Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 02:23 AM GMT

PDB ID	:	2GY7
Title	:	Angiopoietin-2/Tie2 Complex Crystal Structure
Authors	:	Barton, W.A.; Nikolov, D.B.
Deposited on	:	2006-05-09
Resolution	:	3.70 Å(reported)

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

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

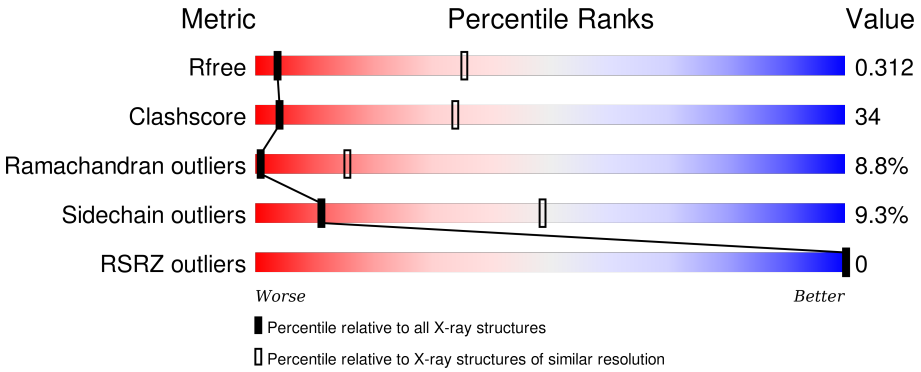
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	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 3.70 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	91344	1101 (3.90-3.50)
Clashscore	102246	1224 (3.90-3.50)
Ramachandran outliers	100387	1172 (3.90-3.50)
Sidechain outliers	100360	1170 (3.90-3.50)
RSRZ outliers	91569	1108 (3.90-3.50)

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	216	38% 52% 9%
2	B	423	43% 45% 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
3	NAG	B	1140	X	-	-	-

2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 5169 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 Angiopoietin-2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	216	1743	1103	294	335	11	0	0	0

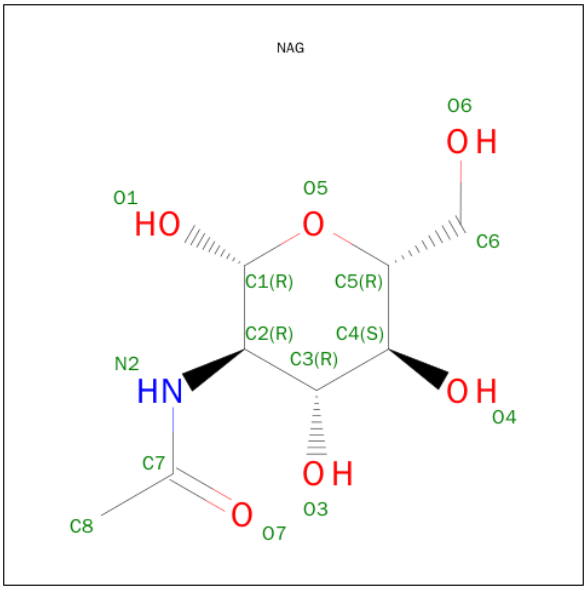
There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	280	GLU	-	CLONING ARTIFACT	UNP O15123

- Molecule 2 is a protein called Angiopoietin-1 receptor.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	B	423	3289	2063	583	604	39	0	0	0

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



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

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

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	B	4	Total	C	N	O	0	0
			56	32	4	20		

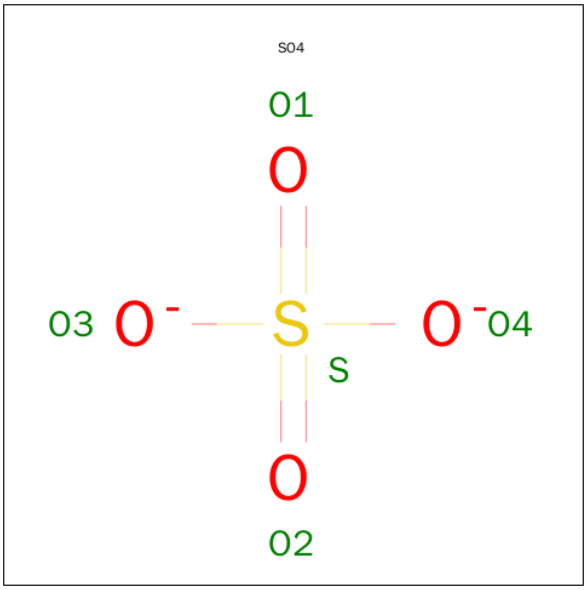
- Molecule 5 is a polymer of unknown type called SUGAR (2-MER).

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

- Molecule 6 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	1	Total	Ca	0	0
			1	1		

- Molecule 7 is SULFATE ION (three-letter code: SO4) (formula: O_4S).



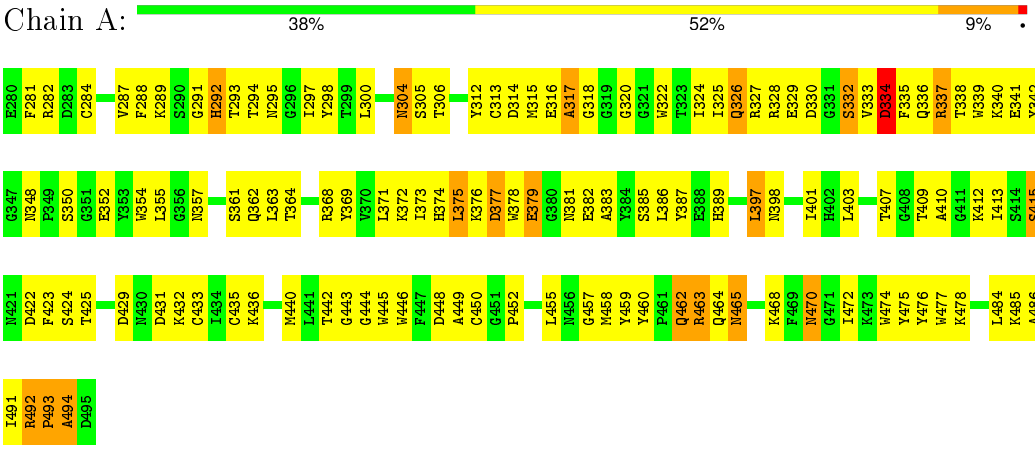
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	B	1	Total O S 5 4 1	0	0
7	B	1	Total O S 5 4 1	0	0

3 Residue-property plots (i)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density (RSRZ > 2). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

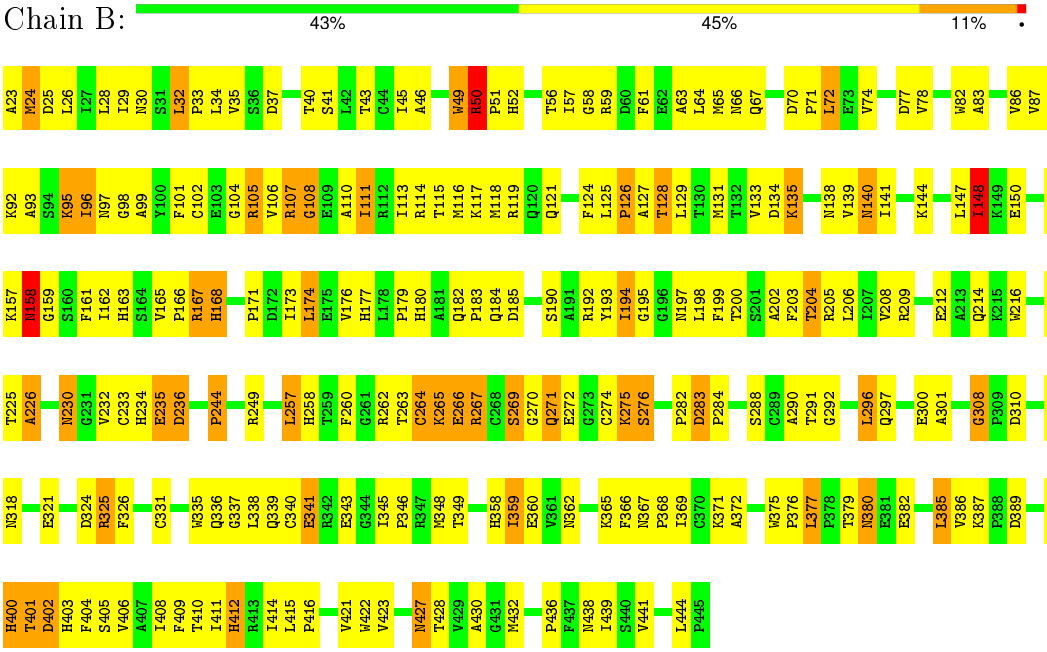
- Molecule 1: Angiopoietin-2

Chain A:



- Molecule 2: Angiopoietin-1 receptor

Chain B:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 41 21 2	Depositor
Cell constants a, b, c, α, β, γ	165.64Å 165.64Å 115.31Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	8.00 – 3.70 49.80 – 3.49	Depositor EDS
% Data completeness (in resolution range)	88.4 (8.00-3.70) 94.6 (49.80-3.49)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.33 (at 3.48Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.240 , 0.317 0.252 , 0.312	Depositor DCC
R_{free} test set	697 reflections (4.65%)	DCC
Wilson B-factor (Å^2)	39.2	Xtriage
Anisotropy	0.255	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.32 , 35.3	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.39$, $< L^2 > = 0.22$	Xtriage
Outliers	0 of 34173 reflections	Xtriage
F_o,F_c correlation	0.74	EDS
Total number of atoms	5169	wwPDB-VP
Average B, all atoms (Å^2)	6.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.95% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: CA, 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	0.46	0/1792	0.70	1/2419 (0.0%)
2	B	0.54	1/3372 (0.0%)	0.83	3/4571 (0.1%)
All	All	0.51	1/5164 (0.0%)	0.79	4/6990 (0.1%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
2	B	0	1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	158	ASN	C-N	-13.80	1.08	1.33

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	158	ASN	O-C-N	-16.48	95.18	123.20
2	B	158	ASN	CA-C-N	9.16	134.52	116.20
2	B	50	ARG	N-CA-C	-5.11	97.20	111.00
1	A	449	ALA	N-CA-C	-5.08	97.28	111.00

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	B	158	ASN	Mainchain

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	1743	0	1623	108	1
2	B	3289	0	3186	228	0
3	B	14	0	13	1	0
4	B	56	0	49	8	0
5	B	56	0	50	4	0
6	A	1	0	0	0	0
7	B	10	0	0	1	0
All	All	5169	0	4921	338	1

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 34.

All (338) 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)
2:B:158:ASN:HD22	4:B:1158:NAG:C1	1.08	1.59
2:B:438:ASN:HD21	5:B:1438:NAG:C1	1.45	1.20
1:A:418:GLN:HB3	1:A:419:PRO:HD2	1.17	1.09
4:B:1160:NAG:H5	4:B:1161:NDG:HA	1.08	1.08
1:A:328:ARG:HB2	1:A:487:THR:HB	1.37	1.06
4:B:1160:NAG:H5	4:B:1161:NDG:N2	1.90	0.86
1:A:418:GLN:CB	1:A:419:PRO:HD2	2.06	0.86
1:A:418:GLN:HB3	1:A:419:PRO:CD	2.05	0.85
2:B:64:LEU:HB3	2:B:67:GLN:HE21	1.40	0.84
2:B:158:ASN:HD22	4:B:1158:NAG:C2	1.89	0.84
1:A:432:LYS:HE2	1:A:432:LYS:HA	1.60	0.83
2:B:41:SER:HB3	2:B:87:VAL:HG12	1.60	0.83
2:B:397:ASP:HB3	2:B:408:ILE:HD11	1.60	0.83
2:B:234:HIS:ND1	2:B:284:PRO:HG2	1.93	0.82
2:B:106:VAL:HG12	2:B:107:ARG:H	1.45	0.82
2:B:64:LEU:HD22	2:B:98:GLY:HA2	1.63	0.81

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:376:LYS:HB2	1:A:486:ALA:HB3	1.63	0.81
2:B:95:LYS:HA	2:B:95:LYS:NZ	1.96	0.81
2:B:157:LYS:HB2	2:B:162:ILE:HD11	1.63	0.81
1:A:462:GLN:HG3	1:A:463:ARG:HD2	1.64	0.80
1:A:377:ASP:OD2	1:A:381:ASN:HB2	1.85	0.77
2:B:125:LEU:HD23	2:B:126:PRO:HD2	1.67	0.77
2:B:64:LEU:HB3	2:B:67:GLN:NE2	2.01	0.76
2:B:115:THR:HG22	2:B:116:MET:H	1.50	0.76
2:B:133:VAL:HG11	2:B:139:VAL:HG11	1.67	0.76
2:B:35:VAL:HG22	2:B:40:THR:HG21	1.68	0.75
1:A:295:ASN:ND2	1:A:316:GLU:HB2	2.02	0.75
2:B:158:ASN:ND2	4:B:1158:NAG:C2	2.46	0.74
2:B:158:ASN:ND2	4:B:1158:NAG:N2	2.35	0.74
2:B:414:ILE:HG12	2:B:441:VAL:HG21	1.71	0.73
2:B:194:ILE:HG23	2:B:195:GLY:H	1.54	0.73
2:B:153:ALA:HB3	2:B:165:VAL:HB	1.70	0.72
1:A:465:ASN:H	1:A:465:ASN:HD22	1.37	0.71
2:B:182:GLN:HB3	2:B:183:PRO:HD2	1.73	0.71
2:B:365:LYS:H	2:B:365:LYS:HD2	1.56	0.71
2:B:25:ASP:CG	2:B:262:ARG:HB2	2.11	0.70
2:B:223:LEU:H	2:B:223:LEU:HD23	1.57	0.69
1:A:369:TYR:HA	1:A:493:PRO:HA	1.74	0.68
2:B:372:ALA:O	2:B:404:PHE:HA	1.92	0.68
2:B:369:ILE:HG12	2:B:408:ILE:HG22	1.74	0.68
1:A:339:TRP:HZ3	1:A:423:PHE:O	1.76	0.68
2:B:335:TRP:CD2	2:B:343:GLU:HG2	2.28	0.68
2:B:35:VAL:HG21	2:B:96:ILE:HG13	1.73	0.68
2:B:30:ASN:HD22	2:B:115:THR:HG21	1.59	0.68
2:B:26:LEU:HD13	2:B:49:TRP:HZ2	1.58	0.68
1:A:433:CYS:C	1:A:435:CYS:H	1.97	0.68
1:A:328:ARG:HD3	1:A:335:PHE:CZ	2.29	0.67
1:A:374:HIS:NE2	1:A:376:LYS:HE2	2.10	0.67
2:B:371:LYS:HA	2:B:405:SER:O	1.95	0.66
1:A:363:LEU:HD13	1:A:363:LEU:O	1.95	0.66
2:B:34:LEU:H	2:B:297:GLN:HE22	1.44	0.66
2:B:267:ARG:HH11	2:B:267:ARG:HG3	1.60	0.65
2:B:366:PHE:CE2	2:B:368:PRO:HG3	2.30	0.65
2:B:232:VAL:HG12	2:B:233:CYS:N	2.11	0.65
2:B:49:TRP:O	2:B:51:PRO:HD3	1.97	0.65
1:A:325:ILE:HD11	1:A:491:ILE:CD1	2.26	0.65
2:B:50:ARG:HB2	2:B:82:TRP:CH2	2.31	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:386:VAL:CG2	2:B:423:VAL:HB	2.28	0.64
2:B:264:CYS:O	2:B:265:LYS:HG2	1.98	0.64
2:B:197:ASN:O	2:B:200:THR:HG22	1.96	0.64
2:B:56:THR:O	2:B:102:CYS:HB2	1.97	0.64
2:B:64:LEU:O	2:B:67:GLN:HG3	1.99	0.63
2:B:95:LYS:HE3	2:B:199:PHE:CD1	2.33	0.63
2:B:401:THR:HG23	2:B:403:HIS:O	1.97	0.63
2:B:400:HIS:ND1	2:B:401:THR:N	2.46	0.63
1:A:345:GLY:HA3	1:A:355:LEU:O	1.98	0.63
2:B:399:ASN:O	2:B:400:HIS:HB2	1.99	0.63
2:B:133:VAL:HG11	2:B:139:VAL:CG1	2.29	0.63
2:B:29:ILE:HB	2:B:43:THR:HB	1.81	0.63
2:B:138:ASN:HD22	2:B:180:HIS:H	1.46	0.62
2:B:438:ASN:HD21	5:B:1438:NAG:C2	2.11	0.61
2:B:119:ARG:NE	2:B:200:THR:HA	2.16	0.61
2:B:65:MET:HG2	2:B:158:ASN:O	2.00	0.61
1:A:326:GLN:HG2	1:A:489:MET:HG3	1.83	0.61
1:A:340:LYS:O	1:A:343:LYS:HB3	2.00	0.61
2:B:45:ILE:HA	2:B:83:ALA:HB2	1.82	0.60
2:B:225:THR:O	2:B:226:ALA:C	2.38	0.60
2:B:399:ASN:HB2	2:B:406:VAL:HB	1.83	0.60
2:B:288:SER:HB2	2:B:310:ASP:OD1	2.01	0.60
2:B:138:ASN:HA	2:B:179:PRO:HA	1.84	0.60
2:B:272:GLU:OE2	2:B:275:LYS:HD2	2.02	0.59
2:B:271:GLN:HG2	2:B:272:GLU:H	1.67	0.59
1:A:339:TRP:HA	1:A:425:THR:HG21	1.83	0.59
1:A:445:TRP:CZ3	1:A:455:LEU:HB2	2.37	0.59
1:A:368:ARG:HG3	1:A:389:HIS:CE1	2.36	0.59
1:A:387:TYR:CD1	1:A:403:LEU:HB3	2.37	0.59
2:B:375:TRP:C	2:B:377:LEU:H	2.04	0.59
1:A:373:ILE:HD12	1:A:474:TRP:CH2	2.38	0.59
2:B:95:LYS:HZ2	2:B:95:LYS:HA	1.65	0.59
2:B:438:ASN:HD22	5:B:1438:NAG:C1	2.07	0.58
2:B:95:LYS:HZ3	2:B:95:LYS:HA	1.67	0.58
5:B:1438:NAG:O3	5:B:1439:NAG:H2	2.02	0.58
2:B:25:ASP:OD1	2:B:262:ARG:HB2	2.03	0.58
2:B:336:GLN:HE21	2:B:346:PRO:HA	1.69	0.58
2:B:28:LEU:HD23	2:B:102:CYS:SG	2.44	0.57
2:B:57:ILE:HG22	2:B:58:GLY:N	2.19	0.57
2:B:67:GLN:HE22	2:B:99:ALA:H	1.52	0.57
4:B:1160:NAG:O3	4:B:1160:NAG:H83	2.05	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:328:ARG:O	1:A:486:ALA:HA	2.04	0.56
2:B:336:GLN:NE2	2:B:346:PRO:HA	2.19	0.56
2:B:161:PHE:CZ	2:B:163:HIS:HA	2.40	0.56
2:B:308:GLY:H	2:B:313:LEU:HB2	1.71	0.56
2:B:40:THR:HB	2:B:117:LYS:NZ	2.20	0.56
1:A:413:ILE:N	1:A:413:ILE:HD12	2.19	0.56
1:A:328:ARG:HD3	1:A:335:PHE:CE2	2.41	0.56
2:B:397:ASP:O	2:B:408:ILE:HG12	2.05	0.56
1:A:429:ASP:OD1	1:A:436:LYS:HG2	2.06	0.56
2:B:23:ALA:HB3	2:B:24:MET:SD	2.46	0.56
1:A:340:LYS:NZ	1:A:343:LYS:NZ	2.54	0.56
2:B:45:ILE:HG23	2:B:83:ALA:HB2	1.89	0.55
2:B:249:ARG:HG3	2:B:428:THR:O	2.05	0.55
2:B:97:ASN:OD1	2:B:118:MET:HA	2.06	0.55
2:B:124:PHE:HA	2:B:144:LYS:O	2.06	0.55
1:A:333:VAL:HG11	1:A:337:ARG:HH22	1.71	0.55
2:B:154:VAL:HG22	2:B:192:ARG:O	2.06	0.55
1:A:340:LYS:HZ2	1:A:343:LYS:NZ	2.05	0.55
2:B:64:LEU:CD2	2:B:98:GLY:HA2	2.34	0.54
1:A:325:ILE:HD11	1:A:491:ILE:HD13	1.88	0.54
2:B:126:PRO:HB2	2:B:128:THR:O	2.07	0.54
2:B:167:ARG:HD2	2:B:167:ARG:C	2.27	0.54
1:A:329:GLU:HG3	1:A:330:ASP:OD1	2.07	0.54
2:B:385:LEU:HB2	2:B:409:PHE:CE2	2.42	0.54
2:B:105:ARG:H	2:B:111:ILE:HG22	1.72	0.54
1:A:289:LYS:C	1:A:291:GLY:H	2.11	0.54
1:A:383:ALA:HB1	1:A:409:THR:OG1	2.08	0.54
1:A:433:CYS:C	1:A:435:CYS:N	2.61	0.54
1:A:314:ASP:OD2	1:A:317:ALA:HB2	2.08	0.54
2:B:275:LYS:HG2	2:B:275:LYS:O	2.08	0.54
2:B:50:ARG:NH2	2:B:421:VAL:HG23	2.23	0.53
2:B:385:LEU:HB2	2:B:409:PHE:CZ	2.44	0.53
2:B:111:ILE:O	2:B:111:ILE:HG23	2.07	0.53
2:B:301:ALA:HB1	2:B:325:ARG:CZ	2.39	0.52
2:B:67:GLN:NE2	2:B:99:ALA:H	2.08	0.52
2:B:106:VAL:HG12	2:B:107:ARG:N	2.20	0.52
2:B:40:THR:HB	2:B:117:LYS:HZ1	1.74	0.52
1:A:493:PRO:O	1:A:494:ALA:HB2	2.09	0.52
2:B:396:LYS:HD3	2:B:410:THR:HB	1.90	0.52
2:B:65:MET:HG2	2:B:159:GLY:HA3	1.92	0.52
2:B:367:ASN:HA	2:B:409:PHE:O	2.09	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:380:ASN:HD22	2:B:380:ASN:H	1.58	0.52
2:B:125:LEU:HD22	2:B:296:LEU:HD13	1.91	0.52
1:A:312:TYR:CD1	1:A:324:ILE:HD12	2.45	0.52
2:B:339:GLN:HB2	2:B:341:GLU:HG3	1.91	0.52
1:A:418:GLN:O	1:A:419:PRO:C	2.47	0.51
2:B:119:ARG:HE	2:B:200:THR:HA	1.75	0.51
1:A:354:TRP:O	1:A:355:LEU:HB3	2.10	0.51
2:B:110:ALA:O	2:B:111:ILE:HB	2.10	0.51
1:A:297:ILE:H	1:A:297:ILE:HD12	1.74	0.51
2:B:96:ILE:H	2:B:96:ILE:HD13	1.76	0.51
2:B:127:ALA:O	2:B:128:THR:HB	2.11	0.51
1:A:326:GLN:HG2	1:A:489:MET:HB2	1.92	0.51
2:B:267:ARG:HG3	2:B:267:ARG:NH1	2.26	0.51
2:B:116:MET:HG2	2:B:203:PHE:CB	2.41	0.51
1:A:377:ASP:HB3	1:A:477:TRP:CH2	2.46	0.51
2:B:118:MET:HE1	2:B:202:ALA:HB1	1.93	0.51
2:B:29:ILE:N	2:B:43:THR:O	2.41	0.50
2:B:65:MET:HG3	2:B:66:ASN:ND2	2.27	0.50
2:B:224:CYS:O	2:B:226:ALA:N	2.44	0.50
2:B:134:ASP:HB3	2:B:212:GLU:HA	1.94	0.50
2:B:33:PRO:HG3	2:B:129:LEU:HD11	1.93	0.50
1:A:298:TYR:HD2	1:A:313:CYS:SG	2.34	0.50
2:B:162:ILE:HG22	2:B:163:HIS:ND1	2.26	0.50
1:A:332:SER:HB2	1:A:352:GLU:CD	2.32	0.50
2:B:216:TRP:HB2	2:B:235:GLU:HA	1.92	0.50
2:B:126:PRO:HB3	2:B:203:PHE:O	2.12	0.49
2:B:49:TRP:HD1	2:B:49:TRP:H	1.60	0.49
2:B:209:ARG:HB2	2:B:235:GLU:HG2	1.93	0.49
2:B:193:TYR:O	2:B:194:ILE:C	2.50	0.49
1:A:338:THR:HG23	1:A:341:GLU:OE1	2.13	0.49
1:A:424:SER:O	1:A:444:GLY:HA2	2.12	0.49
1:A:452:PRO:HG3	2:B:166:PRO:HB3	1.94	0.49
2:B:376:PRO:HG2	2:B:430:ALA:HB2	1.94	0.49
1:A:281:PHE:O	1:A:300:LEU:HA	2.11	0.49
2:B:46:ALA:HB1	2:B:49:TRP:NE1	2.28	0.49
2:B:32:LEU:HD13	2:B:297:GLN:OE1	2.12	0.49
1:A:377:ASP:HB3	1:A:477:TRP:CZ3	2.48	0.49
1:A:330:ASP:HA	1:A:459:TYR:CZ	2.48	0.48
2:B:359:ILE:HB	2:B:439:ILE:HA	1.94	0.48
2:B:148:ILE:HA	2:B:193:TYR:OH	2.13	0.48
2:B:98:GLY:O	2:B:116:MET:HG3	2.13	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:116:MET:HG2	2:B:203:PHE:HB3	1.95	0.48
2:B:155:ILE:HD11	2:B:174:LEU:HD22	1.96	0.48
2:B:116:MET:HE3	2:B:205:ARG:N	2.28	0.48
2:B:88:TRP:CD1	2:B:96:ILE:HG22	2.49	0.48
2:B:135:LYS:HE3	2:B:182:GLN:OE1	2.13	0.48
2:B:216:TRP:CB	2:B:235:GLU:HA	2.44	0.48
1:A:305:SER:OG	1:A:306:THR:N	2.47	0.48
1:A:340:LYS:NZ	1:A:343:LYS:HZ3	2.12	0.48
1:A:386:LEU:HB3	1:A:407:THR:OG1	2.14	0.48
1:A:348:ASN:ND2	1:A:350:SER:OG	2.47	0.48
1:A:487:THR:HG22	1:A:487:THR:O	2.13	0.48
1:A:465:ASN:N	1:A:465:ASN:HD22	2.10	0.48
2:B:362:ASN:HB3	2:B:444:LEU:HG	1.94	0.48
2:B:41:SER:HA	2:B:86:VAL:O	2.14	0.48
2:B:194:ILE:HG23	2:B:195:GLY:N	2.27	0.47
2:B:193:TYR:HB2	7:B:4:SO4:O2	2.14	0.47
2:B:359:ILE:O	2:B:360:GLU:HB2	2.14	0.47
1:A:315:MET:O	1:A:320:GLY:HA2	2.15	0.47
1:A:385:SER:OG	1:A:410:ALA:HB3	2.15	0.47
2:B:34:LEU:HB2	2:B:297:GLN:CD	2.34	0.47
2:B:167:ARG:HD2	2:B:167:ARG:O	2.14	0.47
2:B:106:VAL:O	2:B:107:ARG:C	2.52	0.47
2:B:97:ASN:HA	2:B:117:LYS:O	2.14	0.47
2:B:335:TRP:CE2	2:B:343:GLU:HG2	2.50	0.47
2:B:427:ASN:ND2	2:B:432:MET:HB2	2.30	0.47
1:A:335:PHE:HB3	1:A:342:TYR:OH	2.14	0.47
2:B:95:LYS:HE3	2:B:199:PHE:CE1	2.50	0.47
2:B:45:ILE:HA	2:B:83:ALA:CB	2.44	0.47
2:B:375:TRP:C	2:B:377:LEU:N	2.64	0.47
2:B:65:MET:O	2:B:66:ASN:HB2	2.15	0.47
2:B:232:VAL:HG12	2:B:233:CYS:H	1.79	0.47
1:A:401:ILE:HB	1:A:446:TRP:NE1	2.29	0.47
2:B:77:ASP:OD2	2:B:78:VAL:N	2.48	0.47
2:B:232:VAL:CG1	2:B:233:CYS:N	2.77	0.47
2:B:375:TRP:HB3	2:B:376:PRO:HD3	1.96	0.46
2:B:274:CYS:O	2:B:276:SER:N	2.39	0.46
2:B:301:ALA:HB1	2:B:325:ARG:NH1	2.31	0.46
2:B:162:ILE:CG2	2:B:163:HIS:ND1	2.79	0.46
1:A:378:TRP:CZ2	1:A:485:LYS:HG3	2.51	0.46
2:B:90:ARG:C	2:B:92:LYS:H	2.19	0.46
2:B:260:PHE:O	2:B:266:GLU:HB2	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:74:VAL:HG22	2:B:86:VAL:HG22	1.98	0.46
2:B:141:ILE:HB	2:B:176:VAL:HB	1.97	0.46
1:A:492:ARG:CG	1:A:493:PRO:N	2.78	0.46
1:A:341:GLU:HB3	1:A:346:PHE:HD1	1.80	0.46
2:B:173:ILE:HG13	2:B:173:ILE:O	2.14	0.46
2:B:101:PHE:HA	2:B:113:ILE:O	2.15	0.46
1:A:328:ARG:HH21	1:A:457:GLY:H	1.64	0.46
2:B:183:PRO:HA	2:B:208:VAL:HB	1.96	0.46
1:A:369:TYR:O	1:A:389:HIS:HA	2.15	0.46
2:B:33:PRO:CB	2:B:129:LEU:HD21	2.45	0.46
2:B:257:LEU:HD22	2:B:258:HIS:CD2	2.51	0.46
2:B:95:LYS:HE3	2:B:199:PHE:HD1	1.79	0.46
1:A:378:TRP:HB3	1:A:462:GLN:OE1	2.16	0.46
2:B:183:PRO:C	2:B:185:ASP:H	2.17	0.46
2:B:106:VAL:O	2:B:108:GLY:N	2.49	0.45
1:A:297:ILE:HD12	1:A:297:ILE:N	2.31	0.45
2:B:358:HIS:O	2:B:359:ILE:HG12	2.17	0.45
2:B:72:LEU:H	2:B:72:LEU:HD23	1.80	0.45
2:B:126:PRO:HB3	2:B:204:THR:HB	1.98	0.45
2:B:156:TYR:HB2	2:B:190:SER:HB2	1.98	0.45
1:A:398:ASN:HB2	1:A:422:ASP:HB3	1.98	0.45
2:B:155:ILE:HG22	2:B:162:ILE:HD12	1.98	0.45
2:B:32:LEU:HD22	2:B:297:GLN:HA	1.99	0.45
1:A:314:ASP:CG	1:A:317:ALA:HB2	2.37	0.45
1:A:472:ILE:HG22	1:A:484:LEU:HD12	1.99	0.45
2:B:29:ILE:CD1	2:B:45:ILE:HD11	2.46	0.45
2:B:167:ARG:NH2	2:B:168:HIS:ND1	2.64	0.45
1:A:304:ASN:HA	1:A:304:ASN:HD22	1.62	0.45
2:B:34:LEU:HD23	2:B:118:MET:HG3	1.97	0.45
2:B:244:PRO:HG2	2:B:290:ALA:HA	1.98	0.45
1:A:287:VAL:O	1:A:292:HIS:HB2	2.17	0.45
2:B:125:LEU:HA	2:B:126:PRO:HD2	1.73	0.44
1:A:401:ILE:O	1:A:420:GLY:HA3	2.16	0.44
2:B:114:ARG:HD2	2:B:205:ARG:NH2	2.32	0.44
2:B:34:LEU:HD12	2:B:297:GLN:HG2	1.99	0.44
2:B:348:MET:HG3	2:B:375:TRP:H	1.82	0.44
2:B:23:ALA:HB3	2:B:24:MET:CE	2.47	0.44
2:B:96:ILE:O	2:B:117:LYS:HB3	2.17	0.44
2:B:415:LEU:HB3	2:B:416:PRO:HD2	1.99	0.44
2:B:127:ALA:O	2:B:128:THR:CB	2.66	0.44
2:B:198:LEU:O	2:B:199:PHE:HD2	2.01	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:193:TYR:O	2:B:195:GLY:N	2.50	0.44
2:B:321:GLU:HG2	2:B:331:CYS:HA	1.99	0.44
2:B:56:THR:HG22	2:B:57:ILE:N	2.32	0.44
1:A:412:LYS:C	1:A:413:ILE:HD12	2.38	0.44
2:B:140:ASN:CG	3:B:1140:NAG:C1	2.84	0.44
2:B:399:ASN:HB3	2:B:400:HIS:H	1.69	0.44
1:A:325:ILE:O	1:A:325:ILE:HG22	2.17	0.44
2:B:59:ARG:HH11	2:B:59:ARG:HG3	1.81	0.44
2:B:158:ASN:HD21	4:B:1158:NAG:C7	2.31	0.43
1:A:295:ASN:HB2	1:A:316:GLU:OE2	2.17	0.43
2:B:163:HIS:ND1	2:B:163:HIS:N	2.67	0.43
1:A:314:ASP:HB3	1:A:322:TRP:HB2	2.00	0.43
2:B:292:GLY:HA2	2:B:325:ARG:O	2.18	0.43
2:B:300:GLU:HG2	2:B:301:ALA:O	2.17	0.43
2:B:212:GLU:OE1	2:B:212:GLU:N	2.52	0.43
1:A:477:TRP:CE3	1:A:478:LYS:HG2	2.54	0.43
2:B:263:THR:O	2:B:264:CYS:HB2	2.19	0.43
2:B:52:HIS:CE1	2:B:389:ASP:HA	2.53	0.43
2:B:140:ASN:HD21	2:B:177:HIS:CD2	2.37	0.43
1:A:336:GLN:HG2	1:A:443:GLY:H	1.84	0.43
1:A:376:LYS:HG2	1:A:382:GLU:HB3	2.00	0.43
2:B:230:ASN:HB2	2:B:313:LEU:HD21	2.00	0.43
2:B:126:PRO:O	2:B:127:ALA:HB3	2.19	0.42
2:B:34:LEU:HB2	2:B:297:GLN:NE2	2.33	0.42
2:B:57:ILE:CG2	2:B:58:GLY:N	2.82	0.42
2:B:234:HIS:NE2	2:B:236:ASP:HB2	2.34	0.42
1:A:368:ARG:HE	1:A:389:HIS:CG	2.38	0.42
1:A:292:HIS:O	1:A:294:THR:N	2.51	0.42
2:B:379:THR:O	2:B:382:GLU:N	2.52	0.42
1:A:412:LYS:HB2	1:A:413:ILE:HD12	2.02	0.42
2:B:422:TRP:CE2	2:B:439:ILE:HD12	2.55	0.42
2:B:249:ARG:HD2	2:B:382:GLU:HG2	2.01	0.42
2:B:380:ASN:HD22	2:B:380:ASN:N	2.16	0.42
1:A:375:LEU:HD22	1:A:484:LEU:HD13	2.00	0.42
2:B:29:ILE:HD12	2:B:45:ILE:HD11	2.00	0.42
2:B:339:GLN:O	2:B:340:CYS:HB2	2.20	0.42
1:A:375:LEU:HD22	1:A:484:LEU:CD1	2.50	0.42
2:B:72:LEU:HD12	2:B:86:VAL:HG11	2.01	0.41
2:B:167:ARG:CD	2:B:167:ARG:C	2.89	0.41
1:A:288:PHE:O	1:A:291:GLY:N	2.53	0.41
2:B:257:LEU:O	2:B:258:HIS:HB2	2.19	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:70:ASP:HA	2:B:71:PRO:HD3	1.93	0.41
2:B:403:HIS:O	2:B:404:PHE:CB	2.69	0.41
2:B:402:ASP:HB2	2:B:403:HIS:ND1	2.34	0.41
1:A:334:ASP:O	1:A:337:ARG:NH1	2.53	0.41
1:A:460:TYR:CZ	1:A:468:LYS:HD2	2.55	0.41
1:A:326:GLN:HG2	1:A:489:MET:CG	2.51	0.41
1:A:340:LYS:HZ2	1:A:343:LYS:HZ2	1.67	0.41
1:A:460:TYR:CE2	1:A:468:LYS:HD2	2.55	0.41
1:A:415:SER:OG	1:A:474:TRP:CE2	2.63	0.41
1:A:357:ASN:O	1:A:361:SER:N	2.53	0.41
1:A:376:LYS:HB2	1:A:486:ALA:CB	2.40	0.41
2:B:138:ASN:ND2	2:B:180:HIS:H	2.16	0.41
1:A:431:ASP:O	1:A:432:LYS:HE2	2.21	0.41
1:A:470:ASN:C	1:A:470:ASN:HD22	2.22	0.41
1:A:378:TRP:O	1:A:379:GLU:C	2.58	0.41
2:B:49:TRP:O	2:B:51:PRO:CD	2.65	0.41
2:B:92:LYS:HD2	2:B:92:LYS:HA	1.93	0.41
2:B:257:LEU:HD22	2:B:258:HIS:NE2	2.36	0.41
2:B:131:MET:SD	2:B:206:LEU:HD23	2.61	0.41
1:A:328:ARG:NH1	1:A:335:PHE:CE2	2.89	0.41
1:A:440:MET:SD	2:B:194:ILE:HD11	2.61	0.41
1:A:340:LYS:NZ	1:A:343:LYS:HZ2	2.19	0.41
1:A:284:CYS:HA	1:A:287:VAL:HG23	2.03	0.41
1:A:371:LEU:HD12	1:A:372:LYS:N	2.36	0.41
2:B:324:ASP:C	2:B:326:PHE:H	2.25	0.40
2:B:90:ARG:O	2:B:91:GLU:HB2	2.22	0.40
2:B:214:GLN:HA	2:B:224:CYS:HB2	2.03	0.40
2:B:337:GLY:O	2:B:338:LEU:C	2.58	0.40
1:A:328:ARG:CB	1:A:487:THR:HB	2.28	0.40
2:B:275:LYS:O	2:B:276:SER:CB	2.67	0.40
1:A:282:ARG:O	1:A:300:LEU:HB3	2.22	0.40
2:B:387:LYS:HG2	2:B:422:TRP:CH2	2.56	0.40
2:B:234:HIS:CD2	2:B:236:ASP:HB2	2.56	0.40
2:B:411:ILE:O	2:B:412:HIS:C	2.60	0.40
1:A:362:GLN:C	1:A:364:THR:H	2.24	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:463:ARG:NH2	1:A:463:ARG:NH2[7_556]	2.06	0.14

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	214/216 (99%)	152 (71%)	43 (20%)	19 (9%)	1 15
2	B	421/423 (100%)	321 (76%)	63 (15%)	37 (9%)	1 15
All	All	635/639 (99%)	473 (74%)	106 (17%)	56 (9%)	1 15

All (56) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	293	THR
1	A	397	LEU
1	A	419	PRO
1	A	458	MET
1	A	464	GLN
1	A	493	PRO
1	A	494	ALA
2	B	111	ILE
2	B	128	THR
2	B	194	ILE
2	B	275	LYS
2	B	276	SER
2	B	377	LEU
2	B	412	HIS
1	A	318	GLY
1	A	332	SER
1	A	334	ASP
1	A	442	THR
1	A	475	TYR
1	A	476	TYR
2	B	61	PHE
2	B	63	ALA
2	B	93	ALA
2	B	105	ARG
2	B	107	ARG

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Mol	Chain	Res	Type
2	B	121	GLN
2	B	265	LYS
2	B	271	GLN
2	B	325	ARG
1	A	450	CYS
1	A	462	GLN
2	B	135	LYS
2	B	148	ILE
2	B	171	PRO
2	B	174	LEU
2	B	226	ALA
2	B	283	ASP
2	B	32	LEU
2	B	167	ARG
2	B	269	SER
2	B	308	GLY
2	B	318	ASN
2	B	400	HIS
1	A	448	ASP
2	B	50	ARG
2	B	104	GLY
2	B	108	GLY
2	B	244	PRO
1	A	292	HIS
1	A	317	ALA
2	B	204	THR
2	B	264	CYS
1	A	418	GLN
2	B	126	PRO
2	B	270	GLY
2	B	359	ILE

5.3.2 Protein sidechains (i)

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

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

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	184/184 (100%)	168 (91%)	16 (9%)	13 51
2	B	366/367 (100%)	331 (90%)	35 (10%)	10 46
All	All	550/551 (100%)	499 (91%)	51 (9%)	11 49

All (51) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	304	ASN
1	A	326	GLN
1	A	327	ARG
1	A	334	ASP
1	A	337	ARG
1	A	346	PHE
1	A	375	LEU
1	A	377	ASP
1	A	379	GLU
1	A	397	LEU
1	A	415	SER
1	A	419	PRO
1	A	463	ARG
1	A	465	ASN
1	A	470	ASN
1	A	492	ARG
2	B	24	MET
2	B	37	ASP
2	B	49	TRP
2	B	72	LEU
2	B	90	ARG
2	B	95	LYS
2	B	96	ILE
2	B	140	ASN
2	B	147	LEU
2	B	148	ILE
2	B	150	GLU
2	B	168	HIS
2	B	184	GLN
2	B	219	GLU
2	B	230	ASN
2	B	235	GLU

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Mol	Chain	Res	Type
2	B	236	ASP
2	B	257	LEU
2	B	266	GLU
2	B	267	ARG
2	B	269	SER
2	B	282	PRO
2	B	283	ASP
2	B	291	THR
2	B	296	LEU
2	B	316	SER
2	B	341	GLU
2	B	345	ILE
2	B	349	THR
2	B	380	ASN
2	B	385	LEU
2	B	401	THR
2	B	402	ASP
2	B	427	ASN
2	B	436	PRO

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (19) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	304	ASN
1	A	336	GLN
1	A	348	ASN
1	A	362	GLN
1	A	366	GLN
1	A	465	ASN
1	A	470	ASN
2	B	66	ASN
2	B	67	GLN
2	B	138	ASN
2	B	158	ASN
2	B	177	HIS
2	B	197	ASN
2	B	214	GLN
2	B	297	GLN
2	B	318	ASN
2	B	380	ASN
2	B	427	ASN
2	B	438	ASN

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

8 carbohydrates are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
4	NAG	B	1158	2,4	14,14,15	0.72	0	15,19,21	1.01	1 (6%)
4	NAG	B	1159	4	14,14,15	0.69	0	15,19,21	0.60	0
4	NAG	B	1160	4	14,14,15	0.82	0	15,19,21	1.02	1 (6%)
4	NDG	B	1161	4	14,14,15	0.84	1 (7%)	15,19,21	0.65	0
5	NAG	B	1399	2,5	14,14,15	0.78	0	15,19,21	1.68	3 (20%)
5	NAG	B	1400	5	14,14,15	0.64	0	15,19,21	0.73	0
5	NAG	B	1438	2,5	14,14,15	0.82	0	15,19,21	0.83	1 (6%)
5	NAG	B	1439	5	14,14,15	1.05	1 (7%)	15,19,21	1.29	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
4	NAG	B	1158	2,4	-	0/6/23/26	0/1/1/1
4	NAG	B	1159	4	-	0/6/23/26	0/1/1/1
4	NAG	B	1160	4	-	0/6/23/26	0/1/1/1
4	NDG	B	1161	4	-	0/6/23/26	0/1/1/1
5	NAG	B	1399	2,5	-	0/6/23/26	0/1/1/1
5	NAG	B	1400	5	-	0/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	NAG	B	1438	2,5	-	0/6/23/26	0/1/1/1
5	NAG	B	1439	5	-	0/6/23/26	0/1/1/1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	1161	NDG	C1-C2	2.01	1.55	1.52
5	B	1439	NAG	C1-C2	2.70	1.56	1.52

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	B	1158	NAG	C2-N2-C7	-2.96	119.23	123.04
4	B	1160	NAG	C2-N2-C7	-2.92	119.29	123.04
5	B	1399	NAG	C2-N2-C7	-2.31	120.08	123.04
5	B	1438	NAG	C2-N2-C7	-2.23	120.17	123.04
5	B	1439	NAG	C3-C4-C5	2.16	113.97	110.20
5	B	1399	NAG	C3-C4-C5	3.41	116.15	110.20
5	B	1439	NAG	C4-C3-C2	3.55	116.75	111.23
5	B	1399	NAG	C4-C3-C2	4.50	118.22	111.23

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

5 monomers are involved in 12 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	B	1158	NAG	5	0
4	B	1160	NAG	3	0
4	B	1161	NDG	2	0
5	B	1438	NAG	4	0
5	B	1439	NAG	1	0

5.6 Ligand geometry (i)

Of 4 ligands modelled in this entry, 1 is monoatomic - leaving 3 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the chemical component dictionary. The Link

column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
3	NAG	B	1140	2	14,14,15	0.69	0	15,19,21	0.79	1 (6%)
7	SO4	B	3	-	4,4,4	0.51	0	6,6,6	0.25	0
7	SO4	B	4	-	4,4,4	0.50	0	6,6,6	0.12	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	B	1140	2	1/1/5/7	0/6/23/26	0/1/1/1
7	SO4	B	3	-	-	0/0/0/0	0/0/0/0
7	SO4	B	4	-	-	0/0/0/0	0/0/0/0

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	B	1140	NAG	C2-N2-C7	-2.17	120.25	123.04

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
3	B	1140	NAG	C1

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	B	1140	NAG	1	0
7	B	4	SO4	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	216/216 (100%)	-0.24	0	100	100	1, 5, 15, 26	0
2	B	423/423 (100%)	-0.31	0	100	100	1, 3, 16, 37	0
All	All	639/639 (100%)	-0.28	0	100	100	1, 4, 16, 37	0

There are no RSRZ outliers to report.

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

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
4	NAG	B	1158	14/15	0.80	0.24	0.70	4,11,16,26	0
5	NAG	B	1399	14/15	0.75	0.33	0.26	13,21,33,41	0
4	NDG	B	1161	14/15	0.28	0.54	-	49,55,57,57	0
5	NAG	B	1438	14/15	0.73	0.24	-	1,5,9,18	0
4	NAG	B	1160	14/15	0.63	0.32	-	49,52,54,55	0
5	NAG	B	1400	14/15	0.77	0.40	-	46,53,56,58	0
4	NAG	B	1159	14/15	0.80	0.29	-	31,37,38,44	0
5	NAG	B	1439	14/15	0.26	0.45	-	15,21,24,24	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, 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
6	CA	A	1	1/1	0.80	0.17	-1.11	26,26,26,26	0
7	SO4	B	4	5/5	0.97	0.11	-2.25	3,3,4,6	0
3	NAG	B	1140	14/15	0.58	0.45	-	34,39,41,43	0
7	SO4	B	3	5/5	0.94	0.15	-	1,4,5,5	0

6.5 Other polymers (i)

There are no such residues in this entry.