



# Full wwPDB X-ray Structure Validation Report

Feb 26, 2014 – 05:32 PM GMT

PDB ID : 3MJG  
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 validation report for a publicly released PDB entry.  
We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)  
A user guide is available at <http://wwpdb.org/ValidationPDFNotes.html>

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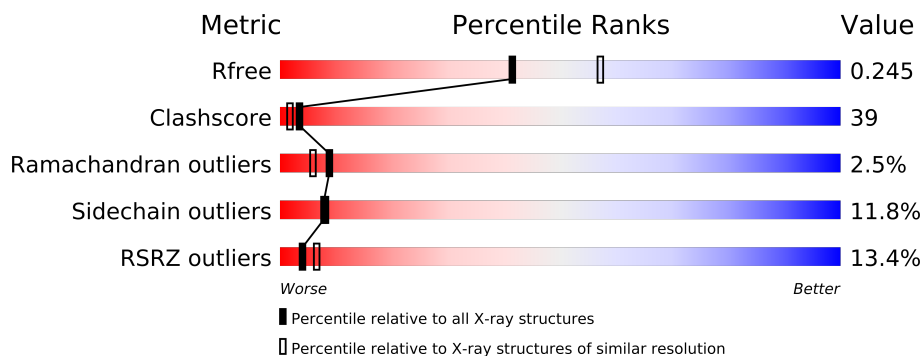
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467  
Mogul : 1.15 2013  
Xtriage (Phenix) : dev-1323  
EDS : stable22639  
Percentile statistics : 21963  
Refmac : 5.8.0049  
CCP4 : 6.3.0 (Settle)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)  
Validation Pipeline (wwPDB-VP) : stable22683

# 1 Overall quality at a glance

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))
$R_{free}$	66092	2929 (2.30-2.30)
Clashscore	79885	3679 (2.30-2.30)
Ramachandran outliers	78287	3642 (2.30-2.30)
Sidechain outliers	78261	3641 (2.30-2.30)
RSRZ outliers	66119	2930 (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 on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Mol	Chain	Length	Quality of chain
1	A	172	
1	B	172	
2	X	289	
2	Y	289	

The following table lists non-polymeric compounds that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Geometry	Electron density
4	NAG	X	4	-	X
4	NAG	X	6	-	X
4	NAG	X	7	-	X
4	NAG	Y	1	-	X

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Mol	Type	Chain	Res	Geometry	Electron density
4	NAG	Y	2	-	X
4	NAG	Y	4	-	X
4	NAG	Y	5	-	X
4	NAG	Y	6	-	X

## 2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 7254 atoms, of which 0 are hydrogen and 0 are deuterium.

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

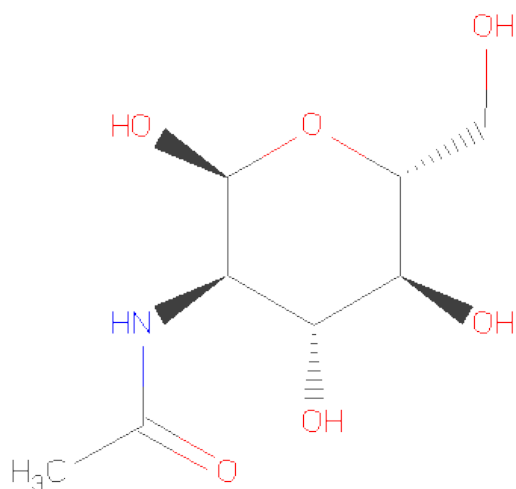
- Molecule 2 is a protein called Beta-type platelet-derived growth factor receptor.

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 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	X	1	Total	C	N	O	0	0
			14	8	1	5		

- Molecule 4 is SUGAR (N-ACETYL-D-GLUCOSAMINE) (three-letter code: 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.

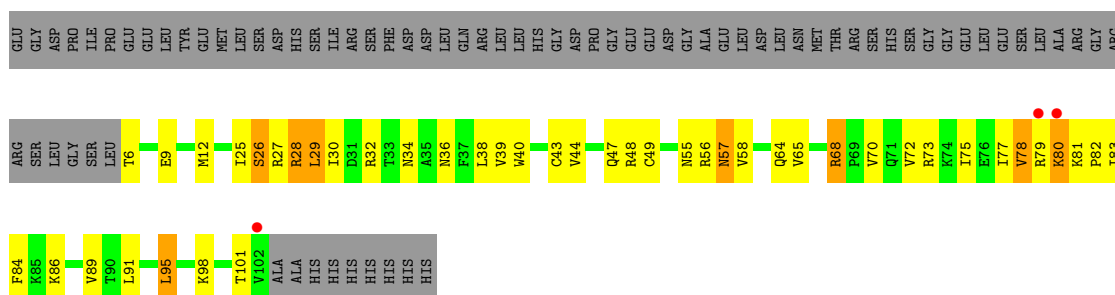
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	204	Total 204	O 204	0	0
5	B	188	Total 188	O 188	0	0
5	X	386	Total 386	O 386	0	0
5	Y	392	Total 392	O 392	0	0

### 3 Residue-property plots

These plots are drawn for all protein, RNA 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.

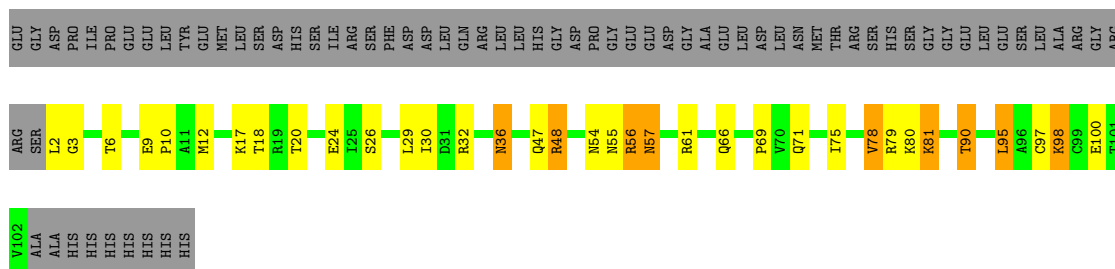
- Molecule 1: Platelet-derived growth factor subunit B

Chain A:



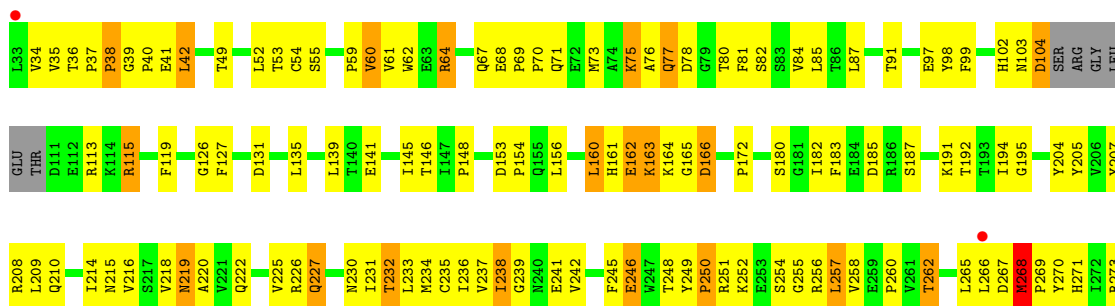
- Molecule 1: Platelet-derived growth factor subunit B

Chain B:



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

Chain X:







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

Chain Y:



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	78.47Å 116.82Å 134.15Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	44.24 – 2.30 44.23 – 2.20	Depositor EDS
% Data completeness (in resolution range)	98.9 (44.24-2.30) 98.6 (44.23-2.20)	Depositor EDS
$R_{merge}$	0.08	Depositor
$R_{sym}$	0.06	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.32 (at 2.20Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, $R_{free}$	0.237 , 0.277 0.244 , 0.245	Depositor DCC
$R_{free}$ test set	3172 reflections (5.36%)	DCC
Wilson B-factor (Å <sup>2</sup> )	44.9	Xtriage
Anisotropy	0.167	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.30 , 60.0	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.31$	Xtriage
Outliers	0 of 62398 reflections	Xtriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	7254	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	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.*

<sup>1</sup>Intensities estimated from amplitudes.

## 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	0.54	0/787	0.79	0/1064
1	B	0.60	0/813	0.86	0/1099
2	X	0.47	0/2205	0.76	1/3013 (0.0%)
2	Y	0.37	0/2197	0.64	0/3002
All	All	0.47	0/6002	0.74	1/8178 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	X	209	LEU	CA-CB-CG	5.24	127.36	115.30

There are no chirality outliers.

There are no planarity outliers.

### 5.2 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 hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	776	0	803	64	0
1	B	802	0	833	47	0
2	X	2159	0	2088	165	0
2	Y	2151	0	2077	220	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	X	14	0	13	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	5983	476	0

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 39.

All (476) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:43:CYS:HB2	5:B:550:HOH:O	1.45	1.15
2:X:268:MET:HB3	2:X:269:PRO:HD3	1.34	1.08
1:B:20:THR:HG22	1:B:47:GLN:HE22	1.11	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:HB2	2:Y:115:ARG:HH11	1.34	0.91
1:A:40:TRP:CH2	1:B:54:ASN:HB2	2.06	0.90
1:B:36:ASN:H	1:B:36:ASN:HD22	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:HD2	1:B:56:ARG:H	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

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
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
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:231:ILE:HB	2:Y:278:ILE:HB	1.70	0.73
1:B:56:ARG:CD	1:B:56:ARG:H	2.02	0.73
2:Y:301:GLN:HG3	4:Y:6:NAG:O7	1.90	0.72
1:B:2:LEU:HD12	1:B:3:GLY:H	1.55	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:O	2:X:182:ILE:HD12	1.90	0.71
2:Y:226:ARG:HD2	5:Y:1214:HOH:O	1.90	0.70
2:X:227:GLN:HB2	5:X:328: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
2:Y:268:MET:CB	2:Y:269:PRO:HD3	2.17	0.69
1:A:30:ILE:HD12	1:A:39:VAL:CG1	2.22	0.69
2:Y:215:ASN:HA	2:Y:302:ASP:OD2	1.93	0.69
2:Y:283:LEU:C	2:Y:285:ASP:H	1.97	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:H	2:X:85:LEU:HD23	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:B:20:THR:HG22	1:B:47:GLN:NE2	1.97	0.68
1:A:68:ARG:HD2	1:B:9:GLU:OE2	1.93	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

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
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:266:LEU:HD23	5:X:388:HOH:O	1.97	0.65
1:A:101:THR:HG22	5:A:661:HOH:O	1.96	0.65
1:A:40:TRP:NE1	2:Y:136:PHE:CE2	2.65	0.65
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
1:A:36:ASN:C	2:Y:242:VAL:HG23	2.18	0.64
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:CG	2:X:64:ARG:HH11	2.09	0.64
2:Y:163:LYS:HB2	2:Y:187:SER:OG	1.97	0.64
2:Y:115:ARG:NH1	2:Y:115:ARG:HB2	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:N	2:Y:249:TYR:CD1	2.67	0.62
4:X:4:NAG:H62	5:X:399:HOH:O	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
1:A:78:VAL:O	1:A:81:LYS:HG2	1.99	0.62
2:X:292:ASN:ND2	4:X:6:NAG:H62	2.15	0.62
2:X:210:GLN:HG2	5:X:930:HOH:O	2.00	0.62
1:B:56:ARG:HG3	2:Y:270:TYR:HE1	1.63	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:X:283:LEU:C	2:X:285:ASP:H	2.04	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:97:GLU:HG2	2:Y:115:ARG:NH1	2.15	0.61

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:Y:49:THR:HA	5:Y:958:HOH:O	2.00	0.61
5:A:797:HOH:O	2:X:267:ASP:HB2	1.99	0.60
2:X:60:VAL:O	2:X:73:MET:HE3	2.00	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:Y:97:GLU:HB3	2:Y:99:PHE:CE1	2.37	0.59
2:X:297:VAL:HG12	2:X:298:ASN:OD1	2.01	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:Y:294:THR:HG23	5:Y:682:HOH:O	2.01	0.59
2:Y:283:LEU:O	2:Y:285:ASP:N	2.35	0.59
2:X:288:THR:HG23	4:X:7:NAG:HN2	1.67	0.59
1:A:70:VAL:HG22	1:A:89:VAL:HG13	1.85	0.59
2:Y:210:GLN:HB3	2:Y:241:GLU:HB2	1.84	0.58
2:Y:119:PHE:O	2:Y:121:PRO:HD3	2.03	0.58
2:Y:99:PHE:CE2	2:Y:115:ARG:HB3	2.39	0.58
2:Y:265:LEU:HB2	2:Y:271:HIS:HB2	1.84	0.58
2:Y:238:ILE:HD12	2:Y:271:HIS:NE2	2.19	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
1:A:12:MET:HE2	5:A:708:HOH:O	2.03	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:HD13	2:Y:306:ILE:N	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:N	1:B:36:ASN:HD22	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
1:B:10:PRO:O	1:B:12:MET:HE2	2.04	0.56
2:X:52:LEU:HB2	2:X:85:LEU:CD2	2.35	0.56

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
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:187:SER:HB3	2:X:205:TYR:CE2	2.41	0.55
2:X:183:PHE:O	2:X:208:ARG:NH2	2.39	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
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:Y:138:PHE:O	2:Y:139:LEU:HD23	2.05	0.55
2:X:162:GLU:O	2:X:163:LYS:C	2.44	0.55
2:Y:64:ARG:HG2	2:Y:64:ARG:HH11	1.72	0.55
2:X:41:GLU:C	2:X:42:LEU:HD23	2.27	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: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
2:Y:298:ASN:O	2:Y:299:ASP:HB2	2.07	0.54
1:A:29:LEU:HD23	1:A:29:LEU:H	1.71	0.54
2:Y:85:LEU:H	2:Y:85:LEU:HD23	1.72	0.54
2:Y:265:LEU:HB2	2:Y:271:HIS:CB	2.38	0.54
1:B:2:LEU:HD21	5:B:1309:HOH:O	2.08	0.54
1:A:83:ILE:HA	5:A:699:HOH:O	2.08	0.54
2:Y:72:GLU:HG3	5:Y:354:HOH:O	2.08	0.53
2:X:283:LEU:HD12	2:X:284:GLU:N	2.24	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
2:Y:238:ILE:HA	2:Y:270:TYR:O	2.08	0.53
2:Y:99:PHE:CD2	2:Y:113:ARG:HD2	2.44	0.53
2:X:64:ARG:HD3	2:X:98:TYR:CZ	2.44	0.53
2:Y:99:PHE:CD2	2:Y:115:ARG:HB3	2.44	0.53
2:X:233:LEU:N	2:X:233:LEU:HD12	2.23	0.53
2:X:53:THR:HG22	5:X:654:HOH:O	2.09	0.53
2:Y:35:VAL:HG12	2:Y:36:THR:N	2.24	0.53
1:B:98:LYS:HD2	5:B:950:HOH:O	2.09	0.53
4:X:5:NAG:H61	4:X:5:NAG:O3	2.09	0.53
2:X:238:ILE:HA	2:X:270:TYR:O	2.09	0.53

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:X:64:ARG:HD3	2:X:98:TYR:CE2	2.43	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
2:Y:257:LEU:HD23	5:Y:932:HOH:O	2.08	0.52
2:Y:225:VAL:CG1	2:Y:229:GLU:HB2	2.38	0.52
1:A:28:ARG:HG3	1:A:32:ARG:HH11	1.72	0.52
1:B:57:ASN:HB3	2:Y:268:MET:SD	2.48	0.52
2:Y:283:LEU:HD13	2:Y:310:VAL:HB	1.92	0.52
1:A:28:ARG:NH1	1:A:32:ARG:HD2	2.24	0.52
1:A:38:LEU:HD11	2:Y:209:LEU:HD11	1.91	0.52
2:X:283:LEU:HD12	2:X:284:GLU:H	1.75	0.52
1:A:77:ILE:O	1:A:77:ILE:HD12	2.09	0.52
1:A:73:ARG:NH1	1:A:73:ARG:HG3	2.25	0.52
2:Y:191:LYS:HD2	2:Y:198:GLU:OE2	2.09	0.52
2:X:36:THR:HA	2:X:53:THR:O	2.10	0.52
1:A:26:SER:H	1:A:29:LEU:HD21	1.75	0.52
1:A:40:TRP:NE1	2:Y:136:PHE:HE2	2.06	0.51
2:X:275:ILE:HG13	2:X:275:ILE:O	2.09	0.51
2:X:153:ASP:HB3	2:X:156:LEU:HG	1.93	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:NH1	2:X:64:ARG:CG	2.72	0.51
2:Y:222:GLN:HG3	2:Y:225:VAL:HG22	1.92	0.51
2:X:172:PRO:HA	5:X:864:HOH:O	2.11	0.51
2:X:269:PRO:HD2	5:X:388:HOH:O	2.11	0.51
2:X:258:VAL:HG21	2:X:278:ILE:HG12	1.92	0.51
1:A:86:LYS:HE3	5:A:1229:HOH:O	2.10	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:Y:44:LEU:O	2:Y:121:PRO:HD2	2.11	0.51
2:X:256:ARG:HD2	5:X:955:HOH:O	2.10	0.51
2:Y:216:VAL:HB	2:Y:304:LYS:HG2	1.93	0.51
1:A:56:ARG:HD2	5:A:797:HOH:O	2.10	0.51
2:Y:225:VAL:O	2:Y:310:VAL:HA	2.11	0.50
2:Y:60:VAL:CG2	2:Y:100:CYS:SG	3.00	0.50
2:X:225:VAL:HG12	2:X:226:ARG:N	2.25	0.50
1:A:98:LYS:NZ	5:A:947:HOH:O	2.44	0.50
2:X:286:SER:HA	2:X:308:ILE:O	2.11	0.50
2:X:256:ARG:NH1	5:X:928:HOH:O	2.44	0.50
2:X:104:ASP:C	5:X:326:HOH:O	2.48	0.50

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:54:ASN:HB3	5:B:1140:HOH:O	2.10	0.50
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
2:Y:265:LEU:CD1	2:Y:271:HIS:HB3	2.38	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
1:B:61:ARG:HD2	5:B:454:HOH:O	2.10	0.50
2:Y:94:ASP:HA	5:Y:781:HOH:O	2.10	0.50
2:X:139:LEU:HD11	2:X:145:ILE:HD11	1.92	0.50
2:X:84:VAL:HG23	2:X:84:VAL:O	2.10	0.50
2:X:161:HIS:NE2	2:X:191:LYS:HE3	2.26	0.50
2:X:268:MET:CB	2:X:269:PRO:HD3	2.25	0.50
2:X:64:ARG:HD2	2:X:97:GLU:O	2.11	0.50
2:Y:69:PRO:HB2	2:Y:70:PRO:CD	2.42	0.50
2:Y:98:TYR:CD1	2:Y:118:ILE:HD12	2.46	0.50
1:B:66:GLN:HB2	1:B:95:LEU:HD21	1.94	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
1:A:79:ARG:C	1:A:81:LYS:H	2.15	0.49
1:B:78:VAL:O	1:B:81:LYS:N	2.35	0.49
2:Y:182:ILE:O	2:Y:182:ILE:HD12	2.12	0.49
2:Y:60:VAL:HG13	2:Y:83:SER:HB2	1.94	0.49
2:Y:288:THR:CG2	4:Y:7:NAG:HN2	2.21	0.49
2:X:91:THR:HG21	5:X:835:HOH:O	2.12	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: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
1:B:29:LEU:C	1:B:29:LEU:HD13	2.34	0.48
2:Y:283:LEU:CD2	5:Y:348:HOH:O	2.59	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
4:Y:6:NAG:H2	5:Y:755:HOH:O	2.13	0.48
2:Y:256:ARG:O	2:Y:256:ARG:HG3	2.14	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
2:Y:119:PHE:C	2:Y:121:PRO:HD3	2.34	0.48
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

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:68:ARG:HB3	1:A:68:ARG:HE	1.52	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:Y:58:ALA:HB1	2:Y:59:PRO:CD	2.44	0.47
2:X:139:LEU:CD1	2:X:145:ILE:HD11	2.44	0.47
2:Y:241:GLU:O	2:Y:272:ILE:HD11	2.14	0.47
2:X:294:THR:CG2	2:X:301:GLN:HG2	2.44	0.47
2:Y:248:THR:HG23	2:Y:290:THR:HB	1.97	0.47
2:X:49:THR:HG23	2:X:87:LEU:O	2.15	0.47
1:A:64:GLN:HG3	1:A:95:LEU:HB2	1.95	0.47
2:Y:264:PHE:CE1	2:Y:272:ILE:HG12	2.49	0.47
2:X:214:ILE:HG23	2:X:237:VAL:CG2	2.42	0.47
1:A:26:SER:HB3	5:A:846:HOH:O	2.14	0.47
2:X:250:PRO:HD3	2:X:288:THR:O	2.13	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:54:CYS:O	2:X:82:SER:HA	2.15	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
2:X:292:ASN:CG	2:X:301:GLN:HE21	2.18	0.47
2:Y:115:ARG:CB	2:Y:115:ARG:HH11	2.18	0.47
2:Y:53:THR:HG22	2:Y:54:CYS:N	2.30	0.47
1:B:32:ARG:O	2:X:262:THR:CG2	2.62	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
5:A:785:HOH:O	2:X:164:LYS:HG2	2.15	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:Y:266:LEU:H	2:Y:271:HIS:HB2	1.78	0.46
2:Y:58:ALA:O	2:Y:81:PHE:HB2	2.15	0.46
2:X:256:ARG:HG3	2:X:256:ARG:O	2.15	0.46
2:X:75:LYS:O	2:X:75:LYS:HD2	2.13	0.46
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
1:A:77:ILE:HD11	5:Y:327:HOH:O	2.15	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:Y:214:ILE:HG22	2:Y:302:ASP:CB	2.46	0.46

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:Y:290:THR:OG1	2:Y:305:ALA:HB2	2.16	0.46
2:X:99:PHE:CD2	2:X:113:ARG:HD2	2.51	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:Y:225:VAL:HG12	2:Y:229:GLU:HB2	1.97	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:X:292:ASN:OD1	2:X:301:GLN:NE2	2.47	0.45
2:X:55:SER:HA	2:X:81:PHE:O	2.16	0.45
2:Y:140:THR:HG23	2:Y:297:VAL:HG13	1.97	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:285:ASP:O	2:Y:289:TYR:HE1	1.99	0.45
2:Y:69:PRO:HB2	2:Y:70:PRO:HD2	1.99	0.45
2:X:39:GLY:HA3	5:X:753:HOH:O	2.17	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:Y:89:ASN:N	5:Y:958:HOH:O	2.48	0.45
2:X:306:ILE:N	2:X:306:ILE:HD13	2.31	0.45
2:Y:249:TYR:HD1	2:Y:249:TYR:N	2.15	0.45
2:X:283:LEU:C	2:X:285:ASP:N	2.70	0.45
2:Y:49:THR:HG22	2:Y:50:PHE:N	2.32	0.45
2:X:236:ILE:HG12	2:X:273:ARG:HB2	1.99	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:162:GLU:O	2:Y:163:LYS:C	2.56	0.45
2:Y:95:THR:HA	2:Y:118:ILE:O	2.16	0.45
2:Y:238:ILE:HG12	5:Y:931:HOH:O	2.17	0.44
2:X:289:TYR:O	2:X:306:ILE:HD13	2.16	0.44
2:X:77:GLN:C	2:X:77:GLN:NE2	2.70	0.44
2:Y:55:SER:HB3	2:Y:82:SER:HB3	1.98	0.44
2:Y:64:ARG:NH1	2:Y:98:TYR:OH	2.50	0.44
2:X:256:ARG:HB2	5:X:630:HOH:O	2.16	0.44
2:Y:298:ASN:O	2:Y:299:ASP:CB	2.66	0.44
2:X:227:GLN:HE21	2:X:227:GLN:HB3	1.57	0.44
2:Y:102:HIS:C	2:Y:103:ASN:HD22	2.19	0.44
2:Y:93:LEU:HB3	5:Y:652:HOH:O	2.16	0.44
2:Y:280:SER:HA	5:Y:695:HOH:O	2.17	0.44

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
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
2:X:38:PRO:HB2	5:X:596:HOH:O	2.17	0.44
1:B:18:THR:HA	1:B:48:ARG:O	2.18	0.44
2:Y:71:GLN:O	2:Y:72:GLU:HG2	2.18	0.44
2:Y:99:PHE:HB3	2:Y:113:ARG:HD2	1.98	0.44
1:A:57:ASN:C	1:A:57:ASN:HD22	2.20	0.44
2:Y:283:LEU:C	2:Y:285:ASP:N	2.64	0.44
2:Y:37:PRO:HD2	2:Y:53:THR:O	2.17	0.44
2:Y:146:THR:HA	2:Y:179:PHE:O	2.18	0.44
2:Y:117:TYR:CD2	2:Y:176:GLN:HG2	2.53	0.44
2:Y:289:TYR:O	2:Y:306:ILE:HD13	2.18	0.44
2:Y:277:HIS:CD2	2:Y:279:PRO:HD3	2.52	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
1:B:24:GLU:HG3	5:B:308:HOH:O	2.16	0.44
2:Y:262:THR:HA	2:Y:273:ARG:O	2.18	0.44
2:Y:85:LEU:N	2:Y:85:LEU:CD2	2.81	0.44
1:A:82:PRO:HG2	1:A:84:PHE:HE1	1.82	0.44
2:Y:288:THR:OG1	4:Y:7:NAG:C1	2.65	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:X:187:SER:HA	2:X:204:TYR:O	2.17	0.43
2:X:266:LEU:H	2:X:271:HIS:HB2	1.84	0.43
2:Y:99:PHE:HD2	2:Y:113:ARG:HD2	1.80	0.43
2:X:283:LEU:CG	2:X:284:GLU:H	2.31	0.43
2:X:102:HIS:HB3	4:X:3:NAG:H2	2.00	0.43
1:B:54:ASN:C	1:B:54:ASN:OD1	2.56	0.43
2:X:215:ASN:HA	2:X:302:ASP:OD2	2.18	0.43
2:X:255:GLY:O	2:X:256:ARG:C	2.56	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
1:B:26:SER:O	1:B:29:LEU:HB3	2.18	0.43
2:Y:294:THR:HG21	4:Y:6:NAG:O7	2.19	0.43
2:X:37:PRO:HD2	2:X:53:THR:HB	2.00	0.43
2:Y:273:ARG:HG2	2:Y:274:SER:N	2.34	0.43
2:Y:58:ALA:HB1	2:Y:59:PRO:HD2	2.00	0.43
1:A:34:ASN:ND2	2:Y:245:PHE:H	2.15	0.43
1:B:12:MET:HG3	5:B:580:HOH:O	2.19	0.43
2:X:42:LEU:N	2:X:42:LEU:HD23	2.34	0.43
2:Y:210:GLN:HB2	5:Y:352:HOH:O	2.18	0.43
2:X:257:LEU:HD12	2:X:257:LEU:H	1.84	0.43

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
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:249:TYR:HB2	2:Y:250:PRO:CD	2.48	0.43
2:X:250:PRO:C	2:X:252:LYS:H	2.23	0.43
2:X:84:VAL:CG2	2:X:84:VAL:O	2.66	0.43
2:Y:240:ASN:HB2	2:Y:243:VAL:HG12	1.99	0.43
2:X:166:ASP:N	5:X:389:HOH:O	2.49	0.43
1:B:36:ASN:N	1:B:36:ASN:ND2	2.60	0.42
2:Y:295:GLU:OE2	2:Y:297:VAL:HB	2.18	0.42
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:48:SER:OG	2:Y:90:LEU:HD12	2.20	0.42
2:Y:72:GLU:HB2	2:Y:84:VAL:HG23	2.01	0.42
1:B:80:LYS:HG2	1:B:80:LYS:O	2.20	0.42
2:Y:177:ARG:NH1	2:Y:177:ARG:HG3	2.35	0.42
2:Y:292:ASN:CG	2:Y:301:GLN:HE21	2.23	0.42
2:Y:251:ARG:O	2:Y:251:ARG:HG2	2.19	0.42
2:Y:238:ILE:HD12	2:Y:271:HIS:CE1	2.55	0.42
1:A:79:ARG:O	1:A:81:LYS:N	2.51	0.42
1:A:73:ARG:HH11	1:A:73:ARG:HG3	1.85	0.42
2:X:153:ASP:HA	2:X:154:PRO:HD3	1.72	0.42
1:B:56:ARG:N	1:B:56:ARG:CD	2.79	0.41
2:Y:250:PRO:HD3	2:Y:288:THR:O	2.19	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:HH11	2:Y:177:ARG:HG3	1.85	0.41
2:X:279:PRO:HG3	5:X:1267:HOH:O	2.20	0.41
2:X:37:PRO:HD2	2:X:53:THR:O	2.20	0.41
2:Y:275:ILE:HD11	2:Y:277:HIS:HB2	2.02	0.41
2:X:292:ASN:ND2	2:X:301:GLN:HE21	2.19	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:B:75:ILE:N	1:B:75:ILE:HD12	2.36	0.41
1:B:56:ARG:HD3	2:Y:241:GLU:OE1	2.21	0.41
1:A:55:ASN:HB3	1:A:57:ASN:H	1.86	0.41
2:X:145:ILE:O	2:X:180:SER:HA	2.20	0.41
2:Y:253:GLU:HB2	5:Y:1083:HOH:O	2.20	0.41
1:A:25:ILE:HD11	1:A:44:VAL:HG13	2.02	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

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
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
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:37:PRO:HA	2:X:38:PRO:HA	1.64	0.41
2:X:37:PRO:HD2	2:X:53:THR:CG2	2.51	0.41
1:A:72:VAL:HG13	1:A:89:VAL:HG12	2.02	0.41
2:Y:253:GLU:HA	5:Y:468:HOH:O	2.19	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
1:B:79:ARG:O	1:B:80:LYS:HB3	2.21	0.41
2:Y:220:ALA:HB1	5:Y:857:HOH:O	2.20	0.41
2:X:248:THR:HG22	2:X:290:THR:HB	1.96	0.41
2:X:68:GLU:HB2	2:X:71:GLN:NE2	2.36	0.40
2:Y:63:GLU:O	2:Y:63:GLU:HG3	2.20	0.40
2:X:231:ILE:C	2:X:232:THR:HG22	2.41	0.40
2:X:146:THR:O	2:X:148:PRO:HD3	2.21	0.40
2:Y:64:ARG:HG3	2:Y:65:MET:HG2	2.03	0.40
2:X:231:ILE:HB	2:X:278:ILE:HB	2.03	0.40
2:Y:241:GLU:HG3	2:Y:270:TYR:CE1	2.57	0.40
2:Y:48:SER:HA	5:Y:1089:HOH:O	2.21	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:292:ASN:ND2	2:Y:301:GLN:HE21	2.19	0.40
2:Y:101:THR:HB	2:Y:102:HIS:H	1.62	0.40
5:A:804:HOH:O	2:X:164:LYS:HG3	2.21	0.40
1:A:44:VAL:HG21	1:A:91:LEU:HD11	2.02	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%)	11   8

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	B	99/172 (58%)	93 (94%)	6 (6%)	0	100	100
2	X	270/289 (93%)	242 (90%)	19 (7%)	9 (3%)	6	3
2	Y	269/289 (93%)	224 (83%)	38 (14%)	7 (3%)	8	5
All	All	733/922 (80%)	648 (88%)	67 (9%)	18 (2%)	9	6

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%)	80 (89%)	10 (11%)	9	9
1	B	93/153 (61%)	80 (86%)	13 (14%)	5	5
2	X	251/264 (95%)	219 (87%)	32 (13%)	6	6
2	Y	250/264 (95%)	224 (90%)	26 (10%)	10	11

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
All	All	684/834 (82%)	603 (88%)	81 (12%)	<b>8</b> <b>8</b>

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	28	ARG
1	A	29	LEU
1	A	57	ASN
1	A	58	VAL
1	A	65	VAL
1	A	68	ARG
1	A	95	LEU
1	B	6	THR
1	B	17	LYS
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	90	THR
1	B	95	LEU
1	B	97	CYS
1	B	98	LYS
2	X	34	VAL
2	X	42	LEU
2	X	60	VAL
2	X	61	VAL
2	X	64	ARG
2	X	75	LYS
2	X	77	GLN
2	X	78	ASP
2	X	103	ASN
2	X	104	ASP
2	X	115	ARG
2	X	131	ASP
2	X	135	LEU
2	X	141	GLU

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Mol	Chain	Res	Type
2	X	160	LEU
2	X	162	GLU
2	X	166	ASP
2	X	219	ASN
2	X	227	GLN
2	X	232	THR
2	X	238	ILE
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	309	THR
2	Y	75	LYS
2	Y	77	GLN
2	Y	80	THR
2	Y	85	LEU
2	Y	103	ASN
2	Y	112	GLU
2	Y	115	ARG
2	Y	130	ASN
2	Y	131	ASP
2	Y	141	GLU
2	Y	151	VAL
2	Y	160	LEU
2	Y	219	ASN
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

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Mol	Chain	Res	Type
2	Y	307	ASN
2	Y	309	THR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (17) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	55	ASN
1	A	57	ASN
1	A	59	GLN
1	B	36	ASN
1	B	47	GLN
1	B	57	ASN
1	B	64	GLN
1	B	71	GLN
2	X	77	GLN
2	X	219	ASN
2	X	222	GLN
2	X	227	GLN
2	Y	77	GLN
2	Y	219	ASN
2	Y	222	GLN
2	Y	227	GLN
2	Y	277	HIS

### 5.3.3 RNA ⓘ

There are no RNA chains 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 carbohydrates 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	$\# Z  > 2$
3	NDG	X	1	-	12,14,15	0.45	0	15,19,21	0.71	0
4	NAG	X	2	2	12,14,15	0.46	0	15,19,21	0.66	0
4	NAG	X	3	2	12,14,15	0.43	0	15,19,21	0.72	0
4	NAG	X	4	2	12,14,15	0.61	0	15,19,21	0.71	0
4	NAG	X	5	2	12,14,15	0.46	0	15,19,21	0.76	0
4	NAG	X	6	2	12,14,15	0.52	0	15,19,21	0.94	1 (6%)
4	NAG	X	7	2	12,14,15	0.46	0	15,19,21	0.56	0
4	NAG	Y	1	2	12,14,15	0.50	0	15,19,21	0.68	0
4	NAG	Y	2	2	12,14,15	0.45	0	15,19,21	0.55	0
4	NAG	Y	3	2	12,14,15	0.45	0	15,19,21	0.70	0
4	NAG	Y	4	2	12,14,15	0.48	0	15,19,21	0.70	0
4	NAG	Y	5	2	12,14,15	0.49	0	15,19,21	0.81	1 (6%)
4	NAG	Y	6	2	12,14,15	0.45	0	15,19,21	0.79	0
4	NAG	Y	7	2	12,14,15	0.52	0	15,19,21	0.69	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	NDG	X	1	-	-	0/6/23/26	0/1/1/1
4	NAG	X	2	2	-	0/6/23/26	0/1/1/1
4	NAG	X	3	2	1/1/5/7	0/6/23/26	0/1/1/1
4	NAG	X	4	2	-	0/6/23/26	0/1/1/1
4	NAG	X	5	2	1/1/5/7	0/6/23/26	0/1/1/1
4	NAG	X	6	2	-	0/6/23/26	0/1/1/1
4	NAG	X	7	2	1/1/5/7	0/6/23/26	0/1/1/1
4	NAG	Y	1	2	1/1/5/7	0/6/23/26	0/1/1/1
4	NAG	Y	2	2	-	0/6/23/26	0/1/1/1
4	NAG	Y	3	2	-	0/6/23/26	0/1/1/1
4	NAG	Y	4	2	-	0/6/23/26	0/1/1/1
4	NAG	Y	5	2	1/1/5/7	0/6/23/26	0/1/1/1
4	NAG	Y	6	2	-	1/6/23/26	1/1/1/1
4	NAG	Y	7	2	-	0/6/23/26	0/1/1/1

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	X	6	NAG	C2-N2-C7	-2.35	119.14	123.09
4	Y	5	NAG	C2-N2-C7	-2.00	119.72	123.09

All (5) chirality outliers are listed below:

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

All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	Y	6	NAG	O7-C7-N2-C2

All (1) ring outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	Y	6	NAG	C1-C2-C3-C4-C5-O5

## 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<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	97/172 (56%)	0.10	3 (3%) 47 56	20, 38, 81, 107	0
1	B	101/172 (58%)	-0.00	0 100 100	21, 36, 57, 93	0
2	X	274/289 (94%)	0.06	2 (0%) 84 91	26, 56, 88, 100	0
2	Y	273/289 (94%)	1.74	94 (34%) 1 1	37, 95, 114, 120	0
All	All	745/922 (80%)	0.67	99 (13%) 4 6	20, 60, 109, 120	0

All (99) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	Y	101	THR	8.1
2	Y	85	LEU	8.1
2	Y	102	HIS	7.9
2	Y	62	TRP	7.3
2	Y	87	LEU	7.2
2	Y	46	VAL	6.9
2	Y	297	VAL	6.2
2	Y	59	PRO	6.1
2	Y	268	MET	6.1
2	Y	82	SER	6.0
2	Y	74	ALA	5.8
2	Y	81	PHE	5.7
1	A	80	LYS	5.5
2	Y	237	VAL	5.3
2	Y	84	VAL	5.1
2	Y	216	VAL	5.0
1	A	79	ARG	4.9
2	Y	269	PRO	4.8
2	Y	252	LYS	4.8
2	Y	104	ASP	4.7
2	Y	215	ASN	4.6

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Mol	Chain	Res	Type	RSRZ
2	Y	126	GLY	4.6
2	Y	61	VAL	4.5
2	Y	254	SER	4.5
2	Y	38	PRO	4.4
2	Y	231	ILE	4.4
2	Y	121	PRO	4.2
2	Y	136	PHE	4.2
2	Y	289	TYR	4.1
2	Y	257	LEU	4.1
2	Y	214	ILE	4.1
2	Y	68	GLU	4.0
2	Y	114	LYS	3.9
2	Y	60	VAL	3.7
2	Y	55	SER	3.7
2	Y	63	GLU	3.7
2	Y	53	THR	3.7
2	Y	300	HIS	3.6
2	Y	58	ALA	3.5
2	Y	78	ASP	3.4
2	Y	266	LEU	3.3
2	Y	272	ILE	3.3
2	Y	225	VAL	3.3
2	Y	116	LEU	3.2
2	Y	112	GLU	3.2
2	Y	278	ILE	3.2
2	Y	47	SER	3.2
2	Y	305	ALA	3.1
2	Y	119	PHE	3.1
2	Y	56	GLY	3.1
2	Y	259	GLU	3.1
2	Y	256	ARG	3.1
2	Y	258	VAL	3.1
2	Y	52	LEU	3.1
2	Y	77	GLN	3.0
2	Y	209	LEU	3.0
2	Y	228	GLY	3.0
2	Y	57	SER	2.9
2	Y	308	ILE	2.9
2	Y	277	HIS	2.9
2	X	266	LEU	2.9
2	Y	298	ASN	2.9
2	Y	307	ASN	2.8

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Mol	Chain	Res	Type	RSRZ
2	Y	79	GLY	2.7
2	Y	267	ASP	2.7
2	Y	265	LEU	2.6
2	Y	83	SER	2.6
2	Y	302	ASP	2.6
2	Y	123	PRO	2.5
2	Y	283	LEU	2.5
2	Y	138	PHE	2.5
2	Y	294	THR	2.5
2	Y	125	VAL	2.5
2	Y	111	ASP	2.5
2	X	33	LEU	2.4
2	Y	43	VAL	2.4
2	Y	103	ASN	2.4
2	Y	304	LYS	2.3
2	Y	93	LEU	2.3
2	Y	288	THR	2.3
2	Y	221	VAL	2.3
2	Y	301	GLN	2.3
2	Y	213	SER	2.3
2	Y	249	TYR	2.3
1	A	102	VAL	2.3
2	Y	292	ASN	2.3
2	Y	48	SER	2.3
2	Y	67	GLN	2.3
2	Y	91	THR	2.3
2	Y	239	GLY	2.2
2	Y	44	LEU	2.2
2	Y	253	GLU	2.1
2	Y	115	ARG	2.1
2	Y	230	ASN	2.1
2	Y	219	ASN	2.1
2	Y	75	LYS	2.1
2	Y	76	ALA	2.0
2	Y	311	VAL	2.0
2	Y	222	GLN	2.0

## 6.2 Non-standard residues in protein, DNA, RNA chains ⓘ

There are no non-standard protein/DNA/RNA residues in this entry.



### 6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

### 6.4 Ligands ⓘ

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<sup>th</sup> 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	RSR	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
4	NAG	X	7	14/15	0.80	13.15	116,119,122,122	0
4	NAG	Y	6	14/15	0.47	10.50	113,118,121,121	0
4	NAG	X	4	14/15	0.32	6.77	106,109,111,111	0
4	NAG	X	6	14/15	0.21	4.84	87,94,100,100	0
4	NAG	Y	2	14/15	0.33	4.12	116,120,122,122	0
4	NAG	Y	4	14/15	0.52	3.11	121,123,123,123	0
4	NAG	Y	5	14/15	0.41	2.12	112,118,121,121	0
4	NAG	Y	1	14/15	0.34	2.10	119,123,125,125	0
4	NAG	Y	7	14/15	0.35	1.50	117,118,119,119	0
4	NAG	X	3	14/15	0.22	1.36	117,119,120,120	0
4	NAG	X	5	14/15	0.14	0.80	87,89,91,91	0
3	NDG	X	1	14/15	0.14	0.17	81,86,89,89	0
4	NAG	Y	3	14/15	0.36	-0.11	114,117,118,118	0
4	NAG	X	2	14/15	0.28	-	96,102,105,107	0

### 6.5 Other polymers ⓘ

There are no such residues in this entry.