR:OG1	2.38	0.41
1:A:177:GLY:HA3	1:A:182:ASP:CB	2.51	0.41
1:B:517:LEU:HD13	1:B:542:GLY:O	2.20	0.41
1:B:389:ASN:OD1	1:B:391:SER:HB3	2.21	0.41
1:B:142:ILE:HG22	1:B:142:ILE:O	2.20	0.41
1:A:561:ARG:HG2	1:A:562:ASP:N	2.36	0.41
1:A:101:MET:CE	1:A:102:LEU:HD12	2.51	0.41
1:B:481:CYS:SG	1:B:490:CYS:N	2.93	0.41
1:B:387:MET:HA	3:B:624:NAG:O6	2.20	0.41
1:A:78:LEU:O	1:A:116:ARG:HB2	2.21	0.40
1:A:203:ASN:HB2	1:A:206:GLN:HG3	2.02	0.40
1:A:521:PRO:O	1:A:523:GLU:HG3	2.21	0.40
1:B:276:VAL:HG21	1:B:292:GLU:HG3	2.02	0.40
1:B:86:VAL:O	1:B:123:ILE:HA	2.21	0.40
1:B:84:ARG:NH2	1:B:119:GLN:HG3	2.36	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	545/621 (88%)	482 (88%)	52 (10%)	11 (2%)	9	18
1	B	580/621 (93%)	525 (90%)	45 (8%)	10 (2%)	11	22
All	All	1125/1242 (91%)	1007 (90%)	97 (9%)	21 (2%)	10	19

All (21) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	317	SER
1	A	460	GLU
1	B	520	GLU
1	B	586	ASP
1	A	296	ASN
1	B	305	GLY
1	B	596	GLU
1	B	600	GLN
1	B	610	CYS
1	A	279	GLN
1	A	577	ALA
1	A	120	LEU
1	A	193	PRO
1	A	288	PRO
1	B	279	GLN
1	B	406	ASN
1	A	306	GLY
1	A	571	PRO
1	B	331	GLY
1	A	574	VAL
1	B	79	PRO

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	474/537 (88%)	398 (84%)	76 (16%)	3	5
1	B	506/537 (94%)	436 (86%)	70 (14%)	4	7
All	All	980/1074 (91%)	834 (85%)	146 (15%)	4	6

All (146) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	11	PRO
1	A	36	ARG
1	A	49	THR
1	A	56	SER
1	A	59	GLN
1	A	73	ASN
1	A	77	THR
1	A	87	ARG
1	A	89	THR
1	A	91	VAL
1	A	98	ILE
1	A	105	ASN
1	A	109	SER
1	A	114	GLN
1	A	116	ARG
1	A	118	THR
1	A	142	ILE
1	A	145	ARG
1	A	151	ARG
1	A	152	ASP
1	A	154	GLU
1	A	181	GLU
1	A	189	THR
1	A	190	ILE
1	A	205	ASN
1	A	210	ASP
1	A	220	GLN

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Mol	Chain	Res	Type
1	A	233	SER
1	A	239	ARG
1	A	247	ASN
1	A	249	LEU
1	A	273	HIS
1	A	276	VAL
1	A	280	THR
1	A	294	ASP
1	A	295	LYS
1	A	298	LEU
1	A	299	LYS
1	A	310	LYS
1	A	312	CYS
1	A	315	THR
1	A	319	SER
1	A	324	VAL
1	A	326	SER
1	A	329	ILE
1	A	341	ASN
1	A	352	ASP
1	A	357	ILE
1	A	367	VAL
1	A	375	THR
1	A	379	ASN
1	A	389	ASN
1	A	397	THR
1	A	402	ARG
1	A	407	ARG
1	A	410	SER
1	A	419	VAL
1	A	431	SER
1	A	441	ARG
1	A	448	SER
1	A	452	THR
1	A	456	ARG
1	A	469	ARG
1	A	499	LEU
1	A	517	LEU
1	A	527	GLU
1	A	529	GLU
1	A	532	SER
1	A	536	GLU

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Mol	Chain	Res	Type
1	A	541	GLU
1	A	549	SER
1	A	551	SER
1	A	561	ARG
1	A	562	ASP
1	A	570	CYS
1	A	575	LEU
1	B	9	VAL
1	B	10	CYS
1	B	13	THR
1	B	36	ARG
1	B	37	CYS
1	B	38	GLU
1	B	49	THR
1	B	74	GLU
1	B	84	ARG
1	B	87	ARG
1	B	95	LYS
1	B	106	THR
1	B	108	SER
1	B	116	ARG
1	B	131	GLU
1	B	142	ILE
1	B	158	LYS
1	B	169	GLU
1	B	181	GLU
1	B	182	ASP
1	B	196	ASN
1	B	205	ASN
1	B	250	THR
1	B	252	GLN
1	B	259	THR
1	B	270	SER
1	B	273	HIS
1	B	276	VAL
1	B	280	THR
1	B	295	LYS
1	B	299	LYS
1	B	300	MET
1	B	307	LEU
1	B	312	CYS
1	B	320	ARG

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Mol	Chain	Res	Type
1	B	327	SER
1	B	329	ILE
1	B	335	CYS
1	B	338	ILE
1	B	341	ASN
1	B	347	THR
1	B	349	LEU
1	B	352	ASP
1	B	356	LYS
1	B	363	GLU
1	B	370	THR
1	B	375	THR
1	B	391	SER
1	B	394	SER
1	B	406	ASN
1	B	420	THR
1	B	425	ARG
1	B	441	ARG
1	B	449	LEU
1	B	477	GLU
1	B	500	SER
1	B	502	ARG
1	B	503	ASN
1	B	520	GLU
1	B	522	ARG
1	B	543	THR
1	B	556	GLN
1	B	561	ARG
1	B	578	LYS
1	B	581	ILE
1	B	596	GLU
1	B	600	GLN
1	B	603	LYS
1	B	606	GLU
1	B	611	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (21) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	138	HIS
1	A	198	HIS
1	A	247	ASN

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Mol	Chain	Res	Type
1	A	256	ASN
1	A	341	ASN
1	A	379	ASN
1	A	381	GLN
1	A	386	HIS
1	A	467	HIS
1	A	468	ASN
1	A	538	GLN
1	A	565	HIS
1	B	138	HIS
1	B	168	HIS
1	B	184	GLN
1	B	205	ASN
1	B	209	HIS
1	B	229	HIS
1	B	467	HIS
1	B	534	HIS
1	B	589	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)

4 carbohydrates are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#|Z| > 2$	Counts	RMSZ	$\#|Z| > 2$
3	NAG	A	624	1,3	14,14,15	0.80	0	15,19,21	1.67	4 (26%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	#|Z| > 2	Counts	RMSZ	#|Z| > 2
3	NAG	A	625	3	14,14,15	0.41	0	15,19,21	1.70	3 (20%)
3	NAG	B	624	1,3	14,14,15	0.43	0	15,19,21	1.31	1 (6%)
3	NAG	B	625	3	14,14,15	0.54	0	15,19,21	0.83	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the chemical component dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	NAG	A	624	1,3	-	0/6/23/26	0/1/1/1
3	NAG	A	625	3	-	0/6/23/26	0/1/1/1
3	NAG	B	624	1,3	-	0/6/23/26	0/1/1/1
3	NAG	B	625	3	-	0/6/23/26	0/1/1/1

There are no bond length outliers.

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	A	624	NAG	C2-N2-C7	-3.35	118.73	123.04
3	A	624	NAG	C3-C2-N2	-2.60	104.33	110.56
3	A	625	NAG	C3-C4-C5	-2.23	106.31	110.20
3	A	624	NAG	O3-C3-C2	-2.01	105.13	109.11
3	A	624	NAG	C4-C3-C2	2.11	114.51	111.23
3	A	625	NAG	C2-N2-C7	2.61	126.39	123.04
3	B	624	NAG	C1-O5-C5	3.56	116.77	112.25
3	A	625	NAG	C1-O5-C5	4.26	117.66	112.25

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	624	NAG	1	0
3	B	624	NAG	1	0

5.6 Ligand geometry (i)

14 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	622	1	14,14,15	0.41	0	15,19,21	2.44	2 (13%)
2	NAG	A	623	1	14,14,15	0.68	0	15,19,21	1.13	2 (13%)
2	NAG	A	626	1	14,14,15	0.60	0	15,19,21	0.99	1 (6%)
2	NAG	A	627	1	14,14,15	0.62	0	15,19,21	1.40	2 (13%)
2	NAG	A	628	1	14,14,15	0.72	0	15,19,21	1.22	3 (20%)
2	NAG	A	629	1	14,14,15	0.80	1 (7%)	15,19,21	1.67	3 (20%)
2	NAG	A	630	1	14,14,15	0.66	0	15,19,21	1.76	2 (13%)
5	SO4	B	5001	-	4,4,4	0.36	0	6,6,6	0.28	0
2	NAG	B	622	1	14,14,15	0.64	0	15,19,21	3.32	6 (40%)
2	NAG	B	623	1	14,14,15	0.68	0	15,19,21	1.61	4 (26%)
4	NDG	B	626	1	14,14,15	0.68	0	15,19,21	1.96	5 (33%)
2	NAG	B	627	1	14,14,15	0.55	0	15,19,21	1.26	1 (6%)
2	NAG	B	628	1	14,14,15	0.66	0	15,19,21	1.81	1 (6%)
2	NAG	B	629	1	14,14,15	1.04	1 (7%)	15,19,21	1.49	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	622	1	-	0/6/23/26	0/1/1/1
2	NAG	A	623	1	-	0/6/23/26	0/1/1/1
2	NAG	A	626	1	1/1/5/7	0/6/23/26	0/1/1/1
2	NAG	A	627	1	-	0/6/23/26	0/1/1/1
2	NAG	A	628	1	1/1/5/7	0/6/23/26	0/1/1/1
2	NAG	A	629	1	-	0/6/23/26	0/1/1/1
2	NAG	A	630	1	-	0/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	SO4	B	5001	-	-	0/0/0/0	0/0/0/0
2	NAG	B	622	1	-	0/6/23/26	0/1/1/1
2	NAG	B	623	1	-	0/6/23/26	0/1/1/1
4	NDG	B	626	1	-	0/6/23/26	0/1/1/1
2	NAG	B	627	1	1/1/5/7	0/6/23/26	0/1/1/1
2	NAG	B	628	1	1/1/5/7	0/6/23/26	0/1/1/1
2	NAG	B	629	1	-	1/6/23/26	0/1/1/1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	629	NAG	C1-C2	2.54	1.56	1.52
2	B	629	NAG	C1-C2	3.14	1.56	1.52

All (34) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	622	NAG	C2-N2-C7	-9.24	111.17	123.04
2	B	628	NAG	C2-N2-C7	-5.55	115.91	123.04
2	A	629	NAG	C2-N2-C7	-3.40	118.67	123.04
2	B	622	NAG	O7-C7-N2	-3.04	115.66	121.86
4	B	626	NDG	C4-C3-C2	-3.04	106.50	111.23
4	B	626	NDG	C3-C4-C5	-2.79	105.34	110.20
2	A	629	NAG	C3-C4-C5	-2.40	106.01	110.20
2	A	623	NAG	C2-N2-C7	-2.25	120.15	123.04
2	A	627	NAG	C2-N2-C7	-2.24	120.16	123.04
2	A	628	NAG	C2-N2-C7	-2.22	120.19	123.04
2	B	622	NAG	C6-C5-C4	-2.13	107.75	113.02
2	A	622	NAG	O4-C4-C5	2.15	114.93	109.24
2	B	623	NAG	C1-O5-C5	2.22	115.06	112.25
2	A	628	NAG	C1-O5-C5	2.30	115.16	112.25
2	B	623	NAG	C2-N2-C7	2.30	126.00	123.04
2	B	629	NAG	C2-N2-C7	2.33	126.03	123.04
2	A	630	NAG	C3-C4-C5	2.36	114.31	110.20
2	A	628	NAG	C4-C3-C2	2.39	114.94	111.23
2	B	623	NAG	C3-C4-C5	2.44	114.45	110.20
4	B	626	NDG	O3-C3-C2	2.54	114.14	109.11
2	A	626	NAG	C3-C4-C5	2.56	114.66	110.20
2	A	623	NAG	C4-C3-C2	2.62	115.30	111.23
2	A	627	NAG	C1-O5-C5	2.69	115.66	112.25
4	B	626	NDG	O-C5-C6	2.76	113.32	107.35
2	B	622	NAG	C3-C4-C5	2.94	115.31	110.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	623	NAG	C4-C3-C2	3.24	116.26	111.23
2	B	627	NAG	C1-O5-C5	3.55	116.76	112.25
2	B	622	NAG	C4-C3-C2	3.56	116.77	111.23
2	A	629	NAG	C1-O5-C5	3.76	117.02	112.25
2	B	629	NAG	C1-O5-C5	4.01	117.33	112.25
4	B	626	NDG	C1-O-C5	4.47	117.92	112.25
2	B	622	NAG	C1-O5-C5	5.92	119.76	112.25
2	A	630	NAG	C1-O5-C5	5.93	119.78	112.25
2	A	622	NAG	C1-O5-C5	8.42	122.93	112.25

All (4) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
2	A	626	NAG	C1
2	B	627	NAG	C1
2	B	628	NAG	C1
2	A	628	NAG	C1

All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	B	629	NAG	O7-C7-N2-C2

There are no ring outliers.

2 monomers are involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	B	5001	SO4	4	0
2	B	627	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	549/621 (88%)	0.95	89 (16%)	3	1	4, 13, 23, 57	0
1	B	584/621 (94%)	0.74	56 (9%)	10	6	6, 17, 28, 66	0
All	All	1133/1242 (91%)	0.84	145 (12%)	5	3	4, 15, 26, 66	0

All (145) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	248	LYS	6.3
1	A	297	GLY	5.9
1	A	578	LYS	5.9
1	A	109	SER	5.9
1	A	296	ASN	5.9
1	A	574	VAL	5.9
1	A	580	PRO	5.4
1	A	561	ARG	5.3
1	A	569	SER	5.1
1	A	560	PHE	5.1
1	A	413	ILE	5.0
1	A	193	PRO	4.9
1	B	52	ASN	4.9
1	B	320	ARG	4.8
1	A	572	HIS	4.8
1	A	298	LEU	4.5
1	A	294	ASP	4.5
1	A	108	SER	4.3
1	A	568	SER	4.3
1	A	245	VAL	4.3
1	A	196	ASN	4.2
1	A	304	CYS	4.1
1	B	607	LEU	4.1
1	A	411	LEU	4.1

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Mol	Chain	Res	Type	RSRZ
1	A	305	GLY	4.1
1	A	273	HIS	4.0
1	A	557	CYS	4.0
1	B	422	LEU	3.9
1	B	390	PHE	3.7
1	A	540	MET	3.7
1	A	461	GLU	3.7
1	A	577	ALA	3.7
1	A	412	LEU	3.6
1	A	303	PRO	3.6
1	B	380	ILE	3.6
1	B	204	PRO	3.6
1	A	380	ILE	3.5
1	A	293	VAL	3.5
1	A	107	ASN	3.5
1	B	424	PHE	3.4
1	A	520	GLU	3.4
1	A	535	PRO	3.4
1	B	120	LEU	3.4
1	B	194	GLN	3.4
1	A	244	LEU	3.4
1	A	194	GLN	3.4
1	A	36	ARG	3.4
1	B	354	TRP	3.3
1	A	246	TYR	3.3
1	B	413	ILE	3.3
1	A	402	ARG	3.2
1	B	460	GLU	3.2
1	B	407	ARG	3.2
1	A	437	ILE	3.1
1	A	306	GLY	3.1
1	A	291	MET	3.1
1	A	11	PRO	3.1
1	A	573	GLY	3.1
1	B	162	ARG	3.1
1	B	411	LEU	3.1
1	A	563	GLY	3.0
1	A	422	LEU	2.9
1	B	68	VAL	2.9
1	A	252	GLN	2.9
1	A	541	GLU	2.9
1	A	378	LEU	2.8

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Mol	Chain	Res	Type	RSRZ
1	A	414	MET	2.8
1	B	318	GLY	2.8
1	B	423	GLY	2.8
1	A	570	CYS	2.8
1	A	571	PRO	2.8
1	A	579	GLY	2.8
1	A	308	CYS	2.8
1	A	443	LEU	2.8
1	B	123	ILE	2.8
1	B	9	VAL	2.8
1	A	321	PHE	2.7
1	A	381	GLN	2.7
1	B	475	VAL	2.7
1	A	507	GLY	2.7
1	A	274	ASN	2.7
1	A	416	ASN	2.7
1	A	289	ASP	2.7
1	B	437	ILE	2.7
1	A	555	ALA	2.7
1	B	107	ASN	2.6
1	B	85	VAL	2.6
1	B	86	VAL	2.6
1	A	551	SER	2.6
1	B	64	VAL	2.6
1	B	121	THR	2.6
1	B	314	GLY	2.6
1	B	378	LEU	2.6
1	B	305	GLY	2.5
1	A	526	HIS	2.5
1	A	195	CYS	2.5
1	A	301	CYS	2.5
1	B	98	ILE	2.5
1	B	167	CYS	2.5
1	B	383	TRP	2.5
1	A	292	GLU	2.5
1	B	359	ALA	2.4
1	B	203	ASN	2.4
1	A	536	GLU	2.4
1	B	71	ALA	2.4
1	A	151	ARG	2.4
1	A	290	LYS	2.4
1	A	295	LYS	2.4

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Mol	Chain	Res	Type	RSRZ
1	A	382	SER	2.4
1	B	205	ASN	2.4
1	B	596	GLU	2.4
1	A	320	ARG	2.4
1	B	308	CYS	2.3
1	B	321	PHE	2.3
1	A	438	SER	2.3
1	A	249	LEU	2.3
1	A	344	PHE	2.3
1	A	390	PHE	2.2
1	B	458	PRO	2.2
1	B	83	LEU	2.2
1	B	62	ARG	2.2
1	B	393	PHE	2.2
1	B	307	LEU	2.2
1	A	272	PRO	2.2
1	B	109	SER	2.1
1	A	204	PRO	2.1
1	A	575	LEU	2.1
1	A	286	CYS	2.1
1	A	379	ASN	2.1
1	B	315	THR	2.1
1	A	537	CYS	2.1
1	A	243	PRO	2.1
1	A	159	ASP	2.1
1	A	288	PRO	2.1
1	A	472	ARG	2.1
1	B	472	ARG	2.1
1	B	436	TYR	2.1
1	B	66	GLY	2.0
1	B	551	SER	2.0
1	A	424	PHE	2.0
1	A	559	HIS	2.0
1	B	386	HIS	2.0
1	B	408	GLY	2.0
1	B	313	GLU	2.0
1	B	106	THR	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)

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, 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	LLDF	B-factors(Å^2)	Q<0.9
3	NAG	A	624	14/15	0.91	0.23	0.85	44,55,62,66	0
3	NAG	B	624	14/15	0.86	0.20	-0.51	53,65,68,75	0
3	NAG	B	625	14/15	0.77	0.40	-	82,87,89,90	0
3	NAG	A	625	14/15	0.85	0.22	-	73,78,80,81	0

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. 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, 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	LLDF	B-factors(Å^2)	Q<0.9
5	SO4	B	5001	5/5	0.89	0.27	2.78	86,87,88,89	0
2	NAG	A	627	14/15	0.84	0.28	2.40	58,68,70,72	0
2	NAG	B	622	14/15	0.67	0.36	2.25	46,59,64,64	0
4	NDG	B	626	14/15	0.85	0.31	1.41	64,73,80,81	0
2	NAG	A	629	14/15	0.78	0.21	1.22	58,70,74,74	0
2	NAG	B	628	14/15	0.91	0.25	1.04	53,62,65,65	0
2	NAG	B	629	14/15	0.71	0.23	0.59	63,72,75,77	0
2	NAG	A	622	14/15	0.89	0.20	0.23	42,49,52,54	0
2	NAG	B	627	14/15	0.85	0.18	-	59,69,73,74	0
2	NAG	A	623	14/15	0.72	0.21	-	65,75,77,79	0
2	NAG	B	623	14/15	0.68	0.19	-	65,76,78,79	0
2	NAG	A	630	14/15	0.78	0.35	-	67,76,79,80	0
2	NAG	A	626	14/15	0.83	0.28	-	62,74,79,81	0
2	NAG	A	628	14/15	0.89	0.23	-	63,71,75,76	0

6.5 Other polymers (i)

There are no such residues in this entry.