



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 01:25 PM UTC

PDB ID : 3MJG / pdb_00003mjg
Title : The structure of a platelet derived growth factor receptor complex
Authors : Shim, A.H.R.; He, X.
Deposited on : 2010-04-12
Resolution : 2.30 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

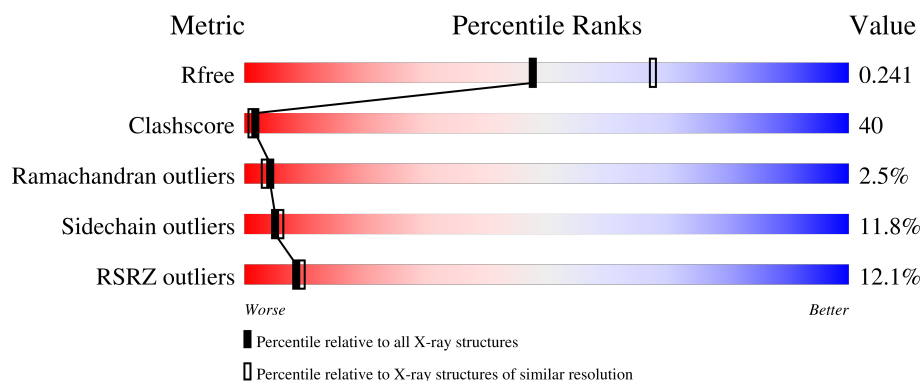
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.30 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}	180053	6319 (2.30-2.30)
Clashscore	190562	6919 (2.30-2.30)
Ramachandran outliers	187476	6854 (2.30-2.30)
Sidechain outliers	187428	6854 (2.30-2.30)
RSRZ outliers	180081	6325 (2.30-2.30)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. 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	172	2% 28% 23% 5% 44%
1	B	172	% 35% 18% 5% 41%
2	X	289	3% 40% 44% 10% 5%
2	Y	289	27% 39% 46% 10% 6%

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

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
4	NAG	X	3	X	-	-	-
4	NAG	X	5	X	-	-	-
4	NAG	X	7	X	-	-	-
4	NAG	Y	1	X	-	-	-
4	NAG	Y	5	X	-	-	-

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 7254 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 Platelet-derived growth factor subunit B.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	97	Total	C	N	O	S	0	0	0
			776	483	147	137	9			
1	B	101	Total	C	N	O	S	0	0	0
			802	500	151	142	9			

There are 14 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	105	HIS	-	expression tag	UNP P01127
A	106	HIS	-	expression tag	UNP P01127
A	107	HIS	-	expression tag	UNP P01127
A	108	HIS	-	expression tag	UNP P01127
A	109	HIS	-	expression tag	UNP P01127
A	110	HIS	-	expression tag	UNP P01127
A	111	HIS	-	expression tag	UNP P01127
B	105	HIS	-	expression tag	UNP P01127
B	106	HIS	-	expression tag	UNP P01127
B	107	HIS	-	expression tag	UNP P01127
B	108	HIS	-	expression tag	UNP P01127
B	109	HIS	-	expression tag	UNP P01127
B	110	HIS	-	expression tag	UNP P01127
B	111	HIS	-	expression tag	UNP P01127

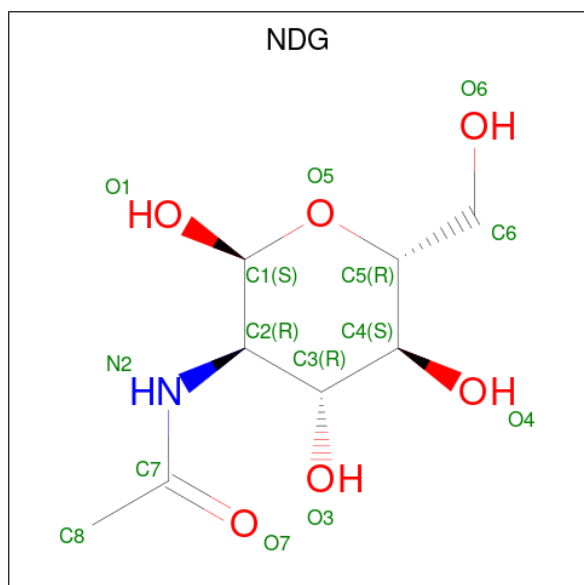
- Molecule 2 is a protein called Beta-type platelet-derived growth factor receptor.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	X	274	Total	C	N	O	S	0	0	0
			2159	1367	352	430	10			
2	Y	273	Total	C	N	O	S	0	0	0
			2151	1361	351	429	10			

There are 14 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
X	315	HIS	-	expression tag	UNP P09619
X	316	HIS	-	expression tag	UNP P09619
X	317	HIS	-	expression tag	UNP P09619
X	318	HIS	-	expression tag	UNP P09619
X	319	HIS	-	expression tag	UNP P09619
X	320	HIS	-	expression tag	UNP P09619
X	321	HIS	-	expression tag	UNP P09619
Y	315	HIS	-	expression tag	UNP P09619
Y	316	HIS	-	expression tag	UNP P09619
Y	317	HIS	-	expression tag	UNP P09619
Y	318	HIS	-	expression tag	UNP P09619
Y	319	HIS	-	expression tag	UNP P09619
Y	320	HIS	-	expression tag	UNP P09619
Y	321	HIS	-	expression tag	UNP P09619

- Molecule 3 is 2-acetamido-2-deoxy- α -D-glucopyranose (CCD ID: NDG) (formula: $C_8H_{15}NO_6$).



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

- Molecule 4 is 2-acetamido-2-deoxy- β -D-glucopyranose (CCD ID: NAG) (formula: $C_8H_{15}NO_6$).



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

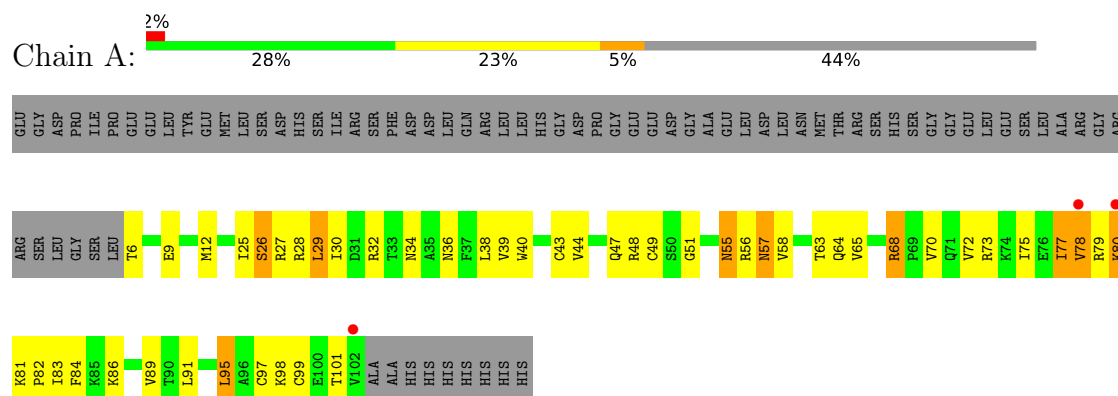
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	204	Total 204	O 204	0	0
5	B	188	Total 188	O 188	0	0
5	X	386	Total 386	O 386	0	0
5	Y	392	Total 392	O 392	0	0

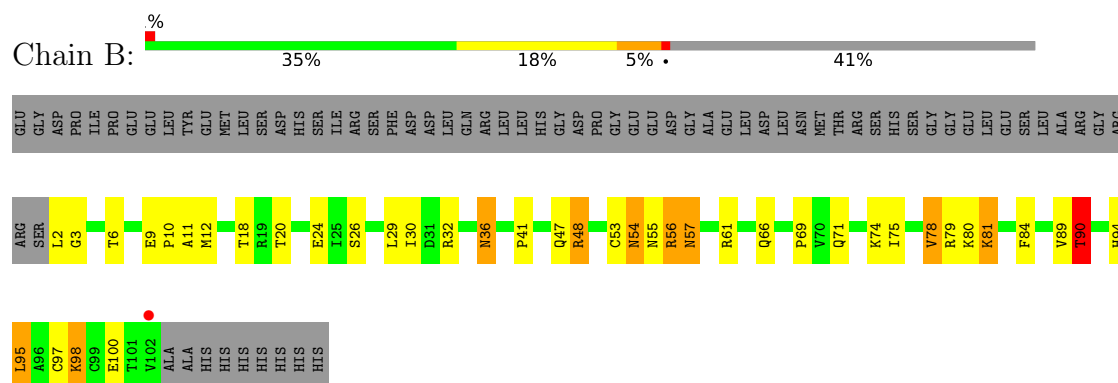
3 Residue-property plots

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

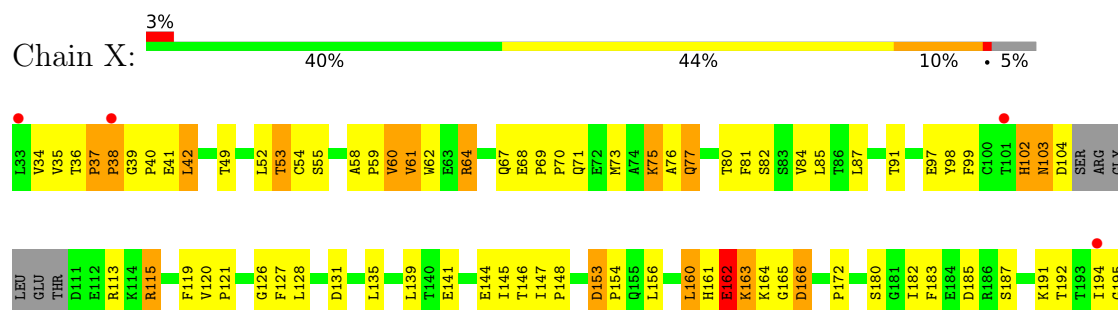
• Molecule 1: Platelet-derived growth factor subunit B

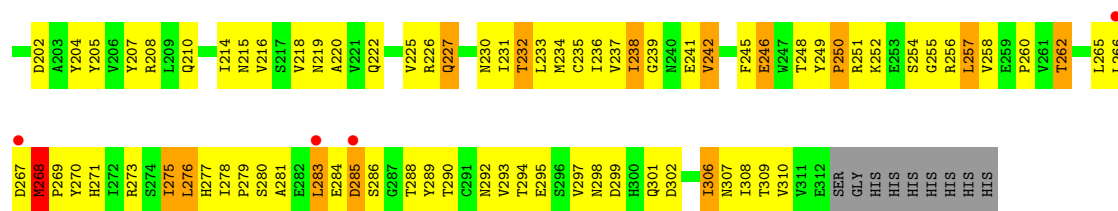


• Molecule 1: Platelet-derived growth factor subunit B

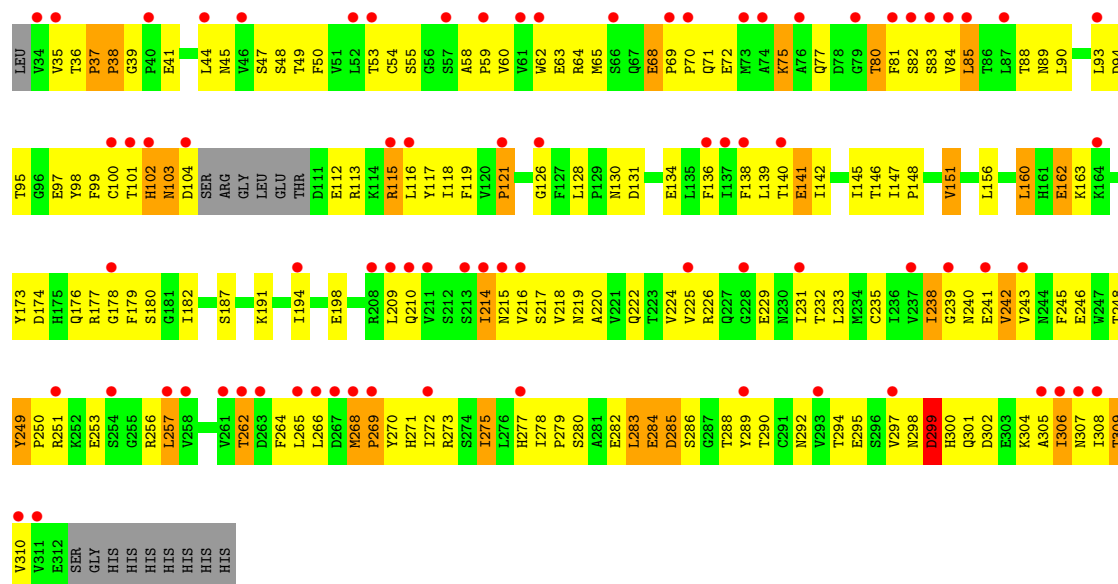


• Molecule 2: Beta-type platelet-derived growth factor receptor





● Molecule 2: Beta-type platelet-derived growth factor receptor



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	78.47Å 116.82Å 134.15Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	44.24 – 2.30 44.24 – 2.30	Depositor EDS
% Data completeness (in resolution range)	98.9 (44.24-2.30) 98.8 (44.24-2.30)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	0.06	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.32 (at 2.20Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.237 , 0.277 0.242 , 0.241	Depositor DCC
R_{free} test set	3172 reflections (5.08%)	wwPDB-VP
Wilson B-factor (Å ²)	44.9	Xtriage
Anisotropy	0.167	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 75.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	7254	wwPDB-VP
Average B, all atoms (Å ²)	66.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.60% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 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, NDG

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	0.70	0/787	1.03	3/1064 (0.3%)
1	B	0.77	2/813 (0.2%)	1.20	6/1099 (0.5%)
2	X	0.57	0/2205	1.11	13/3013 (0.4%)
2	Y	0.45	0/2197	0.94	10/3002 (0.3%)
All	All	0.58	2/6002 (0.0%)	1.05	32/8178 (0.4%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	54	ASN	CG-OD1	5.35	1.33	1.23
1	B	90	THR	CA-CB	5.23	1.60	1.53

All (32) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	X	102	HIS	N-CA-C	10.01	123.58	112.97
2	X	103	ASN	N-CA-C	9.16	124.34	110.14
2	X	147	ILE	N-CA-C	-8.86	99.50	107.56
2	X	162	GLU	N-CA-C	-7.46	98.41	110.20
2	X	268	MET	CA-C-N	-7.32	110.69	119.84
2	X	268	MET	C-N-CA	-7.32	110.69	119.84
1	B	74	LYS	N-CA-C	-6.86	97.55	108.73
1	B	53	CYS	N-CA-C	-6.81	99.20	110.17
2	Y	162	GLU	N-CA-C	-6.58	100.74	110.48
1	B	84	PHE	N-CA-C	6.51	118.89	108.41
2	Y	68	GLU	CA-C-N	6.47	127.05	120.38
2	Y	68	GLU	C-N-CA	6.47	127.05	120.38
2	X	202	ASP	N-CA-C	-6.41	102.07	110.53
1	A	51	GLY	N-CA-C	-6.36	103.56	111.70
1	B	41	PRO	CA-C-N	6.36	125.93	119.19

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	41	PRO	C-N-CA	6.36	125.93	119.19
2	X	61	VAL	N-CA-C	6.33	118.25	108.44
2	X	153	ASP	CA-C-N	6.26	126.38	119.87
2	X	153	ASP	C-N-CA	6.26	126.38	119.87
2	Y	147	ILE	CA-C-N	6.10	127.47	119.84
2	Y	147	ILE	C-N-CA	6.10	127.47	119.84
2	Y	285	ASP	N-CA-C	-6.00	105.06	112.38
1	A	99	CYS	N-CA-C	-5.92	100.19	109.25
2	Y	103	ASN	N-CA-C	5.69	118.06	109.41
1	A	55	ASN	N-CA-C	5.62	117.16	109.18
2	X	285	ASP	N-CA-C	-5.46	105.72	112.38
2	X	144	GLU	N-CA-C	-5.20	103.67	110.53
2	Y	214	ILE	N-CA-C	5.19	115.32	107.80
2	X	37	PRO	N-CA-C	-5.12	104.46	110.70
1	B	94	HIS	N-CA-C	-5.09	100.88	109.07
2	Y	282	GLU	N-CA-C	-5.02	103.42	110.35
2	Y	269	PRO	N-CA-C	-5.01	102.14	112.47

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	776	0	803	64	0
1	B	802	0	833	49	0
2	X	2159	0	2088	170	0
2	Y	2151	0	2077	221	0
3	X	14	0	12	0	0
4	X	84	0	78	10	0
4	Y	98	0	91	13	0
5	A	204	0	0	15	0
5	B	188	0	0	11	0
5	X	386	0	0	33	0
5	Y	392	0	0	44	0
All	All	7254	0	5982	484	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 40.

All (484) 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:43:CYS:HB2	5:B:550:HOH:O	1.45	1.15
1:B:20:THR:HG22	1:B:47:GLN:HE22	1.11	1.08
2:X:268:MET:HB3	2:X:269:PRO:HD3	1.34	1.08
2:Y:268:MET:HB3	2:Y:269:PRO:HD3	1.37	1.04
1:A:49:CYS:HB2	5:A:553:HOH:O	1.58	1.01
2:Y:219:ASN:ND2	2:Y:220:ALA:H	1.61	0.98
2:X:219:ASN:HD22	2:X:220:ALA:N	1.62	0.98
2:X:268:MET:HB3	2:X:269:PRO:CD	1.95	0.96
1:A:40:TRP:HH2	1:B:54:ASN:HB2	1.31	0.95
2:X:219:ASN:ND2	2:X:220:ALA:H	1.68	0.92
2:Y:300:HIS:HB3	5:Y:13:HOH:O	1.69	0.91
2:Y:115:ARG:HH11	2:Y:115:ARG:HB2	1.34	0.91
1:A:40:TRP:CH2	1:B:54:ASN:HB2	2.06	0.90
1:B:36:ASN:HD22	1:B:36:ASN:H	1.16	0.88
2:Y:131:ASP:HB2	2:Y:134:GLU:HG2	1.56	0.86
2:Y:250:PRO:HA	5:Y:1224:HOH:O	1.75	0.86
2:Y:104:ASP:HA	5:Y:681:HOH:O	1.75	0.85
2:Y:88:THR:HA	5:Y:958:HOH:O	1.75	0.84
1:B:56:ARG:H	1:B:56:ARG:HD2	1.41	0.84
2:X:248:THR:CG2	2:X:290:THR:HB	2.08	0.83
1:A:12:MET:HG3	5:A:708:HOH:O	1.80	0.82
2:X:97:GLU:OE2	2:X:115:ARG:NH1	2.14	0.81
1:A:98:LYS:HD2	5:A:584:HOH:O	1.81	0.81
2:Y:136:PHE:HB3	2:Y:138:PHE:HE1	1.45	0.80
2:X:219:ASN:HD22	2:X:220:ALA:H	0.85	0.80
2:Y:288:THR:HG23	4:Y:7:NAG:HN2	1.46	0.80
2:Y:265:LEU:HD12	2:Y:271:HIS:HB3	1.64	0.79
1:A:36:ASN:HA	2:Y:242:VAL:HG23	1.63	0.79
2:Y:219:ASN:HD22	2:Y:220:ALA:H	1.30	0.79
2:Y:292:ASN:ND2	4:Y:6:NAG:H62	1.97	0.79
2:Y:126:GLY:HA2	2:Y:194:ILE:CD1	2.14	0.78
2:Y:140:THR:HG23	2:Y:297:VAL:CG1	2.15	0.77
2:Y:268:MET:HB3	2:Y:269:PRO:CD	2.13	0.77
2:Y:136:PHE:HB3	2:Y:138:PHE:CE1	2.20	0.77
2:X:248:THR:HG23	2:X:290:THR:HB	1.67	0.76
2:X:64:ARG:HG2	2:X:64:ARG:HH11	1.49	0.76
2:Y:295:GLU:OE1	2:Y:298:ASN:HB2	1.85	0.76

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:57:ASN:HB3	5:A:848:HOH:O	1.85	0.75
2:X:37:PRO:HD3	5:X:654:HOH:O	1.87	0.74
2:Y:295:GLU:HB2	5:Y:325:HOH:O	1.87	0.73
2:Y:283:LEU:C	2:Y:285:ASP:H	1.97	0.73
2:Y:231:ILE:HB	2:Y:278:ILE:HB	1.70	0.73
1:B:56:ARG:H	1:B:56:ARG:CD	2.02	0.73
1:B:2:LEU:HD12	1:B:3:GLY:H	1.55	0.72
2:Y:301:GLN:HG3	4:Y:6:NAG:O7	1.90	0.72
1:B:55:ASN:HA	1:B:56:ARG:NH1	2.04	0.72
2:X:69:PRO:O	2:X:71:GLN:HG3	1.89	0.71
2:X:214:ILE:HG23	2:X:237:VAL:HG21	1.73	0.71
2:X:182:ILE:HD12	2:X:182:ILE:O	1.90	0.71
2:X:227:GLN:HB2	5:X:328:HOH:O	1.90	0.70
2:Y:226:ARG:HD2	5:Y:1214:HOH:O	1.90	0.70
2:Y:286:SER:HA	2:Y:308:ILE:O	1.90	0.70
1:A:30:ILE:HD12	1:A:39:VAL:HG11	1.73	0.70
1:B:48:ARG:HG2	5:B:113:HOH:O	1.91	0.69
2:X:248:THR:HG22	5:X:704:HOH:O	1.90	0.69
2:X:214:ILE:HD11	2:X:295:GLU:HG3	1.74	0.69
2:Y:102:HIS:HB3	4:Y:3:NAG:H82	1.74	0.69
1:A:30:ILE:HD12	1:A:39:VAL:CG1	2.22	0.69
1:A:36:ASN:C	2:Y:242:VAL:HG23	2.18	0.69
2:Y:268:MET:CB	2:Y:269:PRO:HD3	2.17	0.69
2:Y:215:ASN:HA	2:Y:302:ASP:OD2	1.93	0.69
1:B:36:ASN:HA	2:X:242:VAL:HG23	1.75	0.69
2:Y:273:ARG:HD3	2:Y:275:ILE:HG22	1.74	0.69
2:X:85:LEU:HD23	2:X:85:LEU:H	1.59	0.68
2:Y:219:ASN:ND2	2:Y:220:ALA:N	2.37	0.68
2:Y:68:GLU:HB2	2:Y:71:GLN:NE2	2.09	0.68
1:A:68:ARG:HD2	1:B:9:GLU:OE2	1.93	0.68
1:B:20:THR:HG22	1:B:47:GLN:NE2	1.97	0.68
2:X:126:GLY:HA2	2:X:194:ILE:CD1	2.24	0.67
1:A:36:ASN:CA	2:Y:242:VAL:HG23	2.25	0.67
2:Y:75:LYS:HD2	2:Y:75:LYS:O	1.96	0.66
1:A:28:ARG:HG3	1:A:32:ARG:NH1	2.09	0.66
1:B:29:LEU:HD12	1:B:30:ILE:HD12	1.78	0.65
2:Y:173:TYR:CE1	2:Y:178:GLY:HA2	2.31	0.65
2:X:283:LEU:C	2:X:285:ASP:H	2.04	0.65
1:A:101:THR:HG22	5:A:661:HOH:O	1.96	0.65
2:X:266:LEU:HD23	5:X:388:HOH:O	1.97	0.65
1:A:40:TRP:NE1	2:Y:136:PHE:CE2	2.65	0.65

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:X:214:ILE:HD11	2:X:295:GLU:CG	2.26	0.65
2:Y:198:GLU:HB3	5:Y:1317:HOH:O	1.96	0.65
2:X:52:LEU:HB2	2:X:85:LEU:HD21	1.79	0.64
2:X:76:ALA:HA	5:X:1171:HOH:O	1.98	0.64
2:X:64:ARG:HH11	2:X:64:ARG:CG	2.09	0.64
2:Y:163:LYS:HB2	2:Y:187:SER:OG	1.97	0.64
2:X:60:VAL:O	2:X:73:MET:HE3	1.97	0.63
2:Y:115:ARG:HB2	2:Y:115:ARG:NH1	2.10	0.63
2:Y:216:VAL:O	2:Y:304:LYS:HG3	1.97	0.63
1:B:36:ASN:H	1:B:36:ASN:ND2	1.94	0.63
2:X:257:LEU:HD12	5:X:1134:HOH:O	1.97	0.63
2:Y:68:GLU:HB3	5:Y:659:HOH:O	1.97	0.63
2:X:194:ILE:HG21	5:X:936:HOH:O	1.97	0.63
2:Y:249:TYR:CD1	2:Y:249:TYR:N	2.67	0.62
1:A:78:VAL:O	1:A:81:LYS:HG2	1.99	0.62
2:X:218:VAL:HA	2:X:234:MET:O	1.99	0.62
2:X:288:THR:HG21	4:X:7:NAG:H82	1.81	0.62
2:X:292:ASN:ND2	4:X:6:NAG:H62	2.15	0.62
4:X:4:NAG:H62	5:X:399:HOH:O	1.99	0.62
1:B:56:ARG:HG3	2:Y:270:TYR:HE1	1.63	0.62
2:X:210:GLN:HG2	5:X:930:HOH:O	2.00	0.62
2:Y:209:LEU:HD12	5:Y:599:HOH:O	1.99	0.62
2:X:35:VAL:HG13	5:X:383:HOH:O	1.98	0.62
2:Y:141:GLU:HG3	5:Y:1113:HOH:O	2.00	0.62
2:Y:126:GLY:HA2	2:Y:194:ILE:HD11	1.81	0.62
1:A:80:LYS:O	1:A:80:LYS:HD3	2.00	0.61
2:Y:35:VAL:O	2:Y:54:CYS:HA	2.01	0.61
1:A:38:LEU:HD11	2:Y:209:LEU:CD1	2.29	0.61
2:Y:224:VAL:HG22	2:Y:309:THR:CG2	2.30	0.61
4:Y:4:NAG:H61	5:Y:504:HOH:O	2.00	0.61
4:Y:7:NAG:O3	4:Y:7:NAG:H83	2.01	0.61
1:B:32:ARG:O	2:X:262:THR:HG22	1.99	0.61
1:A:30:ILE:HD11	1:A:72:VAL:HG21	1.82	0.61
2:Y:48:SER:O	2:Y:90:LEU:HG	2.00	0.61
2:Y:49:THR:HA	5:Y:958:HOH:O	2.00	0.61
2:Y:97:GLU:HG2	2:Y:115:ARG:NH1	2.15	0.61
5:A:797:HOH:O	2:X:267:ASP:HB2	1.99	0.60
2:Y:241:GLU:HG3	2:Y:270:TYR:CZ	2.37	0.60
2:Y:292:ASN:OD1	2:Y:301:GLN:NE2	2.35	0.60
2:X:41:GLU:C	2:X:42:LEU:HD23	2.27	0.59
2:X:162:GLU:O	2:X:163:LYS:C	2.44	0.59

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:X:297:VAL:HG12	2:X:298:ASN:OD1	2.01	0.59
2:Y:97:GLU:HB3	2:Y:99:PHE:CE1	2.37	0.59
2:X:270:TYR:HD1	5:X:930:HOH:O	1.84	0.59
2:Y:97:GLU:HG2	2:Y:115:ARG:HH12	1.65	0.59
2:Y:248:THR:CG2	2:Y:290:THR:HB	2.32	0.59
1:A:40:TRP:HH2	1:B:54:ASN:CB	2.12	0.59
2:X:288:THR:HG23	4:X:7:NAG:HN2	1.67	0.59
2:Y:283:LEU:O	2:Y:285:ASP:N	2.35	0.59
2:Y:294:THR:HG23	5:Y:682:HOH:O	2.01	0.59
1:A:70:VAL:HG22	1:A:89:VAL:HG13	1.85	0.59
2:Y:119:PHE:O	2:Y:121:PRO:HD3	2.03	0.58
2:Y:210:GLN:HB3	2:Y:241:GLU:HB2	1.84	0.58
2:Y:99:PHE:CE2	2:Y:115:ARG:HB3	2.39	0.58
2:Y:238:ILE:HD12	2:Y:271:HIS:NE2	2.19	0.58
2:Y:265:LEU:HB2	2:Y:271:HIS:HB2	1.84	0.58
2:X:266:LEU:HB3	5:X:388:HOH:O	2.04	0.58
2:Y:209:LEU:HB3	5:Y:599:HOH:O	2.04	0.58
2:Y:288:THR:OG1	4:Y:7:NAG:H3	2.03	0.58
2:X:102:HIS:O	4:X:3:NAG:H82	2.03	0.57
2:Y:306:ILE:N	2:Y:306:ILE:HD13	2.19	0.57
4:Y:5:NAG:H2	5:Y:809:HOH:O	2.03	0.57
1:B:55:ASN:HA	1:B:56:ARG:HH11	1.69	0.57
2:Y:139:LEU:O	2:Y:209:LEU:HD23	2.03	0.57
1:B:36:ASN:HD22	1:B:36:ASN:N	1.89	0.57
1:B:100:GLU:HG3	5:B:950:HOH:O	2.03	0.57
2:Y:219:ASN:HD22	2:Y:220:ALA:N	1.99	0.57
1:A:47:GLN:O	1:A:48:ARG:HD3	2.03	0.57
2:X:187:SER:HB3	2:X:205:TYR:CD2	2.40	0.57
2:Y:54:CYS:HB2	2:Y:62:TRP:CZ2	2.40	0.56
1:A:73:ARG:HH12	2:Y:136:PHE:HE1	1.53	0.56
2:X:238:ILE:HD12	2:X:271:HIS:CE1	2.40	0.56
2:Y:41:GLU:HB3	5:Y:1191:HOH:O	2.05	0.56
2:Y:218:VAL:HG22	2:Y:304:LYS:HB3	1.86	0.56
2:Y:85:LEU:N	2:Y:85:LEU:HD23	2.21	0.56
2:X:52:LEU:HB2	2:X:85:LEU:CD2	2.35	0.56
2:Y:283:LEU:HD22	5:Y:348:HOH:O	2.05	0.56
1:A:78:VAL:O	1:A:78:VAL:HG13	2.06	0.55
2:X:183:PHE:O	2:X:208:ARG:NH2	2.39	0.55
2:X:187:SER:HB3	2:X:205:TYR:CE2	2.41	0.55
1:B:69:PRO:HA	1:B:90:THR:HA	1.87	0.55
2:Y:224:VAL:HG22	2:Y:309:THR:HG23	1.88	0.55

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:X:294:THR:HG22	2:X:301:GLN:HG2	1.89	0.55
1:A:75:ILE:HD13	2:Y:138:PHE:CZ	2.41	0.55
2:X:222:GLN:HG3	2:X:225:VAL:HG22	1.89	0.55
2:X:104:ASP:C	5:X:326:HOH:O	2.48	0.55
2:Y:138:PHE:O	2:Y:139:LEU:HD23	2.05	0.55
1:B:11:ALA:O	1:B:12:MET:HE2	2.07	0.55
2:Y:64:ARG:HH11	2:Y:64:ARG:HG2	1.72	0.55
1:A:34:ASN:HD21	2:Y:245:PHE:H	1.54	0.54
2:Y:273:ARG:HD3	2:Y:275:ILE:CG2	2.37	0.54
1:A:79:ARG:C	1:A:81:LYS:H	2.15	0.54
1:B:47:GLN:HG3	5:B:589:HOH:O	2.08	0.54
2:Y:63:GLU:HB3	5:Y:659:HOH:O	2.07	0.54
2:X:269:PRO:HB3	5:X:726:HOH:O	2.06	0.54
2:Y:264:PHE:CD1	2:Y:272:ILE:HG12	2.42	0.54
1:A:29:LEU:H	1:A:29:LEU:HD23	1.71	0.54
2:Y:85:LEU:HD23	2:Y:85:LEU:H	1.72	0.54
2:Y:298:ASN:O	2:Y:299:ASP:HB2	2.07	0.54
1:B:2:LEU:HD21	5:B:1309:HOH:O	2.08	0.54
2:Y:265:LEU:HB2	2:Y:271:HIS:CB	2.38	0.54
1:A:83:ILE:HA	5:A:699:HOH:O	2.08	0.54
2:X:283:LEU:HD12	2:X:284:GLU:N	2.24	0.53
2:Y:72:GLU:HG3	5:Y:354:HOH:O	2.08	0.53
2:Y:58:ALA:HB3	2:Y:102:HIS:CE1	2.43	0.53
2:Y:283:LEU:HD12	2:Y:284:GLU:N	2.23	0.53
2:Y:64:ARG:O	2:Y:65:MET:HB2	2.09	0.53
2:Y:77:GLN:HB3	5:Y:392:HOH:O	2.07	0.53
2:X:76:ALA:HB3	2:X:80:THR:HB	1.90	0.53
1:B:29:LEU:C	1:B:29:LEU:HD13	2.34	0.53
2:X:64:ARG:HD3	2:X:98:TYR:CZ	2.44	0.53
2:Y:99:PHE:CD2	2:Y:113:ARG:HD2	2.44	0.53
2:Y:238:ILE:HA	2:Y:270:TYR:O	2.08	0.53
2:X:233:LEU:HD12	2:X:233:LEU:N	2.23	0.53
2:Y:99:PHE:CD2	2:Y:115:ARG:HB3	2.44	0.53
1:B:98:LYS:HD2	5:B:950:HOH:O	2.09	0.53
2:X:53:THR:HG22	5:X:654:HOH:O	2.09	0.53
4:X:5:NAG:H61	4:X:5:NAG:O3	2.09	0.53
2:Y:35:VAL:HG12	2:Y:36:THR:N	2.24	0.53
2:X:64:ARG:HD3	2:X:98:TYR:CE2	2.43	0.53
2:X:238:ILE:HA	2:X:270:TYR:O	2.09	0.53
2:X:245:PHE:CD2	2:X:293:VAL:HG22	2.44	0.53
1:A:26:SER:OG	1:A:29:LEU:HD23	2.09	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:Y:257:LEU:HD23	5:Y:932:HOH:O	2.08	0.52
1:A:28:ARG:HG3	1:A:32:ARG:HH11	1.72	0.52
2:Y:119:PHE:C	2:Y:121:PRO:HD3	2.34	0.52
2:Y:225:VAL:CG1	2:Y:229:GLU:HB2	2.38	0.52
1:B:57:ASN:HB3	2:Y:268:MET:SD	2.48	0.52
1:A:28:ARG:NH1	1:A:32:ARG:HD2	2.24	0.52
2:Y:283:LEU:HD13	2:Y:310:VAL:HB	1.92	0.52
1:A:38:LEU:HD11	2:Y:209:LEU:HD11	1.91	0.52
1:A:77:ILE:HD12	1:A:77:ILE:O	2.09	0.52
2:X:283:LEU:HD12	2:X:284:GLU:H	1.75	0.52
1:A:73:ARG:HG3	1:A:73:ARG:NH1	2.25	0.52
2:Y:191:LYS:HD2	2:Y:198:GLU:OE2	2.09	0.52
1:A:26:SER:H	1:A:29:LEU:HD21	1.75	0.52
2:X:36:THR:HA	2:X:53:THR:O	2.10	0.52
2:X:292:ASN:CG	2:X:301:GLN:HE21	2.18	0.51
1:A:40:TRP:NE1	2:Y:136:PHE:HE2	2.06	0.51
2:X:153:ASP:HB3	2:X:156:LEU:HG	1.93	0.51
2:X:275:ILE:O	2:X:275:ILE:HG13	2.09	0.51
2:Y:151:VAL:HB	2:Y:156:LEU:HD12	1.91	0.51
1:A:75:ILE:HD13	2:Y:138:PHE:CE2	2.45	0.51
2:X:64:ARG:CG	2:X:64:ARG:NH1	2.72	0.51
2:X:172:PRO:HA	5:X:864:HOH:O	2.11	0.51
2:Y:222:GLN:HG3	2:Y:225:VAL:HG22	1.92	0.51
1:A:86:LYS:HE3	5:A:1229:HOH:O	2.10	0.51
2:X:258:VAL:HG21	2:X:278:ILE:HG12	1.92	0.51
2:X:269:PRO:HD2	5:X:388:HOH:O	2.11	0.51
2:X:76:ALA:HB1	5:X:579:HOH:O	2.10	0.51
2:Y:246:GLU:HG2	5:Y:646:HOH:O	2.10	0.51
2:X:231:ILE:HG13	2:X:281:ALA:HB2	1.93	0.51
2:X:126:GLY:HA2	2:X:194:ILE:HD12	1.93	0.51
2:X:256:ARG:HD2	5:X:955:HOH:O	2.10	0.51
2:Y:44:LEU:O	2:Y:121:PRO:HD2	2.11	0.51
1:A:56:ARG:HD2	5:A:797:HOH:O	2.10	0.51
2:Y:216:VAL:HB	2:Y:304:LYS:HG2	1.93	0.51
2:X:225:VAL:HG12	2:X:226:ARG:N	2.25	0.50
2:Y:60:VAL:CG2	2:Y:100:CYS:SG	3.00	0.50
2:Y:225:VAL:O	2:Y:310:VAL:HA	2.11	0.50
1:A:98:LYS:NZ	5:A:947:HOH:O	2.44	0.50
2:X:256:ARG:NH1	5:X:928:HOH:O	2.44	0.50
2:X:286:SER:HA	2:X:308:ILE:O	2.11	0.50
1:B:54:ASN:HB3	5:B:1140:HOH:O	2.10	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:X:37:PRO:HD2	2:X:53:THR:HG22	1.94	0.50
2:Y:306:ILE:HD13	2:Y:306:ILE:H	1.75	0.50
1:A:12:MET:HE2	5:A:708:HOH:O	2.11	0.50
1:B:61:ARG:HD2	5:B:454:HOH:O	2.10	0.50
2:X:62:TRP:CD1	2:X:85:LEU:HD22	2.46	0.50
2:Y:68:GLU:HG2	5:Y:806:HOH:O	2.10	0.50
2:Y:94:ASP:HA	5:Y:781:HOH:O	2.10	0.50
2:Y:265:LEU:CD1	2:Y:271:HIS:HB3	2.38	0.50
2:X:84:VAL:HG23	2:X:84:VAL:O	2.10	0.50
2:X:139:LEU:HD11	2:X:145:ILE:HD11	1.92	0.50
2:X:161:HIS:NE2	2:X:191:LYS:HE3	2.26	0.50
2:X:64:ARG:HD2	2:X:97:GLU:O	2.11	0.50
2:X:268:MET:CB	2:X:269:PRO:HD3	2.25	0.50
2:Y:69:PRO:HB2	2:Y:70:PRO:CD	2.42	0.50
1:B:66:GLN:HB2	1:B:95:LEU:HD21	1.94	0.50
2:Y:98:TYR:CD1	2:Y:118:ILE:HD12	2.46	0.50
2:X:127:PHE:CE1	2:X:192:THR:HG22	2.47	0.50
2:Y:145:ILE:O	2:Y:180:SER:HA	2.12	0.49
2:Y:269:PRO:O	2:Y:271:HIS:ND1	2.45	0.49
2:Y:162:GLU:O	2:Y:163:LYS:C	2.56	0.49
1:B:78:VAL:O	1:B:81:LYS:N	2.35	0.49
2:Y:182:ILE:HD12	2:Y:182:ILE:O	2.12	0.49
2:X:77:GLN:NE2	2:X:77:GLN:C	2.70	0.49
2:Y:60:VAL:HG13	2:Y:83:SER:HB2	1.94	0.49
2:X:91:THR:HG21	5:X:835:HOH:O	2.12	0.49
2:X:97:GLU:CD	2:X:115:ARG:HH12	2.19	0.49
2:Y:102:HIS:C	2:Y:103:ASN:HD22	2.19	0.49
2:Y:288:THR:CG2	4:Y:7:NAG:HN2	2.21	0.49
2:Y:54:CYS:O	2:Y:60:VAL:HG11	2.12	0.49
2:Y:210:GLN:HG3	2:Y:239:GLY:O	2.12	0.49
2:X:283:LEU:C	2:X:285:ASP:N	2.70	0.49
1:A:57:ASN:C	1:A:57:ASN:HD22	2.20	0.48
2:X:230:ASN:HD22	2:X:277:HIS:CE1	2.30	0.48
2:X:268:MET:CB	2:X:269:PRO:CD	2.83	0.48
2:X:292:ASN:ND2	4:X:6:NAG:C6	2.77	0.48
2:Y:128:LEU:HB3	5:Y:1118:HOH:O	2.12	0.48
2:X:255:GLY:O	2:X:256:ARG:C	2.56	0.48
2:X:249:TYR:N	2:X:249:TYR:CD1	2.82	0.48
2:Y:80:THR:HG22	5:Y:994:HOH:O	2.12	0.48
2:Y:283:LEU:CD2	5:Y:348:HOH:O	2.59	0.48
2:Y:256:ARG:O	2:Y:256:ARG:HG3	2.14	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:Y:6:NAG:H2	5:Y:755:HOH:O	2.13	0.48
2:Y:233:LEU:HD23	2:Y:306:ILE:HD11	1.95	0.48
2:Y:248:THR:HG22	2:Y:290:THR:O	2.13	0.48
1:B:54:ASN:C	1:B:54:ASN:OD1	2.56	0.48
1:A:68:ARG:HE	1:A:68:ARG:HB3	1.52	0.47
1:B:56:ARG:HG3	2:Y:270:TYR:CE1	2.48	0.47
2:X:62:TRP:O	2:X:69:PRO:HD2	2.14	0.47
2:X:257:LEU:N	5:X:1134:HOH:O	2.47	0.47
2:X:283:LEU:O	2:X:285:ASP:N	2.47	0.47
2:X:139:LEU:CD1	2:X:145:ILE:HD11	2.44	0.47
2:X:250:PRO:C	2:X:252:LYS:H	2.23	0.47
2:Y:58:ALA:HB1	2:Y:59:PRO:CD	2.44	0.47
1:A:64:GLN:HG3	1:A:95:LEU:HB2	1.95	0.47
2:X:49:THR:HG23	2:X:87:LEU:O	2.15	0.47
2:X:294:THR:CG2	2:X:301:GLN:HG2	2.44	0.47
2:Y:241:GLU:O	2:Y:272:ILE:HD11	2.14	0.47
2:Y:248:THR:HG23	2:Y:290:THR:HB	1.97	0.47
1:A:26:SER:HB3	5:A:846:HOH:O	2.14	0.47
2:X:54:CYS:O	2:X:82:SER:HA	2.15	0.47
2:X:119:PHE:CG	2:X:154:PRO:HG3	2.50	0.47
2:X:207:TYR:OH	2:X:241:GLU:OE1	2.26	0.47
2:X:214:ILE:HG23	2:X:237:VAL:CG2	2.42	0.47
2:X:250:PRO:HD3	2:X:288:THR:O	2.13	0.47
2:Y:264:PHE:CE1	2:Y:272:ILE:HG12	2.49	0.47
2:Y:283:LEU:C	2:Y:285:ASP:N	2.64	0.47
1:A:70:VAL:CG2	1:A:89:VAL:HG13	2.45	0.47
2:X:215:ASN:HB3	4:X:4:NAG:N2	2.30	0.47
5:A:785:HOH:O	2:X:164:LYS:HG2	2.15	0.47
1:B:32:ARG:O	2:X:262:THR:CG2	2.62	0.47
2:Y:53:THR:HG22	2:Y:54:CYS:N	2.30	0.47
2:Y:115:ARG:HH11	2:Y:115:ARG:CB	2.18	0.47
2:Y:145:ILE:HG22	2:Y:146:THR:N	2.30	0.47
2:Y:182:ILE:CD1	5:Y:551:HOH:O	2.62	0.47
2:Y:292:ASN:CG	2:Y:301:GLN:HE21	2.23	0.47
1:A:28:ARG:HG2	1:A:28:ARG:HH11	1.81	0.46
1:A:32:ARG:HD3	5:A:968:HOH:O	2.14	0.46
4:X:5:NAG:H2	5:X:1232:HOH:O	2.15	0.46
2:X:75:LYS:HD2	2:X:75:LYS:O	2.13	0.46
2:Y:58:ALA:O	2:Y:81:PHE:HB2	2.15	0.46
2:Y:266:LEU:H	2:Y:271:HIS:HB2	1.78	0.46
1:A:77:ILE:HD11	5:Y:327:HOH:O	2.15	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:Y:266:LEU:HD12	2:Y:266:LEU:N	2.29	0.46
2:Y:283:LEU:HD12	2:Y:284:GLU:H	1.80	0.46
2:Y:38:PRO:HD2	2:Y:39:GLY:H	1.80	0.46
2:X:37:PRO:CD	2:X:53:THR:O	2.63	0.46
2:Y:246:GLU:HA	5:Y:329:HOH:O	2.14	0.46
2:X:195:GLY:HA3	5:X:683:HOH:O	2.15	0.46
1:B:20:THR:HG23	5:B:118:HOH:O	2.16	0.46
2:X:99:PHE:CD2	2:X:113:ARG:HD2	2.51	0.46
2:Y:214:ILE:HG22	2:Y:302:ASP:CB	2.46	0.46
2:Y:290:THR:OG1	2:Y:305:ALA:HB2	2.16	0.46
1:A:55:ASN:ND2	2:X:185:ASP:OD2	2.49	0.46
2:X:216:VAL:HG13	2:X:235:CYS:SG	2.56	0.46
2:X:231:ILE:C	2:X:232:THR:HG22	2.41	0.46
2:Y:75:LYS:HD3	5:Y:776:HOH:O	2.16	0.46
2:Y:217:SER:HB2	5:Y:665:HOH:O	2.16	0.46
2:Y:225:VAL:HG12	2:Y:229:GLU:HB2	1.97	0.46
2:X:55:SER:HA	2:X:81:PHE:O	2.16	0.45
2:X:292:ASN:OD1	2:X:301:GLN:NE2	2.47	0.45
2:X:37:PRO:CD	2:X:53:THR:HG22	2.46	0.45
2:X:294:THR:HG22	2:X:301:GLN:CG	2.46	0.45
2:Y:140:THR:HG23	2:Y:297:VAL:HG13	1.97	0.45
2:X:39:GLY:HA3	5:X:753:HOH:O	2.17	0.45
2:Y:69:PRO:HB2	2:Y:70:PRO:HD2	1.99	0.45
2:Y:285:ASP:O	2:Y:289:TYR:HE1	1.99	0.45
1:A:27:ARG:NE	2:Y:264:PHE:CZ	2.84	0.45
2:Y:126:GLY:N	5:Y:1144:HOH:O	2.50	0.45
2:Y:216:VAL:HG13	2:Y:235:CYS:SG	2.56	0.45
2:Y:240:ASN:HB2	2:Y:243:VAL:CG1	2.46	0.45
2:Y:36:THR:HG22	2:Y:54:CYS:HB2	1.97	0.45
1:B:79:ARG:O	1:B:79:ARG:HG3	2.16	0.45
2:X:306:ILE:HD13	2:X:306:ILE:N	2.31	0.45
2:Y:89:ASN:N	5:Y:958:HOH:O	2.48	0.45
2:Y:249:TYR:N	2:Y:249:TYR:HD1	2.15	0.45
2:X:236:ILE:HG12	2:X:273:ARG:HB2	1.99	0.45
2:X:256:ARG:O	2:X:256:ARG:HG3	2.15	0.45
2:Y:49:THR:HG22	2:Y:50:PHE:N	2.32	0.45
2:Y:142:ILE:N	2:Y:142:ILE:HD13	2.31	0.45
1:A:73:ARG:NH1	2:Y:136:PHE:CE1	2.84	0.45
2:Y:95:THR:HA	2:Y:118:ILE:O	2.16	0.45
2:X:289:TYR:O	2:X:306:ILE:HD13	2.16	0.44
2:Y:55:SER:HB3	2:Y:82:SER:HB3	1.98	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:Y:238:ILE:HG12	5:Y:931:HOH:O	2.17	0.44
2:X:256:ARG:HB2	5:X:630:HOH:O	2.16	0.44
2:Y:64:ARG:NH1	2:Y:98:TYR:OH	2.50	0.44
2:X:227:GLN:HE21	2:X:227:GLN:HB3	1.57	0.44
2:Y:93:LEU:HB3	5:Y:652:HOH:O	2.16	0.44
2:Y:298:ASN:O	2:Y:299:ASP:CB	2.66	0.44
2:Y:280:SER:HA	5:Y:695:HOH:O	2.17	0.44
1:A:26:SER:OG	1:A:28:ARG:HB3	2.17	0.44
2:X:67:GLN:HB2	5:X:606:HOH:O	2.17	0.44
1:B:18:THR:HA	1:B:48:ARG:O	2.18	0.44
2:X:38:PRO:HB2	5:X:596:HOH:O	2.17	0.44
2:X:182:ILE:HD12	2:X:182:ILE:C	2.43	0.44
2:Y:71:GLN:O	2:Y:72:GLU:HG2	2.18	0.44
2:Y:115:ARG:C	2:Y:116:LEU:HD12	2.43	0.44
2:Y:37:PRO:HD2	2:Y:53:THR:O	2.17	0.44
2:Y:99:PHE:HB3	2:Y:113:ARG:HD2	1.98	0.44
2:Y:117:TYR:CD2	2:Y:176:GLN:HG2	2.53	0.44
2:Y:146:THR:HA	2:Y:179:PHE:O	2.18	0.44
1:B:24:GLU:HG3	5:B:308:HOH:O	2.16	0.44
2:X:119:PHE:CD1	2:X:154:PRO:HG3	2.53	0.44
2:X:258:VAL:HG13	5:X:376:HOH:O	2.16	0.44
2:Y:277:HIS:CD2	2:Y:279:PRO:HD3	2.52	0.44
2:Y:289:TYR:O	2:Y:306:ILE:HD13	2.18	0.44
1:A:82:PRO:HG2	1:A:84:PHE:HE1	1.82	0.44
2:Y:85:LEU:N	2:Y:85:LEU:CD2	2.81	0.44
2:Y:262:THR:HA	2:Y:273:ARG:O	2.18	0.44
2:X:187:SER:HA	2:X:204:TYR:O	2.17	0.43
2:Y:102:HIS:O	4:Y:3:NAG:H82	2.18	0.43
2:Y:283:LEU:CG	2:Y:284:GLU:H	2.30	0.43
2:Y:288:THR:OG1	4:Y:7:NAG:C1	2.65	0.43
2:X:102:HIS:HB3	4:X:3:NAG:H2	2.00	0.43
2:X:266:LEU:H	2:X:271:HIS:HB2	1.84	0.43
2:X:283:LEU:CG	2:X:284:GLU:H	2.31	0.43
2:Y:99:PHE:HD2	2:Y:113:ARG:HD2	1.80	0.43
2:X:215:ASN:HA	2:X:302:ASP:OD2	2.18	0.43
1:B:26:SER:O	1:B:29:LEU:HB3	2.18	0.43
2:X:238:ILE:HG12	2:X:239:GLY:N	2.33	0.43
2:Y:214:ILE:O	2:Y:302:ASP:OD2	2.36	0.43
2:X:37:PRO:HD2	2:X:53:THR:HB	2.00	0.43
2:Y:294:THR:HG21	4:Y:6:NAG:O7	2.19	0.43
1:A:34:ASN:ND2	2:Y:245:PHE:H	2.15	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:Y:58:ALA:HB1	2:Y:59:PRO:HD2	2.00	0.43
1:B:12:MET:HG3	5:B:580:HOH:O	2.19	0.43
2:X:42:LEU:HD23	2:X:42:LEU:N	2.34	0.43
2:X:120:VAL:O	2:X:121:PRO:C	2.61	0.43
2:X:257:LEU:HD12	2:X:257:LEU:H	1.84	0.43
2:Y:37:PRO:HA	2:Y:38:PRO:HA	1.80	0.43
2:Y:174:ASP:OD1	2:Y:176:GLN:HB2	2.19	0.43
2:Y:210:GLN:HB2	5:Y:352:HOH:O	2.18	0.43
2:X:84:VAL:O	2:X:84:VAL:CG2	2.66	0.43
2:X:166:ASP:N	5:X:389:HOH:O	2.49	0.43
2:Y:240:ASN:HB2	2:Y:243:VAL:HG12	1.99	0.43
2:Y:249:TYR:HB2	2:Y:250:PRO:CD	2.48	0.43
2:X:37:PRO:HD2	2:X:53:THR:CB	2.48	0.42
2:X:165:GLY:HA2	5:X:389:HOH:O	2.19	0.42
2:X:260:PRO:HB3	2:X:276:LEU:HD23	2.01	0.42
2:Y:295:GLU:OE2	2:Y:297:VAL:HB	2.18	0.42
2:Y:48:SER:OG	2:Y:90:LEU:HD12	2.20	0.42
1:B:80:LYS:O	1:B:80:LYS:HG2	2.20	0.42
2:Y:72:GLU:HB2	2:Y:84:VAL:HG23	2.01	0.42
2:Y:177:ARG:NH1	2:Y:177:ARG:HG3	2.35	0.42
2:Y:251:ARG:O	2:Y:251:ARG:HG2	2.19	0.42
1:A:79:ARG:O	1:A:81:LYS:N	2.51	0.42
2:Y:238:ILE:HD12	2:Y:271:HIS:CE1	2.55	0.42
1:A:73:ARG:HG3	1:A:73:ARG:HH11	1.85	0.42
1:B:78:VAL:O	1:B:79:ARG:C	2.63	0.42
2:X:153:ASP:HA	2:X:154:PRO:HD3	1.72	0.42
1:B:56:ARG:CD	1:B:56:ARG:N	2.79	0.41
2:X:279:PRO:HG3	5:X:1267:HOH:O	2.20	0.41
2:X:283:LEU:CD1	2:X:284:GLU:H	2.33	0.41
2:Y:160:LEU:HB2	2:Y:179:PHE:CE2	2.55	0.41
2:Y:177:ARG:HG3	2:Y:177:ARG:HH11	1.85	0.41
2:Y:250:PRO:HD3	2:Y:288:THR:O	2.19	0.41
2:X:37:PRO:HD2	2:X:53:THR:O	2.20	0.41
2:X:292:ASN:ND2	2:X:301:GLN:HE21	2.19	0.41
2:Y:275:ILE:HD11	2:Y:277:HIS:HB2	2.02	0.41
1:B:75:ILE:N	1:B:75:ILE:HD12	2.36	0.41
2:X:283:LEU:O	2:X:284:GLU:HB2	2.20	0.41
2:X:286:SER:HB2	2:X:310:VAL:H	1.84	0.41
1:A:25:ILE:HD11	1:A:44:VAL:HG13	2.02	0.41
1:A:55:ASN:HB3	1:A:57:ASN:H	1.86	0.41
1:B:56:ARG:HD3	2:Y:241:GLU:OE1	2.21	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:X:145:ILE:O	2:X:180:SER:HA	2.20	0.41
2:Y:77:GLN:NE2	2:Y:77:GLN:C	2.78	0.41
2:Y:253:GLU:HB2	5:Y:1083:HOH:O	2.20	0.41
1:B:36:ASN:CA	2:X:242:VAL:HG23	2.47	0.41
2:X:283:LEU:HD13	2:X:310:VAL:HB	2.03	0.41
2:Y:45:ASN:O	2:Y:90:LEU:HD12	2.21	0.41
1:B:10:PRO:O	1:B:12:MET:HE3	2.21	0.41
2:X:139:LEU:HD11	2:X:145:ILE:CD1	2.50	0.41
2:X:160:LEU:HD23	2:X:160:LEU:HA	1.89	0.41
2:X:219:ASN:ND2	2:X:220:ALA:N	2.43	0.41
2:X:246:GLU:HB3	2:X:292:ASN:HB3	2.03	0.41
1:A:72:VAL:HG13	1:A:89:VAL:HG12	2.02	0.41
2:X:37:PRO:HD2	2:X:53:THR:CG2	2.51	0.41
2:X:37:PRO:HA	2:X:38:PRO:HA	1.64	0.41
2:X:280:SER:O	2:X:281:ALA:C	2.64	0.41
2:Y:253:GLU:HA	5:Y:468:HOH:O	2.19	0.41
1:B:79:ARG:O	1:B:80:LYS:HB3	2.21	0.41
2:X:58:ALA:C	2:X:81:PHE:CD2	2.98	0.41
2:X:182:ILE:CD1	5:X:552:HOH:O	2.68	0.41
2:Y:214:ILE:HG22	2:Y:302:ASP:HB3	2.01	0.41
2:Y:222:GLN:HB2	5:Y:1254:HOH:O	2.21	0.41
2:X:248:THR:HG22	2:X:290:THR:HB	1.96	0.41
2:Y:220:ALA:HB1	5:Y:857:HOH:O	2.20	0.41
2:X:68:GLU:HB2	2:X:71:GLN:NE2	2.36	0.40
2:X:146:THR:O	2:X:148:PRO:HD3	2.21	0.40
2:Y:63:GLU:HG3	2:Y:63:GLU:O	2.20	0.40
2:X:231:ILE:HB	2:X:278:ILE:HB	2.03	0.40
2:Y:64:ARG:HG3	2:Y:65:MET:HG2	2.03	0.40
1:B:29:LEU:C	1:B:29:LEU:CD1	2.95	0.40
1:A:77:ILE:HA	1:A:82:PRO:HA	2.03	0.40
2:X:306:ILE:HD13	2:X:306:ILE:H	1.85	0.40
2:Y:48:SER:HA	5:Y:1089:HOH:O	2.21	0.40
2:Y:241:GLU:HG3	2:Y:270:TYR:CE1	2.57	0.40
1:A:44:VAL:HG21	1:A:91:LEU:HD11	2.02	0.40
5:A:804:HOH:O	2:X:164:LYS:HG3	2.21	0.40
2:Y:101:THR:HB	2:Y:102:HIS:H	1.62	0.40
2:Y:292:ASN:ND2	2:Y:301:GLN:HE21	2.19	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	95/172 (55%)	89 (94%)	4 (4%)	2 (2%)	5	4
1	B	99/172 (58%)	93 (94%)	6 (6%)	0	100	100
2	X	270/289 (93%)	242 (90%)	19 (7%)	9 (3%)	3	2
2	Y	269/289 (93%)	224 (83%)	38 (14%)	7 (3%)	4	3
All	All	733/922 (80%)	648 (88%)	67 (9%)	18 (2%)	4	3

All (18) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	X	268	MET
2	Y	299	ASP
2	X	251	ARG
2	X	163	LYS
2	Y	37	PRO
2	Y	38	PRO
2	Y	121	PRO
1	A	78	VAL
2	X	38	PRO
2	X	40	PRO
2	Y	47	SER
2	Y	148	PRO
2	Y	284	GLU
1	A	80	LYS
2	X	254	SER
2	X	59	PRO
2	X	250	PRO
2	X	70	PRO

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	90/153 (59%)	78 (87%)	12 (13%)	4	4
1	B	93/153 (61%)	80 (86%)	13 (14%)	3	3
2	X	251/264 (95%)	218 (87%)	33 (13%)	4	4
2	Y	250/264 (95%)	227 (91%)	23 (9%)	8	11
All	All	684/834 (82%)	603 (88%)	81 (12%)	5	6

All (81) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	6	THR
1	A	9	GLU
1	A	26	SER
1	A	29	LEU
1	A	57	ASN
1	A	58	VAL
1	A	63	THR
1	A	65	VAL
1	A	68	ARG
1	A	77	ILE
1	A	95	LEU
1	A	97	CYS
1	B	6	THR
1	B	36	ASN
1	B	48	ARG
1	B	56	ARG
1	B	57	ASN
1	B	71	GLN
1	B	78	VAL
1	B	81	LYS
1	B	89	VAL
1	B	90	THR
1	B	95	LEU
1	B	97	CYS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	98	LYS
2	X	34	VAL
2	X	42	LEU
2	X	53	THR
2	X	60	VAL
2	X	61	VAL
2	X	64	ARG
2	X	75	LYS
2	X	77	GLN
2	X	103	ASN
2	X	115	ARG
2	X	128	LEU
2	X	131	ASP
2	X	135	LEU
2	X	141	GLU
2	X	160	LEU
2	X	162	GLU
2	X	166	ASP
2	X	227	GLN
2	X	232	THR
2	X	238	ILE
2	X	242	VAL
2	X	246	GLU
2	X	257	LEU
2	X	262	THR
2	X	265	LEU
2	X	268	MET
2	X	275	ILE
2	X	276	LEU
2	X	283	LEU
2	X	299	ASP
2	X	306	ILE
2	X	307	ASN
2	X	309	THR
2	Y	75	LYS
2	Y	80	THR
2	Y	85	LEU
2	Y	102	HIS
2	Y	112	GLU
2	Y	115	ARG
2	Y	130	ASN
2	Y	141	GLU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	Y	151	VAL
2	Y	160	LEU
2	Y	232	THR
2	Y	238	ILE
2	Y	242	VAL
2	Y	249	TYR
2	Y	257	LEU
2	Y	262	THR
2	Y	268	MET
2	Y	275	ILE
2	Y	283	LEU
2	Y	299	ASP
2	Y	306	ILE
2	Y	307	ASN
2	Y	309	THR

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

Mol	Chain	Res	Type
1	A	47	GLN
1	A	57	ASN
1	A	59	GLN
1	B	36	ASN
1	B	47	GLN
1	B	71	GLN
2	X	77	GLN
2	X	130	ASN
2	X	219	ASN
2	X	222	GLN
2	X	227	GLN
2	X	271	HIS
2	Y	77	GLN
2	Y	102	HIS
2	Y	130	ASN
2	Y	219	ASN
2	Y	222	GLN
2	Y	227	GLN
2	Y	277	HIS
2	Y	301	GLN

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 ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

14 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
4	NAG	Y	7	2	14,14,15	0.67	0	17,19,21	0.63	0
4	NAG	Y	2	2	14,14,15	0.60	0	17,19,21	0.67	0
4	NAG	Y	4	2	14,14,15	0.72	0	17,19,21	0.61	0
4	NAG	X	6	2	14,14,15	0.67	0	17,19,21	0.96	1 (5%)
4	NAG	X	2	2	14,14,15	0.56	0	17,19,21	0.70	0
4	NAG	X	3	2	14,14,15	0.66	0	17,19,21	0.76	1 (5%)
3	NDG	X	1	-	14,14,15	0.63	0	17,19,21	0.71	1 (5%)
4	NAG	Y	3	2	14,14,15	0.62	0	17,19,21	0.65	0
4	NAG	Y	1	2	14,14,15	0.67	0	17,19,21	0.67	1 (5%)
4	NAG	X	7	2	14,14,15	0.67	0	17,19,21	0.58	0
4	NAG	Y	6	2	14,14,15	0.78	0	17,19,21	0.81	0
4	NAG	Y	5	2	14,14,15	0.70	0	17,19,21	0.77	1 (5%)
4	NAG	X	4	2	14,14,15	0.72	0	17,19,21	0.85	0
4	NAG	X	5	2	14,14,15	0.55	0	17,19,21	0.73	1 (5%)

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	Y	7	2	-	4/6/23/26	0/1/1/1
4	NAG	Y	2	2	-	3/6/23/26	0/1/1/1
4	NAG	Y	4	2	-	2/6/23/26	0/1/1/1
4	NAG	X	6	2	-	4/6/23/26	0/1/1/1
4	NAG	X	2	2	-	2/6/23/26	0/1/1/1
4	NAG	X	5	2	1/1/5/7	5/6/23/26	0/1/1/1
4	NAG	X	3	2	1/1/5/7	2/6/23/26	0/1/1/1
3	NDG	X	1	-	-	2/6/23/26	0/1/1/1
4	NAG	Y	3	2	-	3/6/23/26	0/1/1/1
4	NAG	Y	1	2	1/1/5/7	4/6/23/26	0/1/1/1
4	NAG	Y	6	2	-	4/6/23/26	0/1/1/1
4	NAG	Y	5	2	1/1/5/7	4/6/23/26	0/1/1/1
4	NAG	X	4	2	-	3/6/23/26	0/1/1/1
4	NAG	X	7	2	1/1/5/7	4/6/23/26	0/1/1/1

There are no bond length outliers.

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	X	6	NAG	C2-N2-C7	-2.81	119.14	122.90
4	Y	5	NAG	C2-N2-C7	-2.37	119.72	122.90
4	X	5	NAG	C2-N2-C7	-2.30	119.81	122.90
4	X	3	NAG	C2-N2-C7	-2.21	119.94	122.90
3	X	1	NDG	C2-N2-C7	-2.16	120.00	122.90
4	Y	1	NAG	C2-N2-C7	-2.03	120.17	122.90

All (5) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
4	X	3	NAG	C1
4	X	5	NAG	C1
4	X	7	NAG	C1
4	Y	1	NAG	C1
4	Y	5	NAG	C1

All (46) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	X	2	NAG	C8-C7-N2-C2
4	X	2	NAG	O7-C7-N2-C2
4	X	3	NAG	C8-C7-N2-C2
4	X	3	NAG	O7-C7-N2-C2
4	X	4	NAG	C3-C2-N2-C7
4	X	4	NAG	C8-C7-N2-C2
4	X	4	NAG	O7-C7-N2-C2
4	X	5	NAG	C8-C7-N2-C2
4	X	5	NAG	O7-C7-N2-C2
4	X	7	NAG	C8-C7-N2-C2
4	X	7	NAG	O7-C7-N2-C2
4	Y	1	NAG	C8-C7-N2-C2
4	Y	1	NAG	O7-C7-N2-C2
4	Y	2	NAG	C1-C2-N2-C7
4	Y	2	NAG	C8-C7-N2-C2
4	Y	2	NAG	O7-C7-N2-C2
4	Y	3	NAG	C8-C7-N2-C2
4	Y	3	NAG	O7-C7-N2-C2
4	Y	4	NAG	C8-C7-N2-C2
4	Y	4	NAG	O7-C7-N2-C2
4	Y	5	NAG	C8-C7-N2-C2
4	Y	5	NAG	O7-C7-N2-C2
4	Y	6	NAG	C8-C7-N2-C2
4	Y	6	NAG	O7-C7-N2-C2
4	Y	7	NAG	C8-C7-N2-C2
4	Y	7	NAG	O7-C7-N2-C2
4	X	6	NAG	C4-C5-C6-O6
3	X	1	NDG	O5-C5-C6-O6
4	X	6	NAG	O5-C5-C6-O6
4	X	5	NAG	O5-C5-C6-O6
4	Y	6	NAG	O5-C5-C6-O6
4	Y	7	NAG	C4-C5-C6-O6
4	Y	1	NAG	C4-C5-C6-O6
4	Y	7	NAG	O5-C5-C6-O6
3	X	1	NDG	C4-C5-C6-O6
4	X	5	NAG	C4-C5-C6-O6
4	Y	1	NAG	O5-C5-C6-O6
4	Y	6	NAG	C4-C5-C6-O6
4	Y	3	NAG	O5-C5-C6-O6
4	Y	5	NAG	O5-C5-C6-O6
4	X	7	NAG	C4-C5-C6-O6
4	X	6	NAG	C8-C7-N2-C2
4	Y	5	NAG	C3-C2-N2-C7

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
4	X	7	NAG	O5-C5-C6-O6
4	X	5	NAG	C3-C2-N2-C7
4	X	6	NAG	O7-C7-N2-C2

There are no ring outliers.

10 monomers are involved in 23 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	Y	7	NAG	5	0
4	Y	4	NAG	1	0
4	X	6	NAG	2	0
4	X	3	NAG	2	0
4	Y	3	NAG	2	0
4	X	7	NAG	2	0
4	Y	6	NAG	4	0
4	Y	5	NAG	1	0
4	X	4	NAG	2	0
4	X	5	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, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	97/172 (56%)	0.11	3 (3%) 51 53	20, 38, 81, 107	0
1	B	101/172 (58%)	-0.03	1 (0%) 79 80	21, 36, 57, 93	0
2	X	274/289 (94%)	0.46	8 (2%) 53 56	26, 56, 88, 100	0
2	Y	273/289 (94%)	1.55	78 (28%) 1 1	37, 95, 114, 120	0
All	All	745/922 (80%)	0.75	90 (12%) 8 9	20, 60, 109, 120	0

All (90) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	Y	87	LEU	5.1
2	Y	85	LEU	4.6
2	Y	62	TRP	4.3
2	Y	297	VAL	4.2
2	Y	34	VAL	4.0
2	Y	231	ILE	3.7
2	Y	269	PRO	3.7
2	Y	209	LEU	3.6
2	Y	311	VAL	3.5
1	A	80	LYS	3.5
2	Y	214	ILE	3.4
2	Y	211	VAL	3.3
2	Y	215	ASN	3.3
2	Y	138	PHE	3.2
2	Y	306	ILE	3.2
2	Y	266	LEU	3.2
2	Y	82	SER	3.1
2	Y	216	VAL	3.1
2	Y	121	PRO	3.1
2	Y	74	ALA	3.1
1	A	102	VAL	3.1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
2	Y	101	THR	3.1
2	Y	102	HIS	3.1
2	Y	262	THR	3.1
2	Y	307	ASN	3.1
2	Y	194	ILE	3.0
2	Y	81	PHE	2.9
2	Y	136	PHE	2.9
2	Y	53	THR	2.9
2	Y	258	VAL	2.9
2	Y	293	VAL	2.9
2	Y	66	SER	2.9
2	Y	225	VAL	2.9
2	Y	265	LEU	2.8
2	Y	178	GLY	2.7
2	Y	257	LEU	2.7
2	Y	305	ALA	2.7
2	Y	310	VAL	2.7
2	X	38	PRO	2.7
2	Y	73	MET	2.7
2	X	33	LEU	2.7
2	X	267	ASP	2.6
2	Y	237	VAL	2.6
1	A	78	VAL	2.6
2	Y	272	ILE	2.6
2	Y	83	SER	2.6
2	Y	289	TYR	2.6
2	Y	308	ILE	2.6
2	Y	44	LEU	2.5
2	Y	70	PRO	2.5
2	Y	35	VAL	2.5
2	Y	268	MET	2.5
2	Y	228	GLY	2.5
2	Y	251	ARG	2.4
2	Y	79	GLY	2.4
2	X	266	LEU	2.4
2	Y	208	ARG	2.4
2	Y	210	GLN	2.4
2	X	285	ASP	2.4
2	Y	46	VAL	2.4
2	Y	61	VAL	2.4
2	Y	164	LYS	2.3
2	Y	241	GLU	2.3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
2	Y	263	ASP	2.3
2	Y	59	PRO	2.3
2	Y	213	SER	2.3
2	Y	126	GLY	2.3
2	Y	267	ASP	2.3
1	B	102	VAL	2.3
2	Y	52	LEU	2.2
2	Y	243	VAL	2.3
2	Y	69	PRO	2.2
2	Y	57	SER	2.2
2	Y	100	CYS	2.2
2	Y	76	ALA	2.2
2	X	283	LEU	2.2
2	Y	277	HIS	2.1
2	X	101	THR	2.1
2	Y	40	PRO	2.1
2	Y	239	GLY	2.1
2	Y	140	THR	2.1
2	Y	115	ARG	2.1
2	Y	93	LEU	2.0
2	Y	104	ASP	2.0
2	Y	116	LEU	2.0
2	X	194	ILE	2.0
2	Y	137	ILE	2.0
2	Y	84	VAL	2.0
2	Y	261	VAL	2.0
2	Y	254	SER	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 oligosaccharides in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum,

median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
4	NAG	Y	4	14/15	0.12	0.17	121,123,123,123	0
4	NAG	X	7	14/15	0.32	0.20	116,119,122,122	0
4	NAG	Y	1	14/15	0.37	0.16	119,123,125,125	0
4	NAG	Y	5	14/15	0.37	0.17	112,118,121,121	0
4	NAG	Y	2	14/15	0.38	0.17	116,120,122,122	0
4	NAG	Y	7	14/15	0.39	0.16	117,118,119,119	0
4	NAG	Y	6	14/15	0.43	0.16	113,118,121,121	0
4	NAG	X	4	14/15	0.56	0.14	106,109,111,111	0
4	NAG	X	2	14/15	0.65	0.13	96,102,105,107	0
4	NAG	X	3	14/15	0.70	0.15	117,119,120,120	0
4	NAG	Y	3	14/15	0.76	0.11	114,117,118,118	0
4	NAG	X	6	14/15	0.77	0.16	87,94,100,100	0
4	NAG	X	5	14/15	0.83	0.11	87,89,91,91	0
3	NDG	X	1	14/15	0.85	0.13	81,86,89,89	0

6.5 Other polymers

There are no such residues in this entry.