Full wwPDB X-ray Structure Validation Report (i)

Feb 1, 2016 – 12:27 AM GMT

PDB ID	:	2AHX
Title	:	Crystal structure of ErbB4/HER4 extracellular domain
Authors	:	Bouyain, S.; Longo, P.A.; Li, S.; Ferguson, K.M.; Leahy, D.J.
Deposited on	:	2005-07-28
Resolution	:	2.40 Å(reported)

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

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

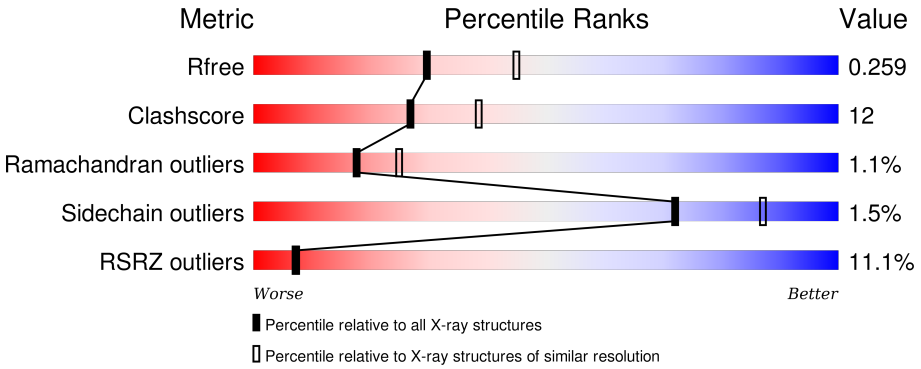
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	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 2.40 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	2919 (2.40-2.40)
Clashscore	102246	3407 (2.40-2.40)
Ramachandran outliers	100387	3351 (2.40-2.40)
Sidechain outliers	100360	3352 (2.40-2.40)
RSRZ outliers	91569	2928 (2.40-2.40)

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	617	11% 74% 24%
1	B	617	11% 76% 23%

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	1008	-	-	-	X
2	NAG	B	1011	-	-	-	X
2	NAG	B	1016	-	-	-	X
4	SO4	B	2003	-	-	-	X

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 9940 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.

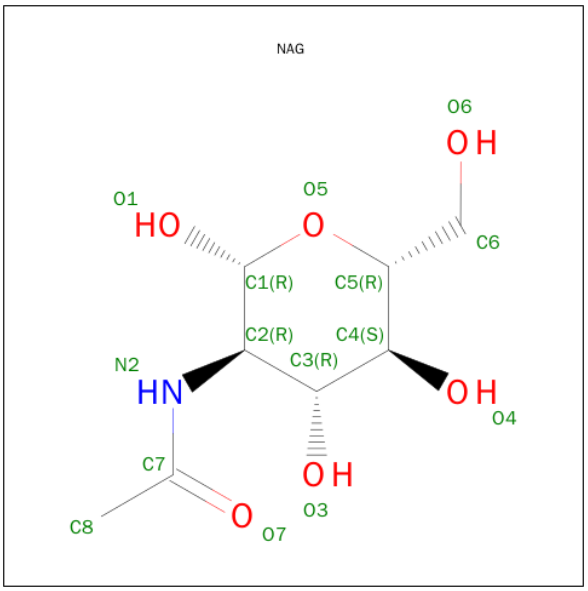
- Molecule 1 is a protein called Receptor tyrosine-protein kinase erbB-4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	611	Total	C	N	O	S	0	0	0
			4767	2961	831	917	58			
1	B	615	Total	C	N	O	S	0	0	0
			4795	2975	837	925	58			

There are 4 discrepancies between the modelled and reference sequences:

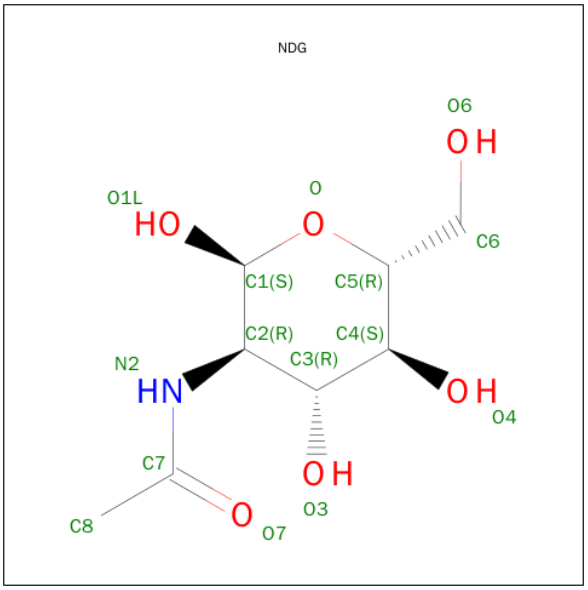
Chain	Residue	Modelled	Actual	Comment	Reference
A	0	ARG	-	CLONING ARTIFACT	UNP Q15303
A	524	ASP	GLY	MUTATION	UNP Q15303
B	0	ARG	-	CLONING ARTIFACT	UNP Q15303
B	524	ASP	GLY	MUTATION	UNP Q15303

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



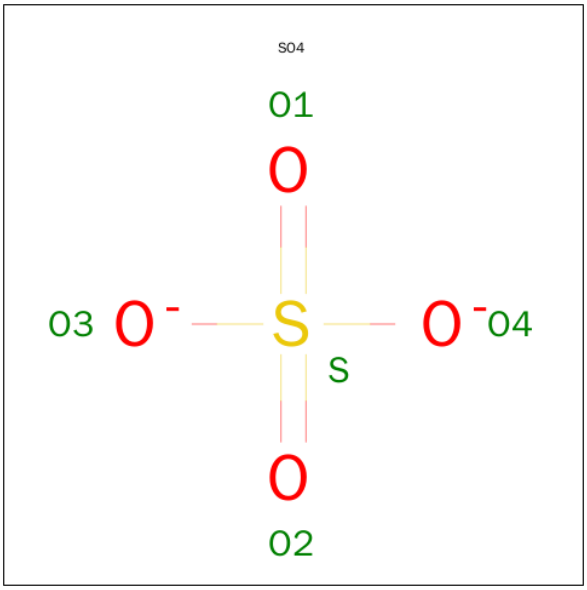
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total C N O 14 8 1 5	0	0
2	A	1	Total C N O 14 8 1 5	0	0
2	A	1	Total C N O 14 8 1 5	0	0
2	A	1	Total C N O 14 8 1 5	0	0
2	A	1	Total C N O 14 8 1 5	0	0
2	B	1	Total C N O 14 8 1 5	0	0
2	B	1	Total C N O 14 8 1 5	0	0
2	B	1	Total C N O 14 8 1 5	0	0
2	B	1	Total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

- Molecule 3 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
3	A	1	Total C N O 14 8 1 5	0	0
3	A	1	Total C N O 14 8 1 5	0	0
3	A	1	Total C N O 14 8 1 5	0	0
3	B	1	Total C N O 14 8 1 5	0	0

- Molecule 4 is SULFATE ION (three-letter code: SO4) (formula: O_4S).



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

- Molecule 5 is YTTRIUM (III) ION (three-letter code: YT3) (formula: Y).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	B	1	Total Y 1 1	0	0

- Molecule 6 is water.

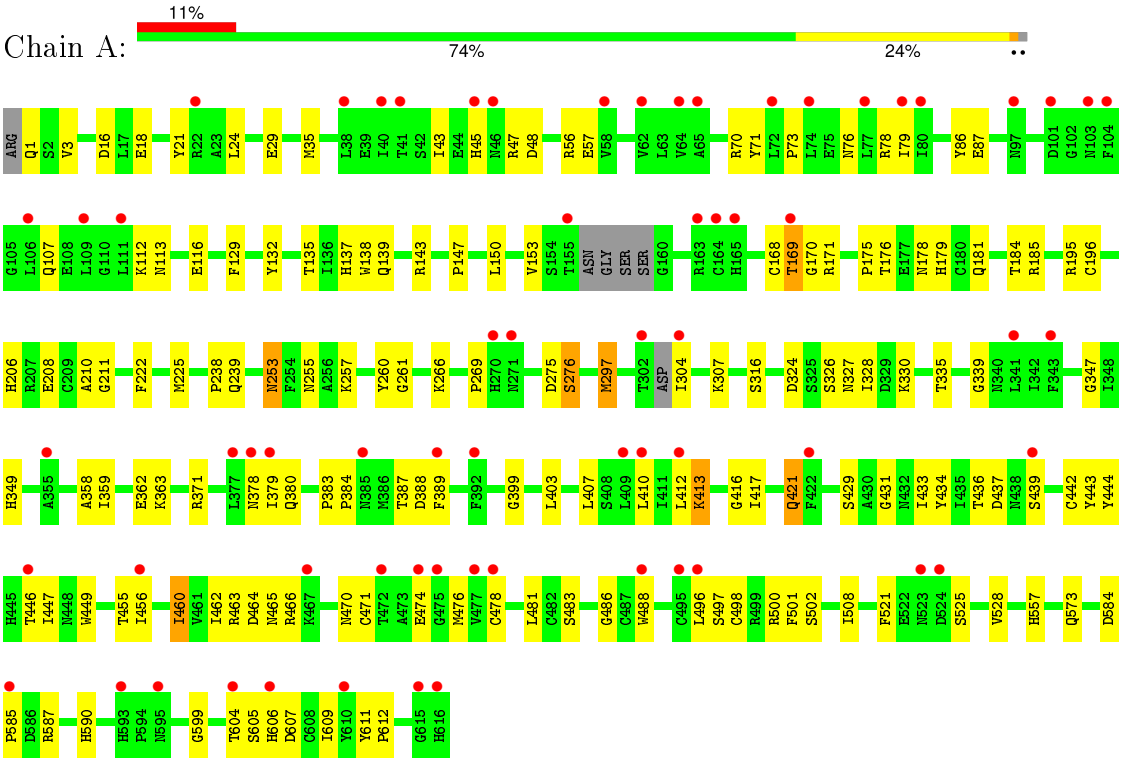
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	56	Total O 56 56	0	0
6	B	82	Total O 82 82	0	0

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.

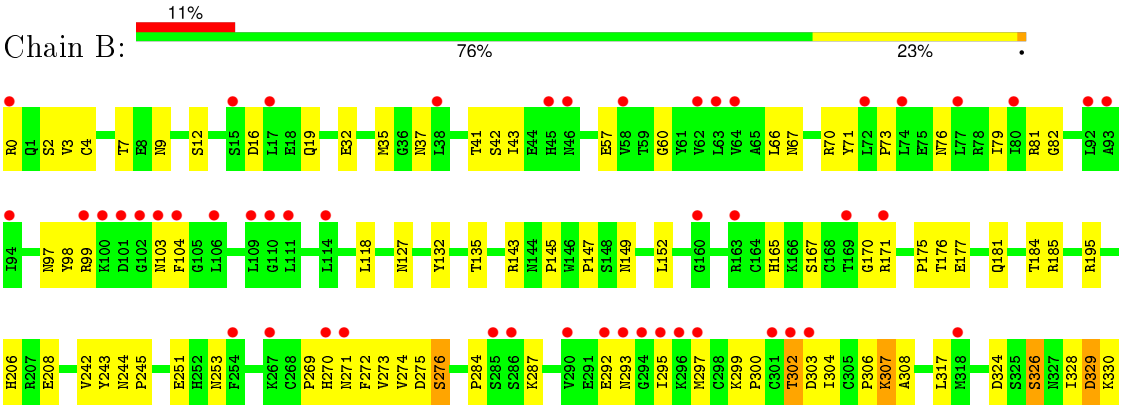
- Molecule 1: Receptor tyrosine-protein kinase erbB-4

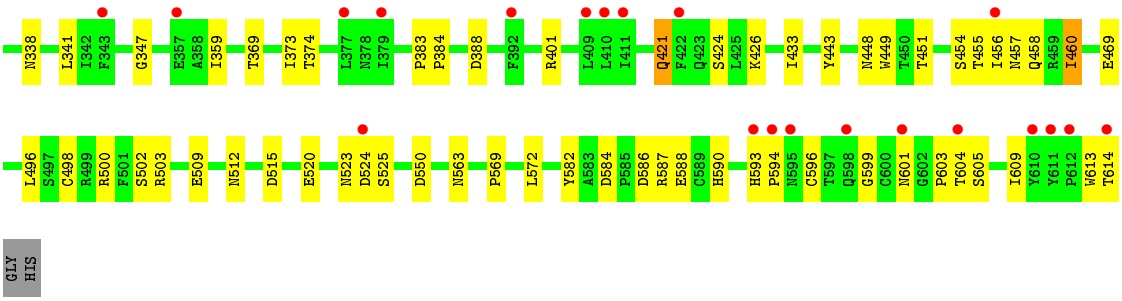
Chain A:



- Molecule 1: Receptor tyrosine-protein kinase erbB-4

Chain B:




N338
L341
I342
F343
G347
E357
A358
I359
T369
I373
T374
L377
N378
I379
P383
P384
D388
F392
R401
L409
I410
I411
Q421
F422
Q423
S424
L425
K426
I433
Y443
N448
W449
T450
T451
S454
T455
I456
N457
Q458
R459
I460
E469
L496
S497
C498
R499
R500
P501
S502
R503
E509
N512
D515
E520
N523
D524
S525
D550
N563
P569
L572
Y582
A583
D584
P585
D586
R587
E588
C589
H590
H593
P594
N595
C596
T597
Q598
G599
C600
N601
G602
P603
T604
S605
I609
Y610
Y611
P612
W613
T614
GLY
HIS

4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α, β, γ	76.96Å 203.09Å 261.32Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	29.88 – 2.40 29.86 – 2.40	Depositor EDS
% Data completeness (in resolution range)	96.4 (29.88-2.40) 96.2 (29.86-2.40)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.51 (at 2.39Å)	Xtriage
Refinement program	REFMAC 5	Depositor
R, R_{free}	0.235 , 0.265 0.227 , 0.259	Depositor DCC
R_{free} test set	4047 reflections (5.49%)	DCC
Wilson B-factor (Å^2)	45.1	Xtriage
Anisotropy	0.426	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.33 , 39.7	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.47$, $< L^2 > = 0.30$	Xtriage
Outliers	0 of 80470 reflections	Xtriage
F_o,F_c correlation	0.93	EDS
Total number of atoms	9940	wwPDB-VP
Average B, all atoms (Å^2)	28.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.88% 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: SO4, YT3, NDG, NAG

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$\|Z\|>5$	RMSZ	#$\|Z\|>5$
1	A	0.40	0/4872	0.67	0/6601
1	B	0.42	0/4901	0.69	1/6644 (0.0%)
All	All	0.41	0/9773	0.68	1/13245 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	302	THR	C-N-CA	-6.73	104.88	121.70

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	4767	0	4496	128	0
1	B	4795	0	4526	102	0
2	A	70	0	65	3	0
2	B	98	0	91	4	0
3	A	42	0	39	6	0
3	B	14	0	13	0	0
4	A	5	0	0	0	0
4	B	10	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	B	1	0	0	1	0
6	A	56	0	0	3	0
6	B	82	0	0	2	0
All	All	9940	0	9230	230	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 (230) 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:407:LEU:HD13	1:A:410:LEU:HD21	1.29	1.11
1:A:78:ARG:HD3	1:A:222:PHE:HB3	1.46	0.94
1:A:470:ASN:OD1	3:A:1007:NDG:H3	1.66	0.94
1:A:446:THR:HG21	1:A:478:CYS:SG	2.07	0.94
1:B:152:LEU:HD11	2:B:1011:NAG:H83	1.54	0.90
1:B:524:ASP:O	1:B:525:SER:OG	1.91	0.89
1:B:176:THR:HG23	6:B:3082:HOH:O	1.72	0.87
1:A:176:THR:CG2	1:A:178:ASN:OD1	2.23	0.86
1:B:454:SER:H	1:B:458:GLN:NE2	1.76	0.83
1:A:143:ARG:HG3	1:A:185:ARG:HH12	1.44	0.82
1:A:24:LEU:HD22	1:A:43:ILE:HD11	1.61	0.82
1:A:137:HIS:HB2	1:A:171:ARG:NH1	1.95	0.81
1:B:99:ARG:HD3	1:B:103:ASN:HD22	1.43	0.81
1:A:436:THR:HG23	1:A:463:ARG:HB2	1.62	0.81
1:A:137:HIS:H	1:A:181:GLN:HE22	1.26	0.81
1:B:165:HIS:HD2	1:B:167:SER:H	1.30	0.80
1:A:176:THR:HG22	1:A:178:ASN:OD1	1.83	0.79
1:A:604:THR:HG22	1:A:606:HIS:H	1.47	0.79
1:A:410:LEU:HD23	1:A:434:TYR:HB3	1.64	0.79
1:B:582:TYR:OH	1:B:603:PRO:HG3	1.83	0.77
1:A:304:ILE:HB	1:A:371:ARG:HH21	1.48	0.77
1:A:471:CYS:HB3	1:A:476:MET:HB2	1.66	0.76
1:A:137:HIS:HB2	1:A:171:ARG:CZ	2.16	0.76
1:A:78:ARG:HD2	6:A:2055:HOH:O	1.86	0.74
1:A:184:THR:HG22	1:A:195:ARG:HB3	1.72	0.72
1:B:448:ASN:ND2	1:B:451:THR:HG23	2.03	0.72
1:B:601:ASN:HB2	1:B:609:ILE:HD11	1.72	0.71
1:A:206:HIS:HD2	1:A:208:GLU:H	1.39	0.70
1:A:253:ASN:ND2	1:A:255:ASN:H	1.89	0.70
1:A:412:LEU:HG	1:A:413:LYS:HG3	1.73	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:451:THR:HG22	2:B:1014:NAG:H82	1.73	0.69
1:A:446:THR:HG22	1:A:486:GLY:HA2	1.74	0.69
1:B:99:ARG:HD3	1:B:103:ASN:ND2	2.09	0.68
1:A:3:VAL:HG13	1:A:35:MET:HG3	1.76	0.68
1:A:455:THR:HG22	1:A:456:ILE:H	1.58	0.67
1:B:132:TYR:OH	1:B:175:PRO:HG3	1.94	0.67
1:B:324:ASP:HA	1:B:359:ILE:HD11	1.75	0.67
1:B:454:SER:H	1:B:458:GLN:HE22	1.44	0.66
1:A:304:ILE:O	1:A:371:ARG:NH2	2.27	0.66
1:A:112:LYS:HD3	2:A:1001:NAG:H82	1.78	0.66
1:A:470:ASN:CG	3:A:1007:NDG:N2	2.49	0.65
1:A:78:ARG:CD	1:A:222:PHE:HB3	2.23	0.65
1:B:588:GLU:OE1	5:B:3001:YT3:Y	1.65	0.64
1:A:327:ASN:O	1:A:330:LYS:HB3	1.98	0.64
1:A:481:LEU:HD13	1:A:508:ILE:HA	1.79	0.63
1:A:147:PRO:HD2	1:A:150:LEU:HD12	1.80	0.63
1:A:407:LEU:HD22	1:A:434:TYR:HB2	1.79	0.63
1:A:78:ARG:HD3	1:A:222:PHE:CB	2.23	0.63
1:A:470:ASN:OD1	3:A:1007:NDG:C3	2.43	0.63
1:A:455:THR:HG22	1:A:456:ILE:N	2.13	0.62
1:A:447:ILE:HG23	1:A:496:LEU:HD11	1.81	0.62
1:A:184:THR:O	1:A:184:THR:HG22	1.97	0.62
1:B:455:THR:H	1:B:458:GLN:HE21	1.47	0.62
1:A:143:ARG:HG3	1:A:185:ARG:NH1	2.14	0.62
1:A:112:LYS:CD	2:A:1001:NAG:H82	2.30	0.60
1:B:601:ASN:HB2	1:B:609:ILE:CD1	2.32	0.59
1:B:57:GLU:HG2	1:B:79:ILE:HG22	1.84	0.58
1:A:470:ASN:OD1	3:A:1007:NDG:N2	2.36	0.58
1:A:171:ARG:HH11	1:A:171:ARG:HG2	1.68	0.58
1:B:297:MET:SD	1:B:299:LYS:HE2	2.43	0.58
1:A:498:CYS:SG	1:A:502:SER:HB3	2.43	0.58
1:A:339:GLY:HA2	6:A:2006:HOH:O	2.04	0.58
1:B:3:VAL:HG11	1:B:35:MET:SD	2.44	0.57
1:A:116:GLU:HB2	1:A:211:GLY:HA2	1.86	0.57
1:A:439:SER:O	1:A:466:ARG:HB2	2.05	0.56
1:B:57:GLU:HG2	1:B:79:ILE:CG2	2.35	0.56
1:B:456:ILE:HG13	1:B:457:ASN:N	2.20	0.56
1:A:176:THR:HG21	1:A:178:ASN:OD1	2.04	0.56
1:A:132:TYR:OH	1:A:175:PRO:HG3	2.05	0.55
1:B:604:THR:HG22	1:B:605:SER:N	2.21	0.55
1:B:269:PRO:O	1:B:272:PHE:HB2	2.06	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:78:ARG:HA	1:A:113:ASN:O	2.07	0.55
1:B:569:PRO:HB3	1:B:572:LEU:HD12	1.89	0.55
1:B:41:THR:O	1:B:43:ILE:HD12	2.08	0.54
1:A:71:TYR:O	1:A:73:PRO:HD3	2.08	0.54
1:A:446:THR:O	1:A:486:GLY:HA3	2.08	0.54
1:A:239:GLN:HG3	1:A:573:GLN:HG2	1.89	0.54
1:A:399:GLY:O	1:A:429:SER:HB2	2.07	0.54
1:B:206:HIS:HD2	1:B:208:GLU:H	1.53	0.54
1:B:613:TRP:O	1:B:614:THR:HB	2.08	0.54
1:A:446:THR:HG22	1:A:486:GLY:CA	2.39	0.53
1:A:137:HIS:H	1:A:181:GLN:NE2	2.00	0.53
1:B:206:HIS:CD2	1:B:208:GLU:H	2.27	0.53
1:B:171:ARG:HG3	1:B:181:GLN:HB3	1.91	0.53
1:B:304:ILE:HD13	1:B:369:THR:HG22	1.91	0.52
1:A:471:CYS:O	1:A:474:GLU:N	2.43	0.52
1:A:488:TRP:CZ2	1:A:496:LEU:HD21	2.45	0.52
1:A:307:LYS:HE2	3:A:1004:NDG:H8C2	1.91	0.51
1:A:307:LYS:H	1:A:335:THR:HB	1.75	0.51
1:A:557:HIS:O	1:A:587:ARG:HD3	2.12	0.50
1:A:257:LYS:HE2	1:A:266:LYS:HG3	1.93	0.50
1:A:407:LEU:HD13	1:A:410:LEU:CD2	2.21	0.50
1:B:42:SER:HA	1:B:66:LEU:O	2.11	0.50
1:A:604:THR:HG22	1:A:605:SER:N	2.26	0.50
1:A:521:PHE:CE2	1:A:528:VAL:HB	2.46	0.50
1:A:462:ILE:HG23	1:A:465:ASN:ND2	2.27	0.50
1:B:9:ASN:HB3	1:B:12:SER:HB2	1.94	0.50
1:B:500:ARG:HD3	1:B:509:GLU:O	2.12	0.50
1:B:97:ASN:HB2	1:B:127:ASN:HD22	1.76	0.49
1:A:57:GLU:HG2	1:A:79:ILE:CG2	2.42	0.49
1:B:242:VAL:HG23	1:B:253:ASN:HB2	1.94	0.49
1:A:403:LEU:HD21	1:A:431:GLY:HA3	1.94	0.49
1:B:604:THR:HG22	1:B:605:SER:H	1.78	0.49
1:B:97:ASN:H	1:B:127:ASN:ND2	2.10	0.49
1:B:60:GLY:O	1:B:82:GLY:HA2	2.13	0.49
1:B:424:SER:O	1:B:426:LYS:HG2	2.11	0.49
1:B:270:HIS:O	1:B:271:ASN:HB2	2.13	0.49
1:B:433:ILE:HB	1:B:460:ILE:HD12	1.96	0.48
1:B:512:ASN:HB3	1:B:515:ASP:O	2.13	0.48
1:B:71:TYR:O	1:B:73:PRO:HD3	2.13	0.48
1:A:185:ARG:HB2	1:A:195:ARG:NH1	2.28	0.48
1:B:582:TYR:HH	1:B:603:PRO:HG3	1.78	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:449:TRP:CD2	1:B:460:ILE:HD13	2.48	0.48
1:A:168:CYS:O	1:A:169:THR:O	2.32	0.48
1:B:0:ARG:HG2	1:B:32:GLU:OE1	2.14	0.48
1:B:16:ASP:OD1	1:B:19:GLN:OE1	2.32	0.48
1:A:137:HIS:CE1	1:A:139:GLN:HG3	2.49	0.47
1:A:403:LEU:CD2	1:A:431:GLY:HA3	2.44	0.47
1:B:388:ASP:HB2	1:B:421:GLN:HG3	1.96	0.47
1:B:81:ARG:HG2	1:B:118:LEU:HD12	1.97	0.47
1:A:436:THR:HG22	1:A:437:ASP:OD2	2.14	0.47
1:B:0:ARG:HG2	1:B:32:GLU:OE2	2.13	0.47
1:B:206:HIS:HD2	1:B:208:GLU:HB2	1.79	0.47
1:A:378:ASN:OD1	1:A:380:GLN:HG3	2.14	0.47
1:A:436:THR:HG22	1:A:437:ASP:N	2.30	0.47
1:B:143:ARG:HA	1:B:185:ARG:NH1	2.30	0.47
1:B:596:CYS:HB3	1:B:599:GLY:O	2.15	0.47
1:A:112:LYS:NZ	2:A:1001:NAG:H82	2.30	0.47
1:A:210:ALA:HB2	1:A:225:MET:SD	2.55	0.47
1:A:16:ASP:OD1	1:A:18:GLU:HB3	2.15	0.47
1:A:86:TYR:O	1:A:87:GLU:HB2	2.15	0.46
1:A:56:ARG:HD3	1:A:76:ASN:HB3	1.97	0.46
1:A:433:ILE:HD13	1:A:449:TRP:CE3	2.51	0.46
1:B:67:ASN:HB2	1:B:97:ASN:OD1	2.15	0.46
1:A:442:CYS:O	1:A:443:TYR:HB2	2.15	0.46
1:B:317:LEU:HD21	1:B:330:LYS:HD3	1.97	0.46
1:A:21:TYR:CE1	1:A:47:ARG:HB3	2.51	0.46
1:A:584:ASP:HB2	1:A:585:PRO:CD	2.45	0.46
1:A:328:ILE:HD13	1:A:363:LYS:HB3	1.96	0.46
1:A:137:HIS:HE1	1:A:139:GLN:HG3	1.80	0.46
1:B:308:ALA:HB1	1:B:338:ASN:ND2	2.31	0.46
1:A:383:PRO:HA	1:A:384:PRO:HD3	1.76	0.45
1:A:1:GLN:HG2	1:A:1:GLN:O	2.16	0.45
1:A:138:TRP:CE2	1:A:153:VAL:HG21	2.51	0.45
1:A:501:PHE:CD2	1:A:525:SER:HA	2.52	0.45
1:B:287:LYS:HE2	1:B:300:PRO:HG3	1.98	0.45
1:A:470:ASN:OD1	3:A:1007:NDG:C2	2.65	0.45
1:A:35:MET:CE	1:A:261:GLY:HA3	2.47	0.45
1:A:465:ASN:O	1:A:466:ARG:C	2.53	0.45
1:B:81:ARG:HA	1:B:118:LEU:HB2	1.97	0.45
1:A:387:THR:HA	1:A:416:GLY:O	2.16	0.45
1:B:503:ARG:HD3	1:B:520:GLU:OE1	2.16	0.45
1:B:550:ASP:HB3	1:B:563:ASN:OD1	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:498:CYS:SG	1:B:502:SER:HB3	2.56	0.45
1:A:599:GLY:C	1:A:609:ILE:HG12	2.37	0.45
1:B:275:ASP:O	1:B:276:SER:HB2	2.17	0.45
1:A:604:THR:HB	1:A:607:ASP:CG	2.37	0.45
1:B:135:THR:HB	1:B:170:GLY:O	2.16	0.45
1:B:165:HIS:CD2	1:B:167:SER:H	2.21	0.44
1:B:2:SER:OG	1:B:32:GLU:HG3	2.17	0.44
1:A:275:ASP:O	1:A:276:SER:HB2	2.18	0.44
1:A:137:HIS:CE1	1:A:139:GLN:HB2	2.53	0.44
1:B:184:THR:OG1	1:B:195:ARG:HD2	2.17	0.44
1:B:383:PRO:HA	1:B:384:PRO:HD3	1.82	0.44
1:A:604:THR:HB	1:A:607:ASP:OD2	2.18	0.44
1:B:582:TYR:CZ	1:B:603:PRO:HG3	2.53	0.44
1:B:524:ASP:O	1:B:525:SER:CB	2.65	0.44
1:B:586:ASP:O	1:B:587:ARG:HB2	2.18	0.44
1:A:324:ASP:OD1	1:A:326:SER:N	2.40	0.44
1:A:462:ILE:HG23	1:A:465:ASN:HD22	1.83	0.44
1:A:138:TRP:NE1	1:A:153:VAL:HG21	2.32	0.44
1:A:407:LEU:CD1	1:A:410:LEU:HD21	2.22	0.43
1:A:521:PHE:CZ	1:A:528:VAL:HB	2.53	0.43
1:B:0:ARG:HG2	1:B:32:GLU:CD	2.38	0.43
1:B:584:ASP:OD2	1:B:588:GLU:HB2	2.18	0.43
1:B:347:GLY:O	1:B:359:ILE:HG13	2.18	0.43
1:A:238:PRO:HD2	1:A:257:LYS:HB2	2.00	0.43
1:A:483:SER:OG	1:A:497:SER:HB2	2.18	0.43
1:A:349:HIS:O	1:A:358:ALA:HB2	2.18	0.43
1:A:260:TYR:CZ	1:A:269:PRO:HG2	2.53	0.43
1:B:7:THR:O	1:B:37:ASN:HB2	2.17	0.43
1:A:176:THR:HB	1:A:179:HIS:HB2	2.01	0.43
1:A:35:MET:HE3	1:A:261:GLY:HA3	2.00	0.43
1:B:374:THR:HB	1:B:401:ARG:HD2	2.00	0.43
1:B:3:VAL:HG12	1:B:4:CYS:N	2.34	0.43
1:B:328:ILE:HG23	1:B:329:ASP:N	2.34	0.43
1:B:341:LEU:HA	1:B:341:LEU:HD23	1.90	0.43
1:A:135:THR:HB	1:A:170:GLY:O	2.19	0.43
1:B:97:ASN:HB2	1:B:127:ASN:ND2	2.34	0.42
1:B:293:ASN:HB2	1:B:295:ILE:CD1	2.49	0.42
1:A:297:MET:HE3	6:A:2056:HOH:O	2.20	0.42
1:A:455:THR:CG2	1:A:456:ILE:H	2.31	0.42
1:A:584:ASP:OD2	1:A:590:HIS:HE1	2.03	0.42
1:A:611:TYR:HA	1:A:612:PRO:HD3	1.88	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:584:ASP:HB2	1:A:585:PRO:HD2	2.02	0.42
1:B:76:ASN:OD1	2:B:1009:NAG:O7	2.38	0.42
1:B:469:GLU:N	1:B:469:GLU:OE1	2.38	0.42
1:B:582:TYR:CE2	1:B:590:HIS:HB2	2.55	0.42
1:A:417:ILE:O	1:A:417:ILE:HG13	2.20	0.42
1:A:460:ILE:N	1:A:460:ILE:HD12	2.35	0.42
1:B:243:TYR:O	1:B:245:PRO:HD3	2.20	0.42
1:B:43:ILE:N	1:B:43:ILE:HD12	2.35	0.41
1:A:362:GLU:OE1	1:A:362:GLU:HA	2.20	0.41
1:B:273:VAL:HG12	1:B:274:VAL:N	2.34	0.41
1:B:448:ASN:ND2	1:B:451:THR:CG2	2.78	0.41
1:A:444:TYR:CE1	1:A:462:ILE:HG21	2.55	0.41
1:A:184:THR:HG23	1:A:196:CYS:O	2.20	0.41
1:B:165:HIS:CE1	1:B:177:GLU:HB2	2.55	0.41
1:B:593:HIS:ND1	1:B:594:PRO:HD2	2.35	0.41
1:A:446:THR:HG22	1:A:446:THR:O	2.21	0.41
1:B:206:HIS:CD2	1:B:208:GLU:HB2	2.55	0.41
1:B:97:ASN:H	1:B:127:ASN:HD22	1.67	0.41
1:B:118:LEU:HD23	1:B:143:ARG:HD2	2.01	0.41
1:B:147:PRO:C	1:B:149:ASN:N	2.72	0.41
1:A:184:THR:CG2	1:A:184:THR:O	2.65	0.41
1:A:442:CYS:C	1:A:444:TYR:H	2.24	0.41
1:B:306:PRO:O	1:B:307:LYS:HB2	2.21	0.41
1:A:388:ASP:CB	1:A:421:GLN:HG3	2.51	0.41
1:B:451:THR:HG22	2:B:1014:NAG:C8	2.48	0.41
1:B:341:LEU:HD12	1:B:373:ILE:HD11	2.03	0.41
1:A:379:ILE:HD13	1:A:389:PHE:CE2	2.56	0.41
1:B:176:THR:CG2	6:B:3082:HOH:O	2.50	0.41
1:A:500:ARG:HB2	1:A:508:ILE:O	2.21	0.41
1:A:488:TRP:HE1	1:A:496:LEU:HD23	1.85	0.40
1:A:347:GLY:O	1:A:359:ILE:HG13	2.21	0.40
1:A:107:GLN:HA	1:A:129:PHE:O	2.21	0.40
1:B:143:ARG:HA	1:B:185:ARG:HH12	1.85	0.40
1:B:244:ASN:HB2	1:B:251:GLU:HG3	2.04	0.40
1:B:324:ASP:OD1	1:B:326:SER:HB3	2.21	0.40
1:B:308:ALA:HB1	1:B:338:ASN:HD21	1.85	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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	605/617 (98%)	545 (90%)	53 (9%)	7 (1%)	16	23
1	B	613/617 (99%)	564 (92%)	42 (7%)	7 (1%)	17	25
All	All	1218/1234 (99%)	1109 (91%)	95 (8%)	14 (1%)	17	25

All (14) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	29	GLU
1	A	169	THR
1	B	307	LYS
1	A	316	SER
1	A	413	LYS
1	A	45	HIS
1	B	276	SER
1	B	284	PRO
1	A	276	SER
1	A	464	ASP
1	B	98	TYR
1	B	292	GLU
1	B	302	THR
1	B	443	TYR

5.3.2 Protein sidechains

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	541/546 (99%)	535 (99%)	6 (1%)	80 92
1	B	545/546 (100%)	535 (98%)	10 (2%)	66 84
All	All	1086/1092 (100%)	1070 (98%)	16 (2%)	72 87

All (16) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	48	ASP
1	A	70	ARG
1	A	253	ASN
1	A	297	MET
1	A	421	GLN
1	A	460	ILE
1	B	70	ARG
1	B	104	PHE
1	B	145	PRO
1	B	303	ASP
1	B	326	SER
1	B	329	ASP
1	B	421	GLN
1	B	460	ILE
1	B	496	LEU
1	B	523	ASN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (25) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	46	ASN
1	A	103	ASN
1	A	137	HIS
1	A	179	HIS
1	A	181	GLN
1	A	206	HIS
1	A	253	ASN
1	A	349	HIS
1	A	354	ASN
1	A	421	GLN
1	A	573	GLN
1	A	590	HIS
1	B	103	ASN
1	B	126	GLN

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Mol	Chain	Res	Type
1	B	127	ASN
1	B	165	HIS
1	B	206	HIS
1	B	321	GLN
1	B	338	ASN
1	B	349	HIS
1	B	445	HIS
1	B	458	GLN
1	B	523	ASN
1	B	595	ASN
1	B	601	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 carbohydrates in this entry.

5.6 Ligand geometry (i)

Of 20 ligands modelled in this entry, 1 is monoatomic - leaving 19 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	$\#\|Z\| > 2$
2	NAG	A	1001	1	14,14,15	0.71	1 (7%)	15,19,21	1.11	2 (13%)
2	NAG	A	1002	1	14,14,15	0.43	0	15,19,21	1.02	1 (6%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
2	NAG	A	1003	1	14,14,15	0.50	0	15,19,21	1.09	1 (6%)
3	NDG	A	1004	1	14,14,15	0.48	0	15,19,21	0.85	1 (6%)
2	NAG	A	1005	1	14,14,15	0.69	0	15,19,21	0.68	0
3	NDG	A	1006	1	14,14,15	0.83	0	15,19,21	0.83	0
3	NDG	A	1007	1	14,14,15	0.82	1 (7%)	15,19,21	0.64	0
2	NAG	A	1008	1	14,14,15	0.71	1 (7%)	15,19,21	0.81	1 (6%)
4	SO4	A	2001	-	4,4,4	0.25	0	6,6,6	0.13	0
2	NAG	B	1009	1	14,14,15	0.51	0	15,19,21	0.57	0
3	NDG	B	1010	1	14,14,15	0.72	1 (7%)	15,19,21	0.96	1 (6%)
2	NAG	B	1011	1	14,14,15	0.45	0	15,19,21	0.92	1 (6%)
2	NAG	B	1012	1	14,14,15	0.66	0	15,19,21	0.85	1 (6%)
2	NAG	B	1013	1	14,14,15	0.64	0	15,19,21	1.03	1 (6%)
2	NAG	B	1014	1	14,14,15	0.55	0	15,19,21	0.77	1 (6%)
2	NAG	B	1015	1	14,14,15	0.54	0	15,19,21	1.01	1 (6%)
2	NAG	B	1016	1	14,14,15	0.55	0	15,19,21	0.94	1 (6%)
4	SO4	B	2002	-	4,4,4	0.25	0	6,6,6	0.12	0
4	SO4	B	2003	-	4,4,4	0.25	0	6,6,6	0.14	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	NAG	A	1001	1	-	0/6/23/26	0/1/1/1
2	NAG	A	1002	1	-	0/6/23/26	0/1/1/1
2	NAG	A	1003	1	-	0/6/23/26	0/1/1/1
3	NDG	A	1004	1	-	1/6/23/26	0/1/1/1
2	NAG	A	1005	1	-	1/6/23/26	0/1/1/1
3	NDG	A	1006	1	-	0/6/23/26	0/1/1/1
3	NDG	A	1007	1	-	0/6/23/26	0/1/1/1
2	NAG	A	1008	1	-	2/6/23/26	0/1/1/1
4	SO4	A	2001	-	-	0/0/0/0	0/0/0/0
2	NAG	B	1009	1	-	0/6/23/26	0/1/1/1
3	NDG	B	1010	1	-	0/6/23/26	0/1/1/1
2	NAG	B	1011	1	-	0/6/23/26	0/1/1/1
2	NAG	B	1012	1	-	0/6/23/26	0/1/1/1
2	NAG	B	1013	1	-	0/6/23/26	0/1/1/1
2	NAG	B	1014	1	-	0/6/23/26	0/1/1/1
2	NAG	B	1015	1	-	0/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	NAG	B	1016	1	-	0/6/23/26	0/1/1/1
4	SO4	B	2002	-	-	0/0/0/0	0/0/0/0
4	SO4	B	2003	-	-	0/0/0/0	0/0/0/0

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	1001	NAG	C1-C2	2.13	1.55	1.52
2	A	1008	NAG	C1-C2	2.21	1.55	1.52
3	B	1010	NDG	C1-C2	2.27	1.55	1.52
3	A	1007	NDG	C1-C2	2.34	1.55	1.52

All (13) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	1013	NAG	C2-N2-C7	-3.23	118.89	123.04
2	A	1002	NAG	C2-N2-C7	-3.18	118.95	123.04
2	A	1003	NAG	C2-N2-C7	-2.97	119.22	123.04
2	A	1001	NAG	C2-N2-C7	-2.86	119.37	123.04
2	B	1016	NAG	C2-N2-C7	-2.81	119.42	123.04
2	B	1011	NAG	C2-N2-C7	-2.74	119.52	123.04
2	B	1012	NAG	C2-N2-C7	-2.70	119.57	123.04
2	B	1015	NAG	C2-N2-C7	-2.64	119.65	123.04
3	A	1004	NDG	C2-N2-C7	-2.57	119.73	123.04
3	B	1010	NDG	C2-N2-C7	-2.51	119.81	123.04
2	B	1014	NAG	C2-N2-C7	-2.12	120.32	123.04
2	A	1008	NAG	C2-N2-C7	-2.03	120.44	123.04
2	A	1001	NAG	C4-C3-C2	2.09	114.47	111.23

There are no chirality outliers.

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	1005	NAG	O7-C7-N2-C2
3	A	1004	NDG	O7-C7-N2-C2
2	A	1008	NAG	O7-C7-N2-C2
2	A	1008	NAG	C8-C7-N2-C2

There are no ring outliers.

6 monomers are involved in 13 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	1001	NAG	3	0
3	A	1004	NDG	1	0
3	A	1007	NDG	5	0
2	B	1009	NAG	1	0
2	B	1011	NAG	1	0
2	B	1014	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

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	611/617 (99%)	0.61	66 (10%)	8 8	8, 26, 40, 53	0
1	B	615/617 (99%)	0.59	70 (11%)	7 7	11, 26, 43, 72	0
All	All	1226/1234 (99%)	0.60	136 (11%)	7 7	8, 26, 41, 72	0

All (136) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	101	ASP	6.9
1	B	0	ARG	6.4
1	B	254	PHE	4.9
1	A	616	HIS	4.8
1	B	271	ASN	4.7
1	A	615	GLY	4.7
1	B	295	ILE	4.6
1	B	379	ILE	4.6
1	B	594	PRO	4.4
1	B	610	TYR	4.2
1	B	111	LEU	4.2
1	A	377	LEU	4.2
1	B	293	ASN	4.2
1	A	163	ARG	4.0
1	B	103	ASN	4.0
1	A	104	PHE	4.0
1	A	392	PHE	3.9
1	A	456	ILE	3.9
1	B	46	ASN	3.8
1	B	456	ILE	3.8
1	B	74	LEU	3.7
1	B	294	GLY	3.7
1	A	304	ILE	3.7
1	B	109	LEU	3.7

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Mol	Chain	Res	Type	RSRZ
1	A	595	ASN	3.7
1	B	169	THR	3.7
1	A	169	THR	3.6
1	B	38	LEU	3.6
1	B	92	LEU	3.6
1	A	64	VAL	3.6
1	B	72	LEU	3.6
1	B	62	VAL	3.5
1	A	111	LEU	3.5
1	B	101	ASP	3.5
1	B	94	ILE	3.5
1	A	38	LEU	3.4
1	B	102	GLY	3.4
1	A	355	ALA	3.4
1	A	604	THR	3.4
1	B	595	ASN	3.3
1	A	270	HIS	3.3
1	A	58	VAL	3.3
1	A	62	VAL	3.3
1	B	64	VAL	3.3
1	A	103	ASN	3.3
1	B	290	VAL	3.3
1	A	46	ASN	3.2
1	B	80	ILE	3.2
1	B	377	LEU	3.2
1	B	601	ASN	3.1
1	A	77	LEU	3.1
1	A	72	LEU	3.1
1	B	100	LYS	3.1
1	A	472	THR	3.1
1	B	114	LEU	3.0
1	B	58	VAL	3.0
1	B	297	MET	3.0
1	B	15	SER	3.0
1	B	104	PHE	3.0
1	A	439	SER	3.0
1	A	477	VAL	2.9
1	B	99	ARG	2.9
1	A	164	CYS	2.9
1	A	422	PHE	2.9
1	A	74	LEU	2.9
1	B	93	ALA	2.8

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Mol	Chain	Res	Type	RSRZ
1	B	612	PRO	2.8
1	B	286	SER	2.8
1	B	270	HIS	2.7
1	A	412	LEU	2.7
1	A	606	HIS	2.7
1	B	392	PHE	2.7
1	A	40	ILE	2.7
1	A	409	LEU	2.7
1	A	389	PHE	2.7
1	B	285	SER	2.7
1	A	610	TYR	2.7
1	B	611	TYR	2.7
1	B	267	LYS	2.7
1	B	303	ASP	2.6
1	A	97	ASN	2.6
1	B	77	LEU	2.6
1	B	17	LEU	2.6
1	B	409	LEU	2.6
1	A	302	THR	2.6
1	B	160	GLY	2.6
1	A	379	ILE	2.5
1	A	106	LEU	2.5
1	A	475	GLY	2.5
1	B	45	HIS	2.5
1	A	271	ASN	2.5
1	A	341	LEU	2.5
1	A	79	ILE	2.5
1	A	495	CYS	2.4
1	B	302	THR	2.4
1	B	318	MET	2.4
1	A	80	ILE	2.4
1	A	378	ASN	2.4
1	A	155	THR	2.4
1	A	488	TRP	2.4
1	B	422	PHE	2.4
1	A	410	LEU	2.3
1	A	165	HIS	2.3
1	A	22	ARG	2.3
1	B	598	GLN	2.3
1	B	292	GLU	2.3
1	B	614	THR	2.3
1	A	45	HIS	2.3

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Mol	Chain	Res	Type	RSRZ
1	B	593	HIS	2.3
1	A	109	LEU	2.3
1	B	110	GLY	2.2
1	A	41	THR	2.2
1	A	524	ASP	2.2
1	A	474	GLU	2.2
1	A	523	ASN	2.2
1	A	585	PRO	2.2
1	B	411	ILE	2.2
1	A	467	LYS	2.2
1	B	106	LEU	2.2
1	B	343	PHE	2.1
1	A	385	ASN	2.1
1	A	593	HIS	2.1
1	B	63	LEU	2.1
1	B	410	LEU	2.1
1	B	296	LYS	2.1
1	B	301	CYS	2.1
1	A	478	CYS	2.1
1	B	604	THR	2.1
1	B	171	ARG	2.1
1	A	65	ALA	2.0
1	B	357	GLU	2.0
1	B	524	ASP	2.0
1	A	446	THR	2.0
1	A	343	PHE	2.0
1	A	496	LEU	2.0
1	B	163	ARG	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 carbohydrates 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. 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	SO4	B	2003	5/5	0.93	0.22	7.03	57,58,70,71	0
2	NAG	B	1011	14/15	0.93	0.31	5.67	35,48,55,58	0
2	NAG	A	1008	14/15	0.93	0.20	5.21	34,44,55,56	0
2	NAG	B	1016	14/15	0.94	0.20	3.05	37,42,45,47	0
2	NAG	A	1003	14/15	0.91	0.23	1.93	29,34,46,49	0
2	NAG	A	1002	14/15	0.95	0.16	0.79	18,23,25,31	0
2	NAG	B	1015	14/15	0.84	0.19	0.44	24,37,50,52	0
2	NAG	B	1012	14/15	0.90	0.25	0.43	24,41,49,53	0
3	NDG	B	1010	14/15	0.91	0.13	-0.45	26,36,43,54	0
2	NAG	A	1001	14/15	0.90	0.15	-0.84	22,28,46,54	0
2	NAG	B	1009	14/15	0.94	0.16	-1.10	16,25,39,45	0
2	NAG	B	1013	14/15	0.83	0.26	-	33,35,42,44	0
3	NDG	A	1006	14/15	0.80	0.35	-	44,48,52,52	0
3	NDG	A	1007	14/15	0.64	0.43	-	61,66,67,68	0
4	SO4	A	2001	5/5	0.97	0.13	-	57,58,66,71	0
2	NAG	B	1014	14/15	0.87	0.23	-	46,54,61,64	0
4	SO4	B	2002	5/5	0.96	0.21	-	73,74,76,76	0
2	NAG	A	1005	14/15	0.86	0.46	-	53,59,68,68	0
3	NDG	A	1004	14/15	0.90	0.17	-	48,56,59,61	0
5	YT3	B	3001	1/1	0.97	0.12	-	38,38,38,38	1

6.5 Other polymers

There are no such residues in this entry.