Full wwPDB X-ray Structure Validation Report (i)

Feb 1, 2016 – 11:55 AM GMT

PDB ID	:	3QCW
Title	:	Structure of neurexin 1 alpha (domains LNS1-LNS6), no splice inserts
Authors	:	Rudenko, G.
Deposited on	:	2011-01-17
Resolution	:	2.65 Å(reported)

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

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

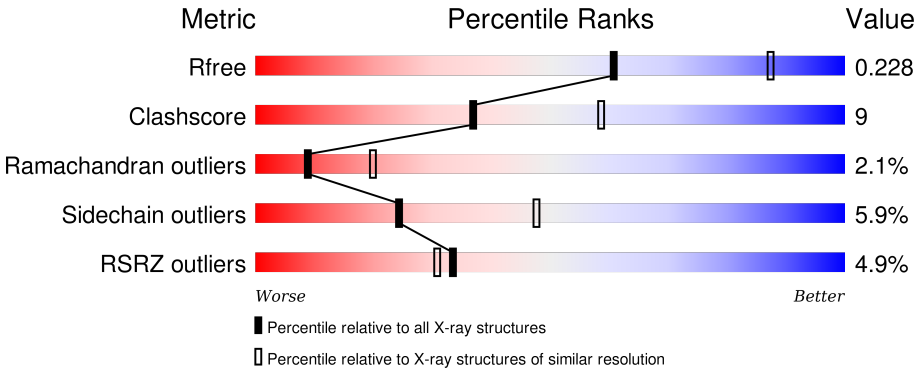
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	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 2.65 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	91344	3152 (2.70-2.62)
Clashscore	102246	3524 (2.70-2.62)
Ramachandran outliers	100387	3469 (2.70-2.62)
Sidechain outliers	100360	3469 (2.70-2.62)
RSRZ outliers	91569	3161 (2.70-2.62)

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	1245	4% 61% 17% • 19%
1	B	1245	4% 62% 16% • 19%

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 15440 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 Neurexin-1-alpha.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	1003	Total	C	N	O	S	0	0	0
			7692	4835	1326	1489	42			
1	B	1003	Total	C	N	O	S	0	0	0
			7692	4835	1326	1489	42			

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	210	GLN	ASN	ENGINEERED MUTATION	UNP Q28146
A	612	GLU	GLN	SEE REMARK 999	UNP Q28146
A	1112	PHE	ILE	SEE REMARK 999	UNP Q28146
B	210	GLN	ASN	ENGINEERED MUTATION	UNP Q28146
B	612	GLU	GLN	SEE REMARK 999	UNP Q28146
B	1112	PHE	ILE	SEE REMARK 999	UNP Q28146

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

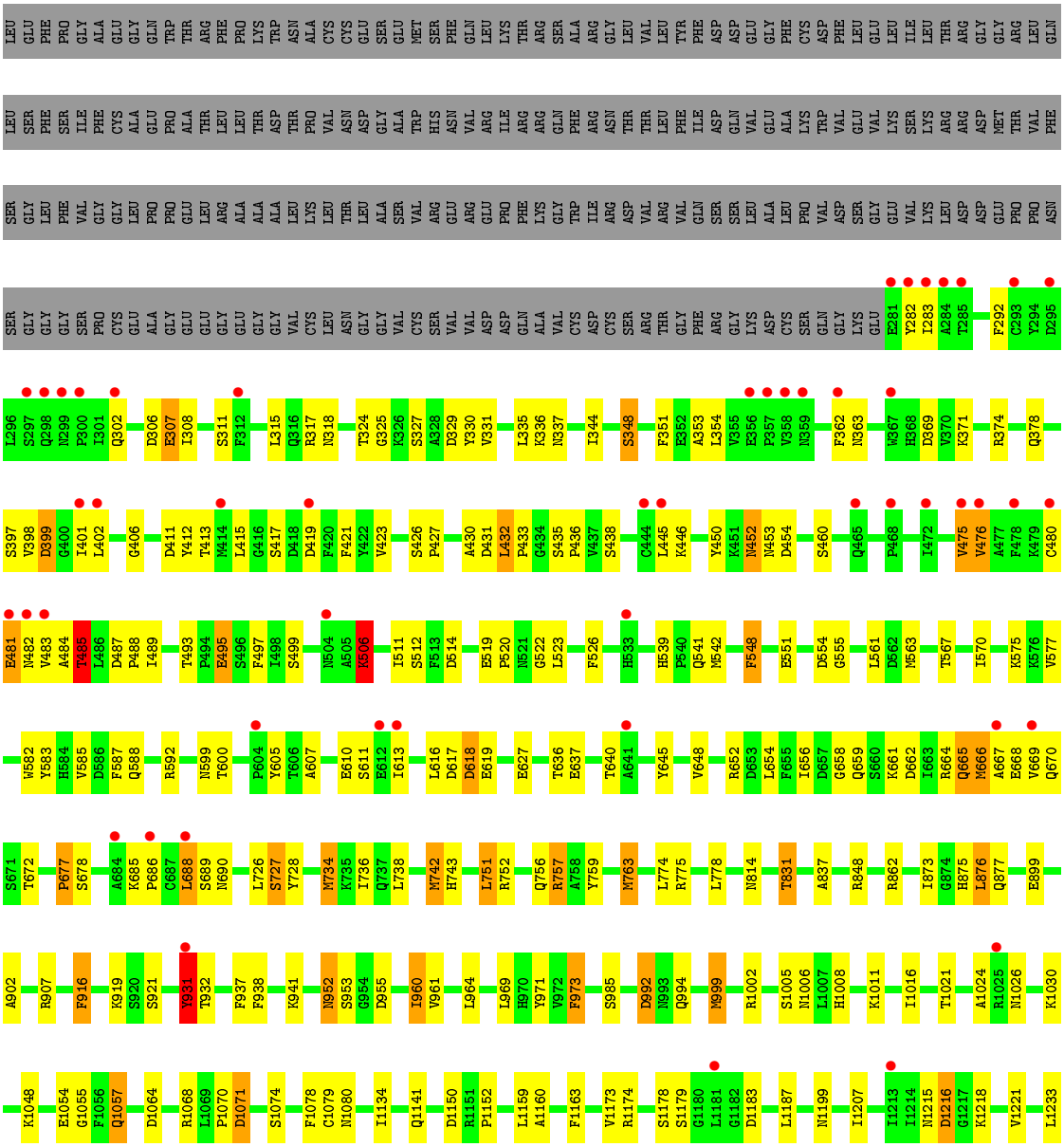
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	2	Total	C	N	O	0	0
			28	16	2	10		
2	B	2	Total	C	N	O	0	0
			28	16	2	10		

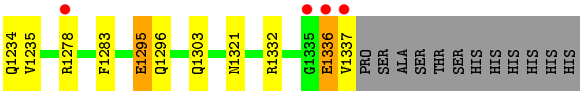
3 Residue-property plots (i)

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: Neurexin-1-alpha

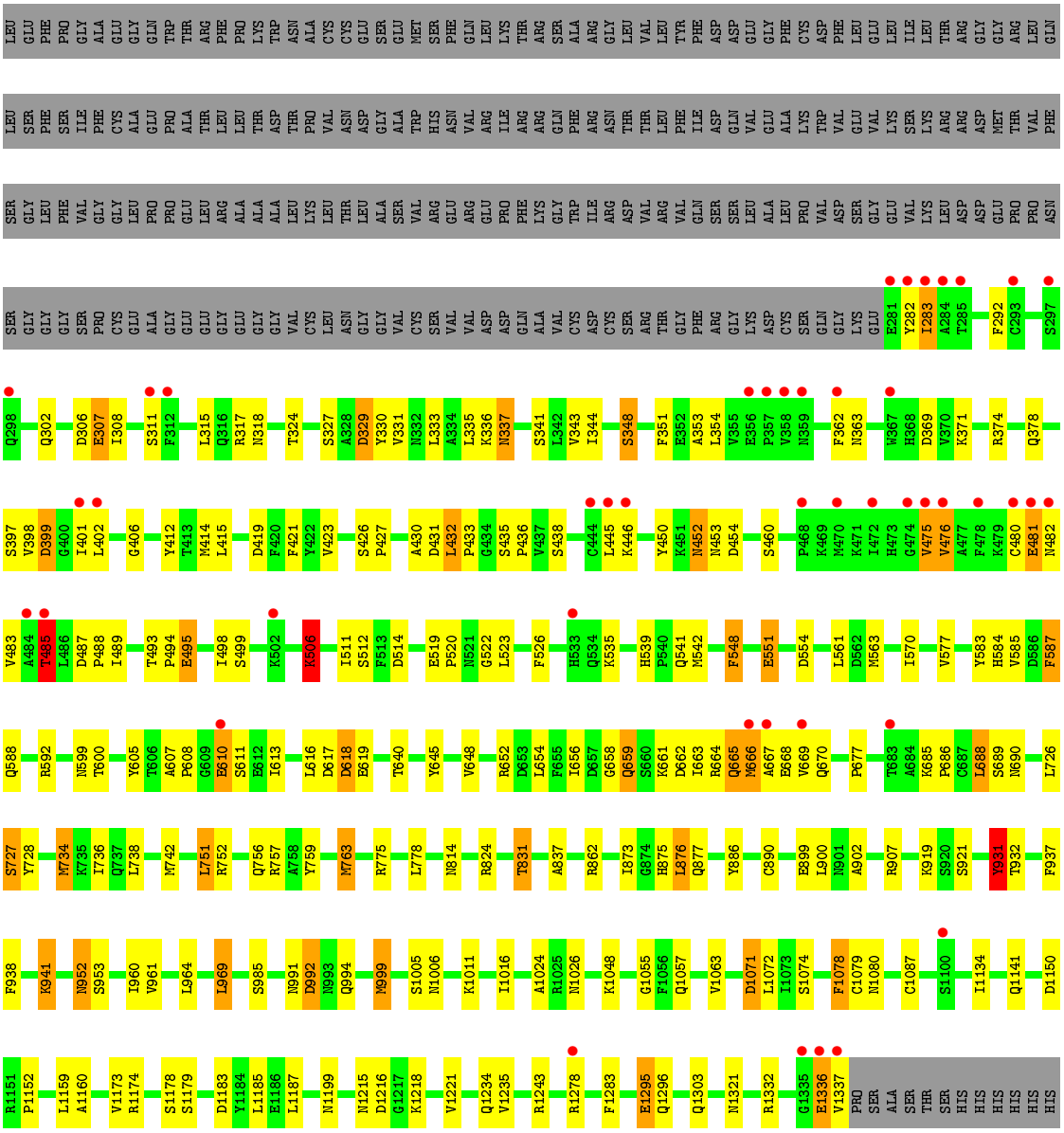
Chain A:





- Molecule 1: Neurexin-1-alpha

Chain B:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α, β, γ	60.95Å 114.54Å 159.58Å 90.61° 90.87° 92.18°	Depositor
Resolution (Å)	30.00 – 2.65 39.18 – 2.65	Depositor EDS
% Data completeness (in resolution range)	98.4 (30.00-2.65) 98.1 (39.18-2.65)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	3.62 (at 2.65Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.208 , 0.230 0.208 , 0.228	Depositor DCC
R_{free} test set	6451 reflections (5.53%)	DCC
Wilson B-factor (Å^2)	48.0	Xtriage
Anisotropy	0.441	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.30 , 47.2	EDS
Estimated twinning fraction	0.126 for h,-k,-l 0.008 for -h,k,-l 0.011 for -h,-k,l	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.33$	Xtriage
Outliers	0 of 123206 reflections	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	15440	wwPDB-VP
Average B, all atoms (Å^2)	65.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.74% 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: 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	0.86	6/7846 (0.1%)	0.84	9/10637 (0.1%)
1	B	0.83	6/7846 (0.1%)	0.83	9/10637 (0.1%)
All	All	0.84	12/15692 (0.1%)	0.83	18/21274 (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
1	A	0	3
1	B	0	2
All	All	0	5

All (12) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	1079	CYS	CB-SG	-11.10	1.63	1.82
1	A	1079	CYS	CB-SG	-10.89	1.63	1.82
1	A	1057	GLN	CG-CD	10.47	1.75	1.51
1	B	1057	GLN	CG-CD	8.90	1.71	1.51
1	A	992	ASP	CB-CG	6.22	1.64	1.51
1	B	992	ASP	CB-CG	6.06	1.64	1.51
1	B	551	GLU	CG-CD	5.87	1.60	1.51
1	B	1078	PHE	CD1-CE1	5.42	1.50	1.39
1	B	890	CYS	CB-SG	-5.17	1.73	1.81
1	A	1054	GLU	CD-OE1	5.16	1.31	1.25
1	A	916	PHE	CE1-CZ	-5.09	1.27	1.37
1	A	973	PHE	CE1-CZ	5.01	1.46	1.37

All (18) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	999	MET	CG-SD-CE	7.72	112.55	100.20
1	B	1071	ASP	CB-CG-OD1	6.73	124.35	118.30
1	A	999	MET	CG-SD-CE	6.63	110.81	100.20
1	A	941	LYS	CD-CE-NZ	-6.49	96.77	111.70
1	A	757	ARG	NE-CZ-NH2	-6.37	117.11	120.30
1	B	824	ARG	NE-CZ-NH2	-6.08	117.26	120.30
1	A	485	THR	N-CA-C	6.04	127.31	111.00
1	B	969	LEU	CA-CB-CG	-5.88	101.79	115.30
1	B	941	LYS	CD-CE-NZ	-5.85	98.24	111.70
1	A	1064	ASP	CB-CG-OD1	5.81	123.53	118.30
1	A	876	LEU	CB-CG-CD1	-5.69	101.33	111.00
1	A	969	LEU	CA-CB-CG	-5.66	102.28	115.30
1	A	992	ASP	CB-CG-OD2	5.52	123.27	118.30
1	B	734	MET	CG-SD-CE	5.32	108.72	100.20
1	A	1071	ASP	CB-CG-OD1	5.30	123.07	118.30
1	B	485	THR	N-CA-C	5.24	125.14	111.00
1	B	876	LEU	CB-CG-CD1	-5.16	102.23	111.00
1	B	992	ASP	CB-CG-OD2	5.15	122.94	118.30

There are no chirality outliers.

All (5) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	1078	PHE	Peptide
1	A	1215	ASN	Peptide
1	A	484	ALA	Peptide
1	B	1078	PHE	Peptide
1	B	1215	ASN	Peptide

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	7692	0	7454	146	1
1	B	7692	0	7454	139	1
2	A	28	0	25	0	0
2	B	28	0	25	0	0
All	All	15440	0	14958	285	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 9.

All (285) 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:1057:GLN:CG	1:A:1057:GLN:CD	1.75	1.51
1:A:931:TYR:HD1	1:A:932:THR:H	1.12	0.93
1:B:931:TYR:HD1	1:B:932:THR:H	1.16	0.93
1:B:667:ALA:HA	1:B:670:GLN:HB2	1.54	0.89
1:A:667:ALA:HA	1:A:670:GLN:HB2	1.56	0.85
1:A:618:ASP:HB3	1:A:619:GLU:OE2	1.86	0.76
1:A:519:GLU:HG3	1:A:648:VAL:HG22	1.70	0.74
1:B:302:GLN:HA	1:B:415:LEU:O	1.89	0.73
1:A:302:GLN:HA	1:A:415:LEU:O	1.89	0.72
1:B:618:ASP:HB3	1:B:619:GLU:OE2	1.90	0.71
1:B:519:GLU:HG3	1:B:648:VAL:HG22	1.71	0.71
1:A:599:ASN:O	1:A:600:THR:HB	1.90	0.70
1:B:599:ASN:O	1:B:600:THR:HB	1.90	0.70
1:B:306:ASP:OD2	1:B:374:ARG:HB3	1.93	0.68
1:B:1141:GLN:HE22	1:B:1295:GLU:HG2	1.57	0.68
1:B:727:SER:HB2	1:B:875:HIS:CD2	2.30	0.67
1:A:1141:GLN:HE22	1:A:1295:GLU:HG2	1.58	0.67
1:A:369:ASP:HB2	1:A:399:ASP:HA	1.77	0.66
1:A:282:TYR:HB3	1:A:460:SER:HB3	1.79	0.65
1:A:688:LEU:C	1:A:690:ASN:N	2.45	0.65
1:B:369:ASP:HB2	1:B:399:ASP:HA	1.79	0.64
1:B:282:TYR:HB3	1:B:460:SER:HB3	1.80	0.63
1:A:1216:ASP:OD2	1:A:1218:LYS:HB2	1.99	0.63
1:A:306:ASP:OD2	1:A:374:ARG:HB3	1.98	0.63
1:B:688:LEU:C	1:B:690:ASN:N	2.46	0.63
1:B:292:PHE:HB2	1:B:423:VAL:HB	1.80	0.63
1:B:668:GLU:C	1:B:670:GLN:H	2.03	0.62
1:B:488:PRO:HB3	1:B:652:ARG:HB3	1.81	0.62
1:A:292:PHE:HB2	1:A:423:VAL:HB	1.82	0.61
1:A:308:ILE:CD1	1:A:450:TYR:HD1	2.13	0.61
1:A:727:SER:HB2	1:A:875:HIS:CD2	2.35	0.61
1:A:452:ASN:ND2	1:A:454:ASP:H	1.99	0.60
1:B:688:LEU:C	1:B:688:LEU:HD12	2.21	0.60
1:B:1216:ASP:OD2	1:B:1218:LYS:HB2	2.01	0.60
1:B:1024:ALA:O	1:B:1026:ASN:ND2	2.35	0.60
1:A:668:GLU:C	1:A:670:GLN:H	2.06	0.59
1:B:430:ALA:HB2	1:B:438:SER:CB	2.31	0.59

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1159:LEU:HD23	1:B:1160:ALA:N	2.18	0.59
1:A:488:PRO:HB3	1:A:652:ARG:HB3	1.83	0.59
1:B:452:ASN:ND2	1:B:454:ASP:H	2.01	0.59
1:A:751:LEU:HD12	1:A:751:LEU:C	2.23	0.59
1:A:1159:LEU:HD23	1:A:1160:ALA:N	2.18	0.59
1:A:430:ALA:HB2	1:A:438:SER:CB	2.31	0.59
1:A:426:SER:HB2	1:A:427:PRO:HD2	1.85	0.59
1:B:308:ILE:CD1	1:B:450:TYR:HD1	2.16	0.58
1:A:751:LEU:HD12	1:A:751:LEU:O	2.03	0.58
1:A:539:HIS:HB2	1:A:542:MET:HE2	1.84	0.58
1:A:688:LEU:C	1:A:690:ASN:H	2.05	0.58
1:A:511:ILE:HD12	1:A:656:ILE:HD13	1.85	0.57
1:A:511:ILE:CG2	1:A:587:PHE:HB3	2.34	0.57
1:A:1011:LYS:HG3	1:A:1016:ILE:HG13	1.87	0.57
1:B:493:THR:HB	1:B:495:GLU:OE2	2.05	0.57
1:B:688:LEU:C	1:B:690:ASN:H	2.06	0.56
1:A:1024:ALA:O	1:A:1026:ASN:ND2	2.38	0.56
1:B:688:LEU:O	1:B:688:LEU:HD12	2.06	0.56
1:B:539:HIS:HB2	1:B:542:MET:HE2	1.86	0.56
1:B:726:LEU:HD22	1:B:902:ALA:HB3	1.88	0.56
1:B:563:MET:CE	1:B:607:ALA:HB3	2.36	0.56
1:B:511:ILE:CG2	1:B:587:PHE:HB3	2.35	0.56
1:B:426:SER:HB2	1:B:427:PRO:HD2	1.87	0.56
1:B:570:ILE:HD11	1:B:605:TYR:HB2	1.88	0.56
1:B:432:LEU:HD12	1:B:435:SER:HB2	1.88	0.55
1:B:331:VAL:HG23	1:B:344:ILE:HG12	1.89	0.55
1:B:511:ILE:HD12	1:B:656:ILE:HD13	1.88	0.55
1:A:563:MET:CE	1:A:607:ALA:HB3	2.37	0.55
1:A:1071:ASP:OD2	1:A:1074:SER:HB2	2.07	0.55
1:A:738:LEU:HD22	1:A:742:MET:HG2	1.89	0.55
1:A:331:VAL:HG23	1:A:344:ILE:HG12	1.90	0.54
1:B:992:ASP:OD2	1:B:994:GLN:NE2	2.41	0.54
1:A:688:LEU:HD12	1:A:688:LEU:C	2.28	0.54
1:A:336:LYS:HD2	1:A:436:PRO:HB2	1.89	0.54
1:A:548:PHE:HB2	1:A:561:LEU:HD12	1.90	0.54
1:A:599:ASN:O	1:A:600:THR:CB	2.55	0.53
1:B:1005:SER:O	1:B:1006:ASN:HB2	2.08	0.53
1:B:336:LYS:HD2	1:B:436:PRO:HB2	1.90	0.53
1:B:523:LEU:HB2	1:B:640:THR:OG1	2.08	0.53
1:B:599:ASN:O	1:B:600:THR:CB	2.56	0.53
1:A:493:THR:HB	1:A:495:GLU:OE2	2.09	0.53

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:475:VAL:O	1:A:476:VAL:HB	2.08	0.53
1:B:738:LEU:HD22	1:B:742:MET:HG2	1.91	0.53
1:A:432:LEU:HD12	1:A:435:SER:HB2	1.91	0.53
1:B:1011:LYS:HG3	1:B:1016:ILE:HG13	1.90	0.53
1:B:475:VAL:O	1:B:476:VAL:HB	2.09	0.52
1:A:1183:ASP:HA	1:A:1199:ASN:O	2.09	0.52
1:B:548:PHE:HB2	1:B:561:LEU:HD12	1.92	0.52
1:B:551:GLU:OE1	1:B:640:THR:HG23	2.10	0.52
1:B:315:LEU:HD13	1:B:485:THR:HG23	1.92	0.52
1:B:324:THR:HG22	1:B:331:VAL:HG12	1.91	0.52
1:A:1150:ASP:O	1:A:1152:PRO:HD3	2.10	0.51
1:A:728:TYR:CE2	1:A:876:LEU:HD12	2.44	0.51
1:B:523:LEU:HD11	1:B:526:PHE:HB2	1.91	0.51
1:B:1278:ARG:CZ	1:B:1278:ARG:HB3	2.40	0.51
1:A:738:LEU:H	1:A:738:LEU:HD12	1.76	0.51
1:A:311:SER:HB2	1:A:446:LYS:HE2	1.93	0.50
1:B:931:TYR:CD1	1:B:932:THR:HG22	2.46	0.50
1:A:1278:ARG:HB3	1:A:1278:ARG:CZ	2.42	0.50
1:A:592:ARG:HH21	1:A:610:GLU:HA	1.77	0.50
1:B:654:LEU:HB3	1:B:661:LYS:HB2	1.93	0.49
1:A:315:LEU:HD13	1:A:485:THR:HG23	1.94	0.49
1:B:919:LYS:HG2	1:B:1055:GLY:O	2.12	0.49
1:B:438:SER:O	1:B:658:GLY:HA3	2.12	0.49
1:A:523:LEU:HD11	1:A:526:PHE:HB2	1.93	0.49
1:B:756:GLN:HG3	1:B:814:ASN:OD1	2.12	0.49
1:A:522:GLY:HA2	1:A:645:TYR:O	2.12	0.49
1:B:736:ILE:HD11	1:B:886:TYR:HB3	1.94	0.49
1:A:318:ASN:HA	1:A:335:LEU:O	2.12	0.49
1:A:351:PHE:CE1	1:A:406:GLY:HA3	2.48	0.48
1:A:315:LEU:O	1:A:363:ASN:HB2	2.13	0.48
1:B:311:SER:HB2	1:B:446:LYS:HE2	1.95	0.48
1:B:1071:ASP:OD2	1:B:1074:SER:HB2	2.12	0.48
1:B:726:LEU:HD22	1:B:902:ALA:CB	2.43	0.48
1:B:728:TYR:CE2	1:B:876:LEU:HD12	2.47	0.48
1:B:522:GLY:HA2	1:B:645:TYR:O	2.14	0.48
1:A:757:ARG:HD2	1:A:873:ILE:HD12	1.96	0.48
1:A:726:LEU:HD22	1:A:902:ALA:HB3	1.96	0.48
1:A:362:PHE:CE1	1:A:398:VAL:HG11	2.48	0.48
1:B:362:PHE:CE1	1:B:398:VAL:HG11	2.48	0.48
1:B:317:ARG:HG2	1:B:337:ASN:HA	1.96	0.48
1:B:324:THR:HG22	1:B:331:VAL:CG1	2.44	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:324:THR:HG22	1:A:331:VAL:HG12	1.94	0.48
1:B:738:LEU:H	1:B:738:LEU:HD12	1.79	0.48
1:A:523:LEU:HB2	1:A:640:THR:OG1	2.13	0.48
1:B:563:MET:HE1	1:B:607:ALA:HB3	1.96	0.47
1:A:563:MET:HE1	1:A:607:ALA:HB3	1.96	0.47
1:B:751:LEU:C	1:B:751:LEU:HD12	2.34	0.47
1:A:667:ALA:O	1:A:672:THR:OG1	2.21	0.47
1:B:1174:ARG:HD3	1:B:1296:GLN:HE21	1.79	0.47
1:B:514:ASP:HA	1:B:583:TYR:O	2.14	0.47
1:A:362:PHE:CZ	1:A:398:VAL:HG11	2.49	0.47
1:B:665:GLN:N	1:B:668:GLU:CB	2.78	0.47
1:B:318:ASN:HA	1:B:335:LEU:O	2.13	0.47
1:B:1150:ASP:O	1:B:1152:PRO:HD3	2.13	0.47
1:A:1174:ARG:HD3	1:A:1296:GLN:HE21	1.79	0.47
1:B:592:ARG:HH21	1:B:610:GLU:HA	1.79	0.47
1:B:759:TYR:HA	1:B:778:LEU:O	2.15	0.47
1:B:1159:LEU:C	1:B:1159:LEU:HD23	2.35	0.47
1:A:751:LEU:C	1:A:751:LEU:CD1	2.83	0.47
1:B:831:THR:HB	1:B:837:ALA:HA	1.96	0.47
1:A:511:ILE:HG23	1:A:587:PHE:HB3	1.96	0.47
1:B:511:ILE:HG22	1:B:587:PHE:HB3	1.96	0.47
1:B:430:ALA:HB2	1:B:438:SER:HB3	1.96	0.47
1:A:480:CYS:SG	1:A:481:GLU:N	2.83	0.47
1:A:577:VAL:O	1:A:583:TYR:HE1	1.98	0.47
1:B:960:ILE:HG12	1:B:961:VAL:N	2.30	0.47
1:A:430:ALA:HB2	1:A:438:SER:HB3	1.95	0.46
1:A:317:ARG:HG2	1:A:337:ASN:HA	1.97	0.46
1:A:688:LEU:O	1:A:688:LEU:HD12	2.15	0.46
1:B:362:PHE:CZ	1:B:398:VAL:HG11	2.51	0.46
1:B:964:LEU:HA	1:B:964:LEU:HD12	1.76	0.46
1:A:756:GLN:HG3	1:A:814:ASN:OD1	2.15	0.46
1:A:324:THR:HG22	1:A:331:VAL:CG1	2.45	0.46
1:A:665:GLN:N	1:A:668:GLU:CB	2.79	0.46
1:B:315:LEU:O	1:B:363:ASN:HB2	2.16	0.46
1:B:751:LEU:O	1:B:751:LEU:HD12	2.15	0.46
1:B:613:ILE:N	1:B:613:ILE:HD12	2.30	0.46
1:A:964:LEU:HD12	1:A:964:LEU:HA	1.74	0.46
1:A:992:ASP:OD2	1:A:994:GLN:NE2	2.49	0.46
1:A:1057:GLN:CG	1:A:1057:GLN:NE2	2.70	0.46
1:B:520:PRO:HB2	1:B:554:ASP:HA	1.98	0.45
1:A:514:ASP:HA	1:A:583:TYR:O	2.15	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:330:TYR:HE1	1:B:343:VAL:HG12	1.82	0.45
1:A:919:LYS:HG2	1:A:1055:GLY:O	2.17	0.45
1:A:636:THR:HG22	1:A:743:HIS:O	2.16	0.45
1:B:668:GLU:C	1:B:670:GLN:N	2.69	0.45
1:A:308:ILE:HD12	1:A:450:TYR:HD1	1.81	0.45
1:A:506:LYS:NZ	1:A:506:LYS:HB2	2.32	0.45
1:A:582:TRP:CZ3	1:A:652:ARG:HG2	2.52	0.45
1:A:570:ILE:HD11	1:A:605:TYR:HB2	1.98	0.45
1:A:613:ILE:N	1:A:613:ILE:HD12	2.31	0.45
1:B:665:GLN:O	1:B:666:MET:C	2.55	0.45
1:A:1159:LEU:C	1:A:1159:LEU:HD23	2.36	0.45
1:A:656:ILE:HG12	1:A:661:LYS:HG3	1.99	0.45
1:B:570:ILE:CD1	1:B:605:TYR:HB3	2.47	0.45
1:A:519:GLU:CG	1:A:648:VAL:HG22	2.45	0.45
1:B:1173:VAL:HG13	1:B:1187:LEU:HB3	1.99	0.45
1:B:487:ASP:HB2	1:B:664:ARG:CB	2.47	0.45
1:B:430:ALA:HB2	1:B:438:SER:HB2	1.98	0.44
1:B:570:ILE:HD13	1:B:605:TYR:HB3	1.99	0.44
1:A:551:GLU:OE1	1:A:640:THR:HG23	2.17	0.44
1:A:931:TYR:CD1	1:A:932:THR:HG22	2.52	0.44
1:A:1005:SER:O	1:A:1006:ASN:HB2	2.17	0.44
1:A:831:THR:HB	1:A:837:ALA:HA	1.98	0.44
1:B:1332:ARG:HG2	1:B:1332:ARG:HH11	1.82	0.44
1:B:351:PHE:CE1	1:B:406:GLY:HA3	2.52	0.44
1:B:480:CYS:SG	1:B:481:GLU:N	2.83	0.44
1:B:371:LYS:HB3	1:B:397:SER:HB3	1.99	0.44
1:A:567:THR:OG1	1:A:637:GLU:HG2	2.17	0.44
1:A:520:PRO:HB2	1:A:554:ASP:HA	2.00	0.44
1:B:498:ILE:HD12	1:B:667:ALA:HB3	1.99	0.44
1:B:1243:ARG:HA	1:B:1243:ARG:HD3	1.83	0.44
1:A:430:ALA:HB2	1:A:438:SER:HB2	1.99	0.44
1:A:511:ILE:HG22	1:A:587:PHE:HB3	1.98	0.44
1:B:763:MET:HE1	1:B:775:ARG:HA	2.00	0.44
1:A:307:GLU:C	1:A:308:ILE:HD13	2.38	0.44
1:A:311:SER:HB2	1:A:446:LYS:HB3	1.99	0.44
1:B:511:ILE:HG23	1:B:587:PHE:HB3	1.99	0.43
1:B:353:ALA:O	1:B:354:LEU:HD12	2.18	0.43
1:A:374:ARG:NH2	1:A:413:THR:O	2.51	0.43
1:A:438:SER:O	1:A:658:GLY:CA	2.66	0.43
1:A:432:LEU:HA	1:A:433:PRO:HD3	1.82	0.43
1:B:941:LYS:HE3	1:B:1087:CYS:SG	2.59	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1163:PHE:HA	1:A:1303:GLN:O	2.18	0.43
1:A:734:MET:HE3	1:A:736:ILE:HD12	2.00	0.43
1:A:955:ASP:OD1	1:A:1030:LYS:HG3	2.19	0.43
1:A:937:PHE:O	1:A:938:PHE:HB3	2.18	0.43
1:A:487:ASP:HB2	1:A:664:ARG:CB	2.49	0.43
1:A:512:SER:HA	1:A:585:VAL:O	2.18	0.43
1:A:1332:ARG:HG2	1:A:1332:ARG:HH11	1.83	0.43
1:B:991:ASN:N	1:B:991:ASN:OD1	2.49	0.43
1:A:426:SER:CB	1:A:427:PRO:HD2	2.49	0.43
1:A:759:TYR:HA	1:A:778:LEU:O	2.19	0.43
1:B:685:LYS:HA	1:B:686:PRO:HD2	1.82	0.43
1:B:1134:ILE:HG12	1:B:1303:GLN:HG2	1.99	0.43
1:A:371:LYS:HB3	1:A:397:SER:HB3	2.01	0.43
1:A:685:LYS:HA	1:A:686:PRO:HD2	1.79	0.43
1:A:688:LEU:O	1:A:690:ASN:N	2.52	0.42
1:A:542:MET:SD	1:A:848:ARG:HD3	2.59	0.42
1:B:282:TYR:CB	1:B:460:SER:HB3	2.46	0.42
1:A:331:VAL:HG13	1:A:331:VAL:O	2.19	0.42
1:A:973:PHE:HZ	1:A:1021:THR:HG21	1.84	0.42
1:B:432:LEU:HA	1:B:433:PRO:HD3	1.83	0.42
1:A:1134:ILE:HG12	1:A:1303:GLN:HG2	2.01	0.42
1:B:1183:ASP:HA	1:B:1199:ASN:O	2.19	0.42
1:A:668:GLU:C	1:A:670:GLN:N	2.72	0.42
1:A:282:TYR:CB	1:A:460:SER:HB3	2.47	0.42
1:A:1173:VAL:HG13	1:A:1187:LEU:HB3	2.00	0.42
1:A:1002:ARG:HH11	1:A:1002:ARG:HG2	1.85	0.42
1:A:1207:ILE:HD13	1:A:1233:LEU:HB2	2.00	0.42
1:B:329:ASP:OD1	1:B:414:MET:O	2.37	0.42
1:A:665:GLN:O	1:A:666:MET:C	2.57	0.42
1:B:570:ILE:CD1	1:B:605:TYR:CB	2.97	0.42
1:B:570:ILE:HD11	1:B:605:TYR:CB	2.49	0.42
1:A:431:ASP:O	1:A:432:LEU:C	2.58	0.42
1:B:506:LYS:HB2	1:B:506:LYS:NZ	2.34	0.42
1:B:577:VAL:O	1:B:583:TYR:HE1	2.02	0.42
1:A:916:PHE:N	1:A:916:PHE:CD2	2.88	0.42
1:A:497:PHE:CD1	1:A:497:PHE:C	2.93	0.42
1:A:374:ARG:HA	1:A:378:GLN:O	2.20	0.42
1:A:677:PRO:HB2	1:A:678:SER:H	1.74	0.42
1:A:931:TYR:CD1	1:A:932:THR:N	2.75	0.42
1:B:311:SER:HB2	1:B:446:LYS:HB3	2.01	0.42
1:A:398:VAL:HB	1:A:402:LEU:HB3	2.02	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:656:ILE:HG12	1:B:661:LYS:HG3	2.01	0.42
1:A:763:MET:HE1	1:A:775:ARG:HA	2.01	0.42
1:B:752:ARG:NH1	1:B:877:GLN:OE1	2.52	0.42
1:B:952:ASN:HD22	1:B:953:SER:N	2.18	0.41
1:B:435:SER:HA	1:B:436:PRO:HD3	1.91	0.41
1:A:960:ILE:HG12	1:A:961:VAL:N	2.35	0.41
1:B:348:SER:HB2	1:B:412:TYR:HB2	2.01	0.41
1:A:306:ASP:CG	1:A:374:ARG:HH11	2.24	0.41
1:A:353:ALA:O	1:A:354:LEU:HD12	2.20	0.41
1:B:426:SER:CB	1:B:427:PRO:HD2	2.51	0.41
1:A:971:TYR:HH	1:A:1008:HIS:CE1	2.38	0.41
1:A:1068:ARG:O	1:A:1070:PRO:HD3	2.20	0.41
1:B:663:ILE:HG13	1:B:663:ILE:H	1.71	0.41
1:B:333:LEU:HD12	1:B:341:SER:O	2.21	0.41
1:B:1063:VAL:HG21	1:B:1072:LEU:HD11	2.01	0.41
1:B:307:GLU:C	1:B:308:ILE:HD13	2.41	0.41
1:A:763:MET:HE1	1:A:774:LEU:HD23	2.02	0.41
1:B:438:SER:O	1:B:658:GLY:CA	2.69	0.41
1:A:654:LEU:HB3	1:A:661:LYS:HB2	2.02	0.41
1:A:555:GLY:O	1:A:577:VAL:HG22	2.21	0.41
1:A:921:SER:HA	1:A:1080:ASN:O	2.21	0.41
1:B:757:ARG:HD2	1:B:873:ILE:HD12	2.02	0.41
1:B:283:ILE:HG12	1:B:446:LYS:HG3	2.03	0.41
1:B:398:VAL:HB	1:B:402:LEU:HB3	2.03	0.41
1:B:921:SER:HA	1:B:1080:ASN:O	2.21	0.41
1:B:607:ALA:HA	1:B:608:PRO:HD3	1.91	0.40
1:B:431:ASP:O	1:B:432:LEU:C	2.60	0.40
1:A:330:TYR:CD2	1:A:433:PRO:HB2	2.56	0.40
1:B:514:ASP:OD1	1:B:584:HIS:ND1	2.54	0.40
1:A:952:ASN:HD22	1:A:953:SER:N	2.19	0.40
1:B:512:SER:HA	1:B:585:VAL:O	2.21	0.40
1:A:752:ARG:NH1	1:A:877:GLN:OE1	2.53	0.40
1:A:325:GLY:HA2	1:A:417:SER:HB2	2.02	0.40
1:B:331:VAL:O	1:B:331:VAL:HG13	2.22	0.40
1:B:659:GLN:HB3	1:B:659:GLN:HE21	1.71	0.40
1:B:937:PHE:O	1:B:938:PHE:HB3	2.21	0.40
1:A:348:SER:HB2	1:A:412:TYR:HB2	2.03	0.40
1:B:688:LEU:O	1:B:690:ASN:N	2.53	0.40
1:A:734:MET:CE	1:A:736:ILE:HD12	2.52	0.40
1:B:665:GLN:H	1:B:668:GLU:CB	2.35	0.40
1:B:494:PRO:HA	1:B:648:VAL:HG12	2.04	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:374:ARG:HA	1:B:378:GLN:O	2.22	0.40
1:A:1030:LYS:HA	1:A:1030:LYS:HD3	1.86	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:411:ASP:OD2	1:B:652:ARG:NH2[1_464]	2.15	0.05

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	1001/1245 (80%)	910 (91%)	70 (7%)	21 (2%)	9 20
1	B	1001/1245 (80%)	913 (91%)	67 (7%)	21 (2%)	9 20
All	All	2002/2490 (80%)	1823 (91%)	137 (7%)	42 (2%)	9 20

All (42) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	327	SER
1	A	506	LYS
1	A	666	MET
1	A	669	VAL
1	A	677	PRO
1	A	1179	SER
1	A	1336	GLU
1	B	327	SER
1	B	485	THR
1	B	506	LYS
1	B	665	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	666	MET
1	B	669	VAL
1	B	677	PRO
1	B	1179	SER
1	B	1336	GLU
1	A	475	VAL
1	A	476	VAL
1	A	483	VAL
1	A	485	THR
1	A	665	GLN
1	A	689	SER
1	A	1048	LYS
1	B	401	ILE
1	B	475	VAL
1	B	476	VAL
1	B	483	VAL
1	B	689	SER
1	B	1048	LYS
1	A	401	ILE
1	A	481	GLU
1	A	618	ASP
1	A	931	TYR
1	B	481	GLU
1	B	618	ASP
1	A	399	ASP
1	A	453	ASN
1	A	1216	ASP
1	B	399	ASP
1	B	453	ASN
1	B	931	TYR
1	B	337	ASN

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.

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	834/1058 (79%)	786 (94%)	48 (6%)	25	48
1	B	834/1058 (79%)	784 (94%)	50 (6%)	24	47
All	All	1668/2116 (79%)	1570 (94%)	98 (6%)	24	48

All (98) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	283	ILE
1	A	307	GLU
1	A	329	ASP
1	A	348	SER
1	A	419	ASP
1	A	421	PHE
1	A	432	LEU
1	A	445	LEU
1	A	452	ASN
1	A	482	ASN
1	A	489	ILE
1	A	495	GLU
1	A	499	SER
1	A	506	LYS
1	A	541	GLN
1	A	548	PHE
1	A	575	LYS
1	A	588	GLN
1	A	611	SER
1	A	616	LEU
1	A	617	ASP
1	A	627	GLU
1	A	659	GLN
1	A	662	ASP
1	A	688	LEU
1	A	727	SER
1	A	734	MET
1	A	742	MET
1	A	751	LEU
1	A	763	MET
1	A	831	THR
1	A	862	ARG

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	899	GLU
1	A	907	ARG
1	A	931	TYR
1	A	952	ASN
1	A	960	ILE
1	A	985	SER
1	A	999	MET
1	A	1178	SER
1	A	1221	VAL
1	A	1234	GLN
1	A	1235	VAL
1	A	1283	PHE
1	A	1295	GLU
1	A	1321	ASN
1	A	1336	GLU
1	A	1337	VAL
1	B	283	ILE
1	B	307	GLU
1	B	329	ASP
1	B	348	SER
1	B	419	ASP
1	B	421	PHE
1	B	432	LEU
1	B	445	LEU
1	B	452	ASN
1	B	482	ASN
1	B	489	ILE
1	B	495	GLU
1	B	499	SER
1	B	506	LYS
1	B	535	LYS
1	B	541	GLN
1	B	548	PHE
1	B	587	PHE
1	B	588	GLN
1	B	610	GLU
1	B	611	SER
1	B	616	LEU
1	B	617	ASP
1	B	659	GLN
1	B	662	ASP
1	B	688	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	727	SER
1	B	734	MET
1	B	751	LEU
1	B	763	MET
1	B	831	THR
1	B	862	ARG
1	B	899	GLU
1	B	900	LEU
1	B	907	ARG
1	B	931	TYR
1	B	952	ASN
1	B	969	LEU
1	B	985	SER
1	B	999	MET
1	B	1178	SER
1	B	1185	LEU
1	B	1221	VAL
1	B	1234	GLN
1	B	1235	VAL
1	B	1283	PHE
1	B	1295	GLU
1	B	1321	ASN
1	B	1336	GLU
1	B	1337	VAL

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (20) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	365	ASN
1	A	439	ASN
1	A	452	ASN
1	A	482	ASN
1	A	659	GLN
1	A	810	ASN
1	A	892	ASN
1	A	994	GLN
1	A	1141	GLN
1	A	1321	ASN
1	B	365	ASN
1	B	452	ASN
1	B	482	ASN
1	B	659	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	810	ASN
1	B	892	ASN
1	B	935	HIS
1	B	1141	GLN
1	B	1188	HIS
1	B	1321	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

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	$\#\|Z\| > 2$
2	NAG	A	2000	1,2	14,14,15	0.74	0	15,19,21	2.32	5 (33%)
2	NAG	A	2001	2	14,14,15	0.71	1 (7%)	15,19,21	1.98	3 (20%)
2	NAG	B	2000	1,2	14,14,15	0.70	0	15,19,21	2.37	5 (33%)
2	NAG	B	2001	2	14,14,15	0.72	0	15,19,21	1.95	3 (20%)

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	2000	1,2	-	0/6/23/26	0/1/1/1
2	NAG	A	2001	2	-	0/6/23/26	0/1/1/1
2	NAG	B	2000	1,2	-	0/6/23/26	0/1/1/1
2	NAG	B	2001	2	-	0/6/23/26	0/1/1/1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	2001	NAG	C1-C2	2.21	1.55	1.52

All (16) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	2001	NAG	C2-N2-C7	-4.69	117.01	123.04
2	B	2001	NAG	C2-N2-C7	-4.52	117.23	123.04
2	A	2000	NAG	O7-C7-C8	-3.47	115.69	122.06
2	B	2000	NAG	O7-C7-C8	-3.46	115.70	122.06
2	B	2001	NAG	C3-C4-C5	-3.00	104.97	110.20
2	A	2001	NAG	C3-C4-C5	-2.91	105.13	110.20
2	B	2000	NAG	O6-C6-C5	2.14	118.40	111.33
2	A	2000	NAG	O6-C6-C5	2.17	118.50	111.33
2	A	2000	NAG	C4-C3-C2	2.19	114.64	111.23
2	B	2000	NAG	C4-C3-C2	2.23	114.69	111.23
2	B	2000	NAG	C2-N2-C7	2.67	126.46	123.04
2	A	2000	NAG	C2-N2-C7	3.55	127.59	123.04
2	B	2001	NAG	O5-C5-C6	4.37	116.82	107.35
2	A	2001	NAG	O5-C5-C6	4.47	117.03	107.35
2	A	2000	NAG	C1-O5-C5	5.56	119.31	112.25
2	B	2000	NAG	C1-O5-C5	6.29	120.23	112.25

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.6 Ligand geometry (i)

There are no ligands in this entry.

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	1003/1245 (80%)	0.06	54 (5%)	29	27	9, 61, 127, 181	0
1	B	1003/1245 (80%)	0.11	45 (4%)	37	35	9, 64, 131, 190	0
All	All	2006/2490 (80%)	0.09	99 (4%)	33	31	9, 62, 128, 190	0

All (99) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	1337	VAL	8.8
1	B	472	ILE	7.4
1	B	481	GLU	6.2
1	A	1337	VAL	5.9
1	A	478	PHE	5.9
1	B	284	ALA	5.5
1	A	481	GLU	5.4
1	A	358	VAL	5.2
1	B	293	CYS	5.2
1	A	359	ASN	5.1
1	A	282	TYR	4.9
1	B	1336	GLU	4.8
1	A	283	ILE	4.8
1	A	480	CYS	4.7
1	B	283	ILE	4.7
1	A	284	ALA	4.7
1	B	475	VAL	4.6
1	B	478	PHE	4.4
1	B	357	PRO	4.2
1	B	1278	ARG	4.2
1	B	358	VAL	4.2
1	B	480	CYS	4.1
1	B	359	ASN	4.0
1	B	356	GLU	4.0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	1335	GLY	3.9
1	B	1335	GLY	3.7
1	B	281	GLU	3.6
1	A	669	VAL	3.6
1	A	300	PRO	3.5
1	A	356	GLU	3.5
1	B	476	VAL	3.5
1	A	1336	GLU	3.5
1	A	472	ILE	3.4
1	B	669	VAL	3.3
1	B	282	TYR	3.3
1	A	445	LEU	3.2
1	B	401	ILE	3.2
1	A	475	VAL	3.2
1	B	470	MET	3.1
1	B	311	SER	3.0
1	A	476	VAL	3.0
1	B	362	PHE	3.0
1	B	298	GLN	3.0
1	B	533	HIS	2.9
1	A	367	TRP	2.9
1	B	485	THR	2.8
1	B	445	LEU	2.8
1	A	613	ILE	2.8
1	A	1278	ARG	2.7
1	A	684	ALA	2.7
1	A	357	PRO	2.7
1	A	444	CYS	2.7
1	A	533	HIS	2.6
1	A	419	ASP	2.6
1	B	666	MET	2.6
1	A	299	ASN	2.5
1	B	444	CYS	2.5
1	A	281	GLU	2.5
1	A	482	ASN	2.5
1	A	667	ALA	2.5
1	B	683	THR	2.5
1	A	297	SER	2.5
1	B	484	ALA	2.5
1	B	482	ASN	2.5
1	A	1213	ILE	2.4
1	A	401	ILE	2.4

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	686	PRO	2.4
1	A	641	ALA	2.4
1	B	367	TRP	2.4
1	A	402	LEU	2.3
1	A	688	LEU	2.3
1	A	293	CYS	2.3
1	B	446	LYS	2.3
1	A	604	PRO	2.3
1	B	667	ALA	2.3
1	A	504	ASN	2.3
1	A	302	GLN	2.3
1	A	1181	LEU	2.3
1	A	483	VAL	2.3
1	B	468	PRO	2.2
1	B	502	LYS	2.2
1	A	468	PRO	2.2
1	A	1025	ARG	2.2
1	A	465	GLN	2.2
1	B	312	PHE	2.2
1	B	474	GLY	2.2
1	B	297	SER	2.1
1	B	610	GLU	2.1
1	A	285	THR	2.1
1	B	285	THR	2.1
1	B	402	LEU	2.1
1	A	612	GLU	2.1
1	A	312	PHE	2.1
1	A	298	GLN	2.1
1	A	295	ASP	2.1
1	B	1100	SER	2.0
1	A	362	PHE	2.0
1	A	414	MET	2.0
1	A	931	TYR	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, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
2	NAG	B	2000	14/15	0.87	0.20	-0.03	59,76,83,85	0
2	NAG	A	2000	14/15	0.89	0.15	-0.62	60,76,81,84	0
2	NAG	A	2001	14/15	0.85	0.29	-	77,89,96,100	0
2	NAG	B	2001	14/15	0.85	0.33	-	79,91,99,102	0

6.4 Ligands (i)

There are no ligands in this entry.

6.5 Other polymers (i)

There are no such residues in this entry.