Full wwPDB X-ray Structure Validation Report (i)

Feb 1, 2016 – 02:56 PM GMT

PDB ID	:	4AY9
Title	:	Structure of follicle-stimulating hormone in complex with the entire ectodomain of its receptor
Authors	:	Jiang, X.; Liu, H.; Chen, X.; He, X.
Deposited on	:	2012-06-19
Resolution	:	2.50 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:

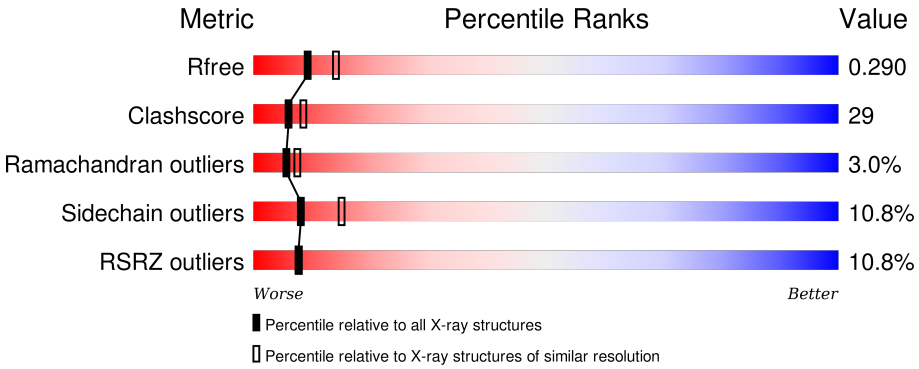
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	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 2.50 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	3553 (2.50-2.50)
Clashscore	102246	4242 (2.50-2.50)
Ramachandran outliers	100387	4156 (2.50-2.50)
Sidechain outliers	100360	4158 (2.50-2.50)
RSRZ outliers	91569	3562 (2.50-2.50)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5% The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	92	4% 51% 39%
1	D	92	7% 55% 35% 5%
1	G	92	4% 52% 37% 5%
2	B	111	4% 63% 31%
2	E	111	7% 62% 30%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
2	H	111	8% 62% 31%
3	X	350	14% 47% 32% 8% 12%
3	Y	350	13% 51% 28% 7% 12%
3	Z	350	10% 50% 29% 9% 12%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	TYS	Y	335	-	-	X	-
3	TYS	Z	335	-	-	X	-
4	NAG	E	1007	-	-	X	-
4	NAG	Y	1191	-	-	-	X

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 12344 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 GLYCOPROTEIN HORMONES, ALPHA POLYPEPTIDE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	88	Total	C	N	O	S	0	0	0
			675	417	118	127	13			
1	D	89	Total	C	N	O	S	0	0	0
			682	422	119	128	13			
1	G	88	Total	C	N	O	S	0	0	0
			675	417	118	127	13			

- Molecule 2 is a protein called FOLLITROPIN SUBUNIT BETA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	107	Total	C	N	O	S	0	0	0
			831	517	140	162	12			
2	E	107	Total	C	N	O	S	0	0	0
			831	517	140	162	12			
2	H	107	Total	C	N	O	S	0	0	0
			831	517	140	162	12			

- Molecule 3 is a protein called FOLLICLE-STIMULATING HORMONE RECEPTOR.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	X	307	Total	C	N	O	S	0	0	0
			2462	1555	429	466	12			
3	Y	307	Total	C	N	O	S	0	0	0
			2462	1555	429	466	12			
3	Z	307	Total	C	N	O	S	0	0	0
			2462	1555	429	466	12			

There are 3 discrepancies between the modelled and reference sequences:

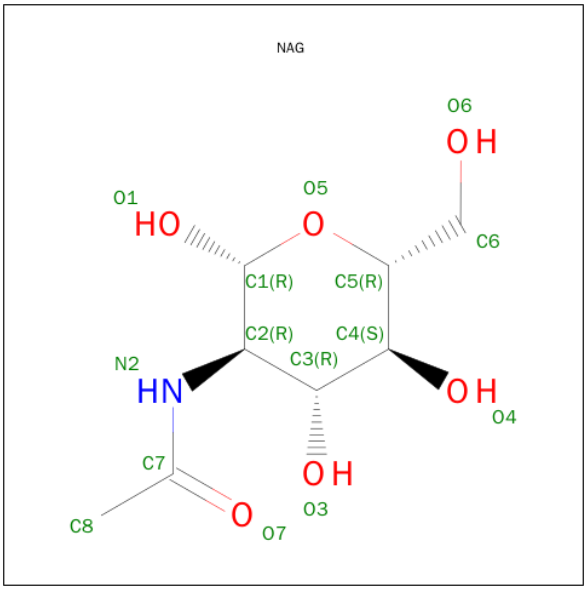
Chain	Residue	Modelled	Actual	Comment	Reference
X	188	SER	CYS	CONFLICT	UNP P23945
Y	188	SER	CYS	CONFLICT	UNP P23945

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
Z	188	SER	CYS	CONFLICT	UNP P23945

- 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	A	1	Total	C	N	O	0	0
			14	8	1	5		
4	A	1	Total	C	N	O	0	0
			14	8	1	5		
4	B	1	Total	C	N	O	0	0
			14	8	1	5		
4	B	1	Total	C	N	O	0	0
			14	8	1	5		
4	D	1	Total	C	N	O	0	0
			14	8	1	5		
4	D	1	Total	C	N	O	0	0
			14	8	1	5		
4	E	1	Total	C	N	O	0	0
			14	8	1	5		
4	E	1	Total	C	N	O	0	0
			14	8	1	5		
4	G	1	Total	C	N	O	0	0
			14	8	1	5		
4	G	1	Total	C	N	O	0	0
			14	8	1	5		

Continued on next page...

Continued from previous page...

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

- Molecule 5 is water.

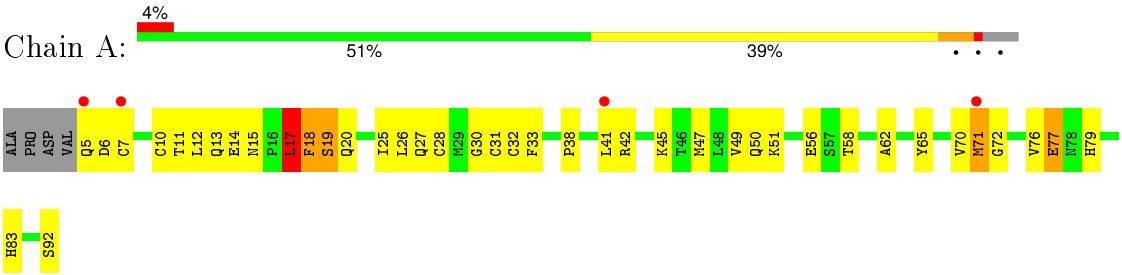
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	19	Total O 19 19	0	0
5	B	15	Total O 15 15	0	0
5	D	18	Total O 18 18	0	0
5	E	21	Total O 21 21	0	0
5	G	18	Total O 18 18	0	0
5	H	14	Total O 14 14	0	0
5	X	28	Total O 28 28	0	0
5	Y	45	Total O 45 45	0	0
5	Z	45	Total O 45 45	0	0

3 Residue-property plots (i)

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

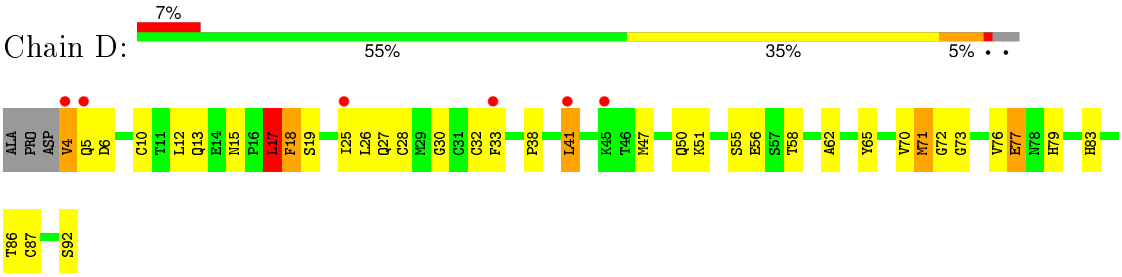
- Molecule 1: GLYCOPROTEIN HORMONES, ALPHA POLYPEPTIDE

Chain A:



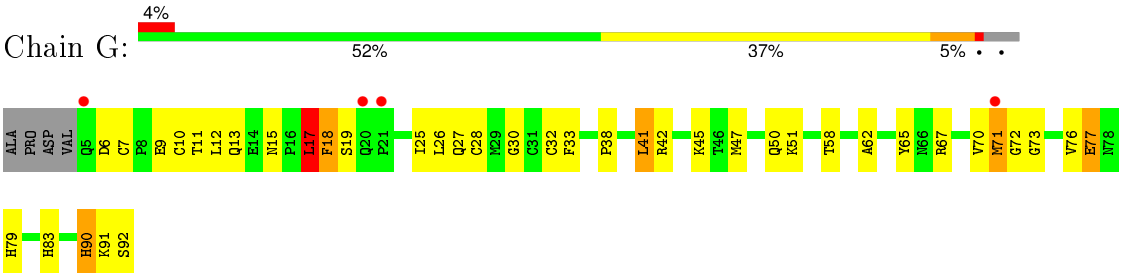
- Molecule 1: GLYCOPROTEIN HORMONES, ALPHA POLYPEPTIDE

Chain D:



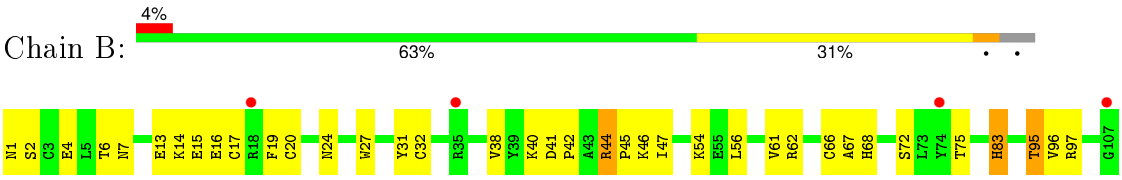
- Molecule 1: GLYCOPROTEIN HORMONES, ALPHA POLYPEPTIDE

Chain G:



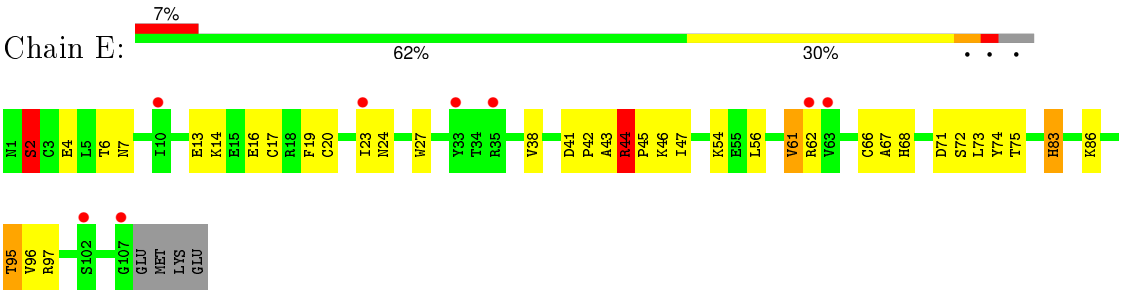
- Molecule 2: FOLLITROPIN SUBUNIT BETA

Chain B:



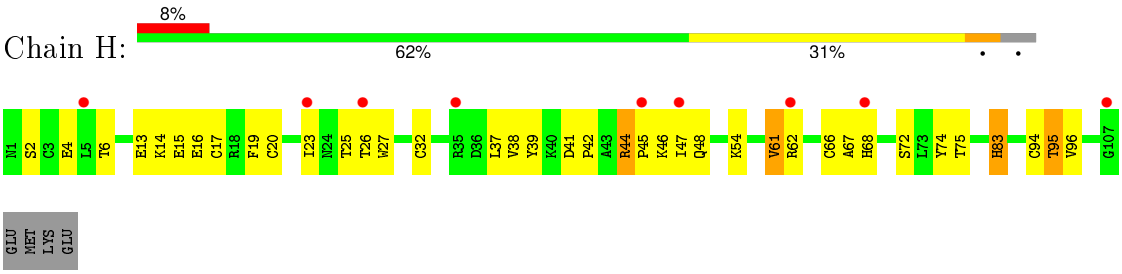
- Molecule 2: FOLLITROPIN SUBUNIT BETA

Chain E:



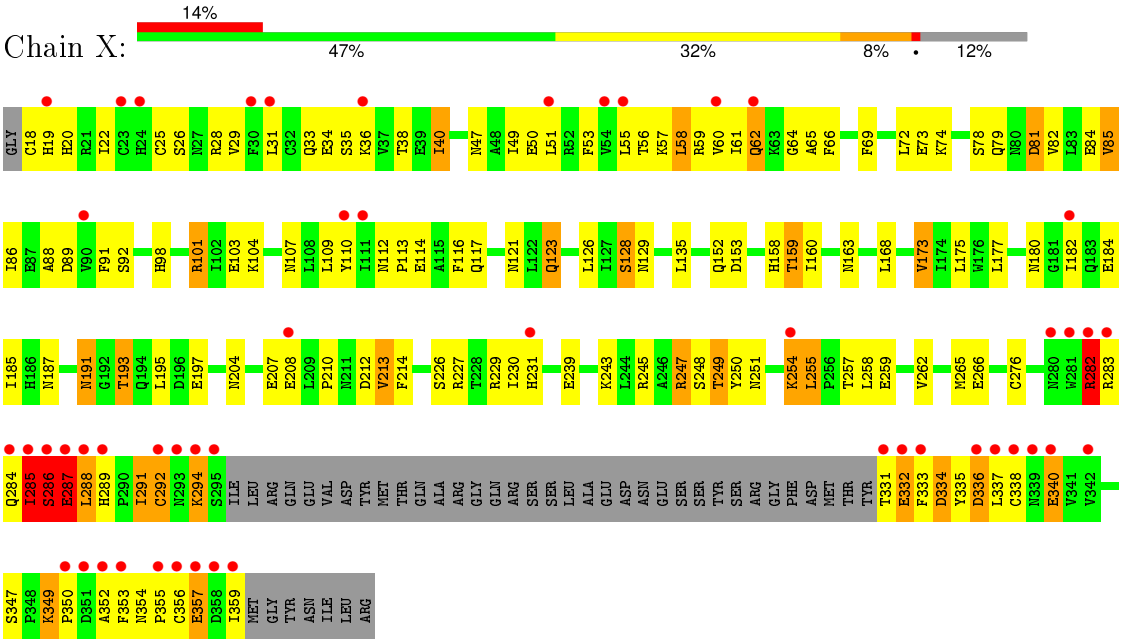
- Molecule 2: FOLLITROPIN SUBUNIT BETA

Chain H:



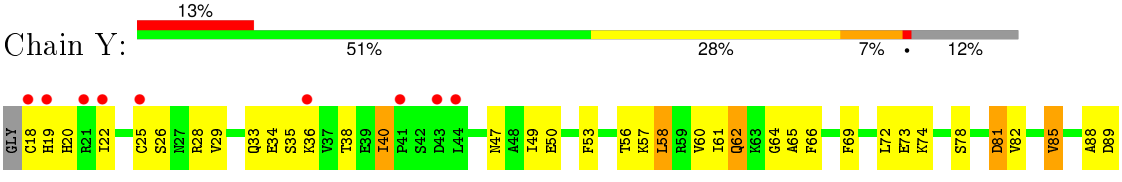
- Molecule 3: FOLLICLE-STIMULATING HORMONE RECEPTOR

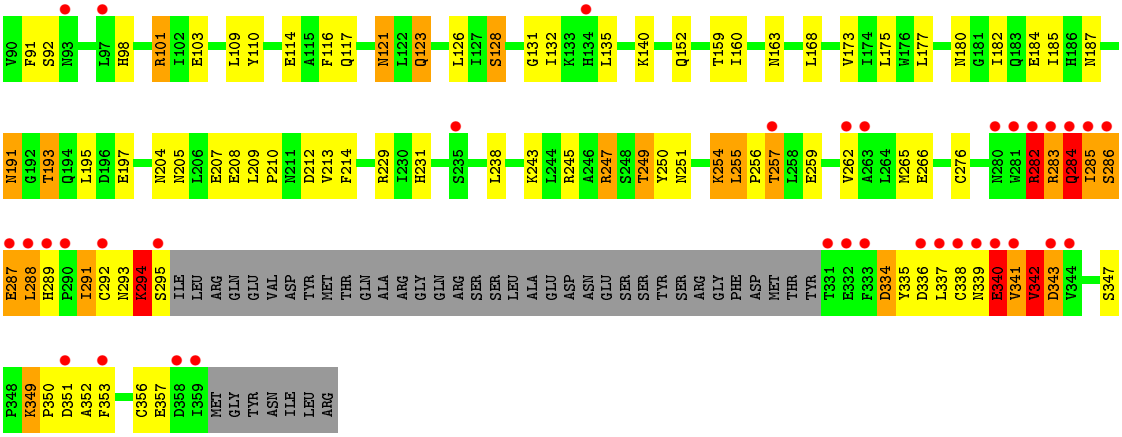
Chain X:



- Molecule 3: FOLLICLE-STIMULATING HORMONE RECEPTOR

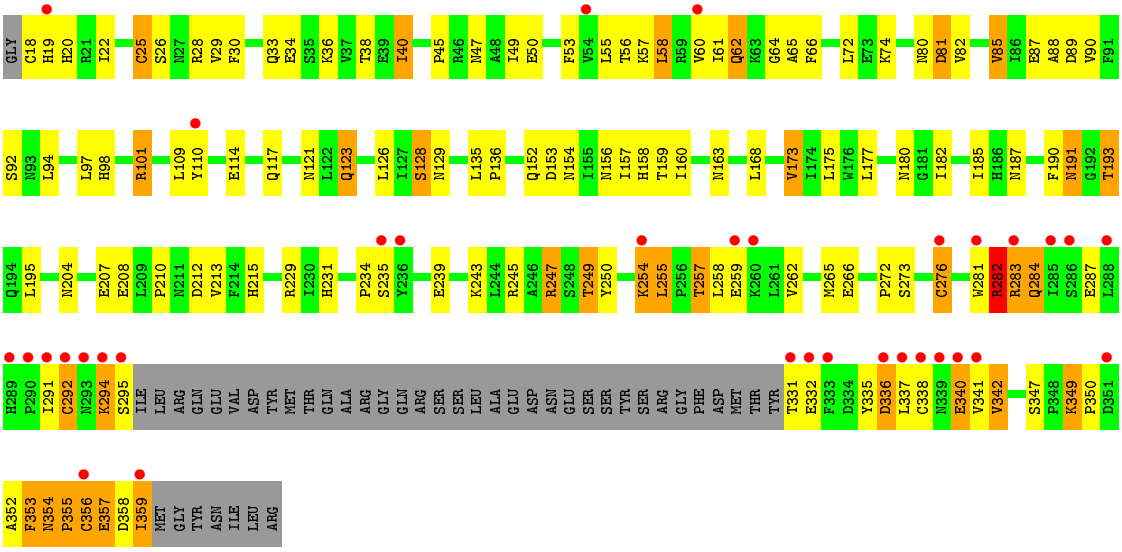
Chain Y:





- Molecule 3: FOLLICLE-STIMULATING HORMONE RECEPTOR

Chain Z:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α, β, γ	70.72Å 95.48Å 95.67Å 60.30° 80.02° 75.35°	Depositor
Resolution (Å)	47.90 – 2.50 47.90 – 2.50	Depositor EDS
% Data completeness (in resolution range)	100.0 (47.90-2.50) 80.3 (47.90-2.50)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	4.11 (at 2.51Å)	Xtriage
Refinement program	REFMAC 5.5.0066	Depositor
R, R_{free}	0.235 , 0.269 0.257 , 0.290	Depositor DCC
R_{free} test set	1989 reflections (2.81%)	DCC
Wilson B-factor (Å^2)	52.4	Xtriage
Anisotropy	0.366	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.31 , 66.5	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.31$	Xtriage
Outliers	0 of 141670 reflections	Xtriage
F_o,F_c correlation	0.92	EDS
Total number of atoms	12344	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 4.23% 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, TYS

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	0.38	0/690	0.56	0/933
1	D	0.37	0/697	0.53	0/943
1	G	0.38	0/690	0.57	0/933
2	B	0.34	0/850	0.55	0/1155
2	E	0.39	0/850	0.60	0/1155
2	H	0.35	0/850	0.57	0/1155
3	X	0.33	0/2493	0.60	0/3380
3	Y	0.34	0/2493	0.61	0/3380
3	Z	0.34	0/2493	0.60	0/3380
All	All	0.35	0/12106	0.59	0/16414

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
3	Y	0	2

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
3	Y	340	GLU	Peptide
3	Y	341	VAL	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	675	0	647	40	0
1	D	682	0	656	49	0
1	G	675	0	647	43	0
2	B	831	0	782	43	0
2	E	831	0	782	51	0
2	H	831	0	782	36	0
3	X	2462	0	2439	153	0
3	Y	2462	0	2440	162	0
3	Z	2462	0	2438	137	0
4	A	28	0	26	3	0
4	B	28	0	26	9	0
4	D	28	0	26	1	0
4	E	28	0	26	12	0
4	G	28	0	26	4	0
4	H	28	0	26	5	0
4	X	14	0	13	5	0
4	Y	14	0	13	5	0
4	Z	14	0	13	1	0
5	A	19	0	0	6	0
5	B	15	0	0	7	0
5	D	18	0	0	4	0
5	E	21	0	0	4	0
5	G	18	0	0	3	0
5	H	14	0	0	0	0
5	X	28	0	0	20	0
5	Y	45	0	0	21	0
5	Z	45	0	0	21	0
All	All	12344	0	11808	681	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 29.

All (681) 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)
3:Y:191:ASN:HD21	4:Y:1191:NAG:C1	1.07	1.58
3:Y:276:CYS:SG	3:Y:350:PRO:HG3	1.58	1.41
4:E:1007:NAG:O6	5:E:2021:HOH:O	1.54	1.25
3:Y:335:TYS:HE2	3:Y:335:TYS:O3	1.38	1.18
3:Z:335:TYS:HD2	3:Z:335:TYS:N	1.53	1.17
3:Y:341:VAL:CG1	3:Y:342:VAL:HG22	1.74	1.15
3:Y:341:VAL:HG22	3:Y:342:VAL:HG13	1.28	1.13
3:Z:276:CYS:HB2	5:Z:2042:HOH:O	1.48	1.11
2:E:44:ARG:HD3	2:E:46:LYS:H	1.07	1.10
2:B:44:ARG:HB2	2:B:45:PRO:HA	1.17	1.10
2:H:44:ARG:HB2	2:H:45:PRO:HA	1.20	1.09
3:X:69:PHE:HB3	5:X:2002:HOH:O	1.56	1.04
3:X:60:VAL:HG13	3:X:85:VAL:HG23	1.37	1.04
3:Y:341:VAL:HG13	3:Y:342:VAL:CG2	1.87	1.04
3:Y:187:ASN:OD1	3:Y:212:ASP:HB2	1.56	1.04
3:X:285:ILE:CG1	3:X:286:SER:HB2	1.87	1.03
3:X:276:CYS:SG	3:X:350:PRO:HG3	1.99	1.02
3:Y:335:TYS:CE2	3:Y:335:TYS:O3	1.97	1.01
3:Y:60:VAL:HG13	3:Y:85:VAL:HG23	1.43	1.00
3:Y:349:LYS:HG2	5:Y:2044:HOH:O	1.60	1.00
3:Y:341:VAL:HG13	3:Y:342:VAL:HG22	1.04	0.99
3:Y:254:LYS:HG3	3:Y:255:LEU:H	1.28	0.99
3:Y:285:ILE:HG23	3:Y:286:SER:H	1.27	0.98
2:B:24:ASN:ND2	4:B:1024:NAG:H4	1.76	0.98
1:A:18:PHE:HB2	1:A:25:ILE:HD11	1.46	0.98
3:X:226:SER:HA	5:X:2018:HOH:O	1.65	0.97
5:G:2003:HOH:O	2:H:32:CYS:HB2	1.64	0.96
2:B:44:ARG:HB2	2:B:45:PRO:CA	1.96	0.96
3:X:285:ILE:HG13	3:X:286:SER:HB2	1.44	0.96
3:Z:98:HIS:HB2	3:Z:123:GLN:HG3	1.47	0.96
3:Y:341:VAL:HG22	3:Y:342:VAL:CG1	1.97	0.95
1:D:17:LEU:O	1:D:19:SER:N	2.00	0.95
2:E:44:ARG:HB2	2:E:45:PRO:CA	1.98	0.94
2:E:44:ARG:HD3	2:E:46:LYS:N	1.82	0.94
1:G:47:MET:HE1	1:G:51:LYS:H	1.32	0.93
3:Y:276:CYS:SG	3:Y:350:PRO:CG	2.55	0.93
1:A:47:MET:HE1	1:A:51:LYS:H	1.32	0.93
3:X:191:ASN:CG	4:X:1191:NAG:C1	2.36	0.93
2:H:44:ARG:HB2	2:H:45:PRO:CA	2.00	0.92
1:G:17:LEU:O	1:G:19:SER:N	2.00	0.92
3:Z:335:TYS:CD2	3:Z:335:TYS:N	2.32	0.91
3:Y:191:ASN:CG	4:Y:1191:NAG:C1	2.39	0.91

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:X:250:TYR:OH	3:Z:208:GLU:OE1	1.88	0.91
2:B:44:ARG:CB	2:B:45:PRO:HA	2.00	0.91
2:E:7:ASN:OD1	4:E:1007:NAG:H2	1.69	0.90
2:E:7:ASN:OD1	4:E:1007:NAG:C2	2.19	0.90
2:H:44:ARG:CB	2:H:45:PRO:HA	2.01	0.90
1:G:47:MET:CE	1:G:51:LYS:H	1.86	0.89
3:Y:98:HIS:HB2	3:Y:123:GLN:HG3	1.52	0.89
3:X:69:PHE:CA	5:X:2002:HOH:O	2.21	0.89
3:Z:187:ASN:OD1	3:Z:212:ASP:HB2	1.72	0.88
3:Z:163:ASN:ND2	3:Z:191:ASN:OD1	2.07	0.88
3:X:98:HIS:HB2	3:X:123:GLN:HG3	1.57	0.87
3:Z:80:ASN:HB3	5:Z:2004:HOH:O	1.74	0.86
3:Z:258:LEU:CB	3:Z:283:ARG:HD2	2.05	0.86
3:Z:245:ARG:HH11	3:Z:245:ARG:HG2	1.38	0.86
3:Y:245:ARG:HH11	3:Y:245:ARG:HG2	1.41	0.86
2:E:44:ARG:HB2	2:E:45:PRO:C	1.95	0.85
3:Y:254:LYS:HA	5:Y:2040:HOH:O	1.77	0.85
3:Z:281:TRP:HB3	3:Z:283:ARG:HG3	1.58	0.84
2:E:38:VAL:N	3:Y:335:TYS:O2	2.09	0.84
3:Z:60:VAL:HG13	3:Z:85:VAL:HG23	1.57	0.83
1:G:6:ASP:O	5:G:2001:HOH:O	1.96	0.83
3:X:163:ASN:ND2	3:X:191:ASN:OD1	2.10	0.83
4:B:1024:NAG:O7	4:B:1024:NAG:C1	2.24	0.83
3:Y:356:CYS:O	3:Y:357:GLU:HG2	1.77	0.83
1:D:32:CYS:HB3	1:D:58:THR:HG23	1.60	0.82
3:X:245:ARG:HG2	3:X:245:ARG:HH11	1.44	0.82
3:X:285:ILE:HA	3:X:286:SER:CB	2.09	0.82
1:G:32:CYS:HB3	1:G:58:THR:HG23	1.60	0.82
3:Z:98:HIS:HB2	3:Z:123:GLN:CG	2.10	0.82
1:A:47:MET:CE	1:A:51:LYS:H	1.93	0.81
5:B:2007:HOH:O	3:X:334:ASP:OD1	1.98	0.81
2:B:44:ARG:CB	2:B:45:PRO:CA	2.58	0.81
3:X:294:LYS:O	3:X:294:LYS:HD2	1.80	0.81
1:D:47:MET:HE1	1:D:51:LYS:H	1.45	0.81
2:H:44:ARG:CB	2:H:45:PRO:CA	2.59	0.80
3:X:60:VAL:HG13	3:X:85:VAL:CG2	2.12	0.79
3:Z:273:SER:HA	5:Z:2042:HOH:O	1.82	0.79
3:Y:98:HIS:HB2	3:Y:123:GLN:CG	2.12	0.79
3:Z:158:HIS:NE2	5:Z:2020:HOH:O	2.13	0.79
3:Z:353:PHE:CA	5:Z:2043:HOH:O	2.29	0.79
3:Y:249:THR:O	5:Y:2039:HOH:O	2.01	0.79

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:Y:257:THR:HA	5:Y:2041:HOH:O	1.81	0.79
5:B:2007:HOH:O	3:X:334:ASP:OD2	2.00	0.79
5:B:2007:HOH:O	3:X:334:ASP:CG	2.22	0.78
4:B:1007:NAG:H81	5:B:2015:HOH:O	1.84	0.78
1:D:47:MET:CE	1:D:51:LYS:H	1.95	0.78
3:X:98:HIS:HB2	3:X:123:GLN:CG	2.13	0.78
3:Y:341:VAL:CG2	3:Y:342:VAL:HG13	2.13	0.77
2:E:13:GLU:HG3	2:E:20:CYS:SG	2.23	0.77
3:X:187:ASN:OD1	3:X:212:ASP:HB2	1.84	0.77
3:Y:28:ARG:NH1	3:Y:47:ASN:O	2.18	0.77
2:B:24:ASN:HD22	4:B:1024:NAG:H4	1.45	0.77
3:Y:40:ILE:HG13	3:Y:62:GLN:NE2	1.99	0.77
4:G:1052:NAG:C3	4:G:1052:NAG:O7	2.31	0.77
3:Y:254:LYS:O	5:Y:2040:HOH:O	2.01	0.76
3:X:227:ARG:N	5:X:2018:HOH:O	2.17	0.76
3:Z:258:LEU:HB3	3:Z:283:ARG:HD2	1.65	0.76
2:B:13:GLU:HG3	2:B:20:CYS:SG	2.26	0.76
3:Z:353:PHE:HA	5:Z:2043:HOH:O	1.86	0.75
3:Y:208:GLU:HA	5:Y:2032:HOH:O	1.86	0.75
3:X:254:LYS:HG3	5:X:2025:HOH:O	1.85	0.75
1:D:73:GLY:N	5:D:2012:HOH:O	2.20	0.74
3:Y:177:LEU:O	3:Y:180:ASN:ND2	2.20	0.74
1:A:32:CYS:HB3	1:A:58:THR:HG23	1.68	0.74
3:Y:288:LEU:HD13	3:Y:339:ASN:HD22	1.50	0.74
4:A:1052:NAG:C3	4:A:1052:NAG:O7	2.32	0.74
2:E:41:ASP:OD1	2:E:42:PRO:HD2	1.88	0.74
2:B:24:ASN:ND2	4:B:1024:NAG:C4	2.49	0.74
3:X:69:PHE:CB	5:X:2002:HOH:O	2.18	0.73
2:H:37:LEU:HD22	3:Z:335:TYS:O2	1.88	0.73
1:D:4:VAL:HG23	5:E:2002:HOH:O	1.89	0.73
4:E:1007:NAG:C3	4:E:1007:NAG:O7	2.36	0.73
1:G:10:CYS:HA	1:G:30:GLY:HA3	1.71	0.73
3:X:193:THR:HA	5:X:2015:HOH:O	1.89	0.73
1:G:18:PHE:CB	1:G:25:ILE:HD11	2.18	0.73
3:Y:116:PHE:O	5:Y:2010:HOH:O	2.07	0.73
3:Y:254:LYS:C	5:Y:2040:HOH:O	2.26	0.72
3:X:28:ARG:NH1	3:X:47:ASN:O	2.23	0.72
1:A:14:GLU:OE2	5:A:2003:HOH:O	2.06	0.72
3:Z:28:ARG:NH1	3:Z:47:ASN:O	2.21	0.72
3:X:285:ILE:HA	3:X:286:SER:OG	1.89	0.72
2:B:41:ASP:OD1	2:B:42:PRO:HD2	1.88	0.72

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:X:335:TYS:HE2	3:X:335:TYS:O3	1.88	0.72
3:X:353:PHE:HB3	5:X:2028:HOH:O	1.89	0.71
3:Y:163:ASN:ND2	3:Y:191:ASN:OD1	2.23	0.71
1:A:17:LEU:O	1:A:19:SER:N	2.23	0.71
4:E:1007:NAG:H3	4:E:1007:NAG:O7	1.90	0.71
3:Y:60:VAL:HG13	3:Y:85:VAL:CG2	2.20	0.71
3:Y:254:LYS:O	3:Y:255:LEU:HB2	1.89	0.71
1:G:18:PHE:HB2	1:G:25:ILE:HD11	1.73	0.71
3:Z:258:LEU:HB2	3:Z:283:ARG:HD2	1.72	0.71
2:B:56:LEU:O	5:B:2011:HOH:O	2.09	0.70
3:Z:338:CYS:HB2	3:Z:340:GLU:HG2	1.72	0.70
1:A:14:GLU:HG2	5:A:2003:HOH:O	1.89	0.70
3:Z:355:PRO:O	3:Z:357:GLU:N	2.24	0.70
2:E:43:ALA:O	2:E:44:ARG:O	2.10	0.70
3:Z:101:ARG:HG3	3:Z:126:LEU:HD23	1.74	0.70
3:X:101:ARG:HG3	3:X:126:LEU:HD23	1.74	0.70
3:Z:356:CYS:C	3:Z:357:GLU:HG3	2.12	0.70
1:A:10:CYS:HA	1:A:30:GLY:HA3	1.74	0.70
3:Y:254:LYS:O	3:Y:255:LEU:CB	2.39	0.70
1:A:18:PHE:HB2	1:A:25:ILE:CD1	2.20	0.70
3:Y:291:ILE:HG23	3:Y:291:ILE:O	1.92	0.69
3:Y:254:LYS:CA	5:Y:2040:HOH:O	2.38	0.69
3:Z:136:PRO:O	5:Z:2017:HOH:O	2.09	0.69
1:D:92:SER:HA	2:E:86:LYS:HD2	1.74	0.69
3:Y:245:ARG:CG	3:Y:245:ARG:HH11	2.06	0.69
3:Y:285:ILE:HG23	3:Y:286:SER:N	2.06	0.69
3:X:283:ARG:NH1	3:X:283:ARG:HB3	2.06	0.69
2:B:7:ASN:ND2	4:B:1007:NAG:O7	2.26	0.69
3:Z:215:HIS:HE1	5:Z:2033:HOH:O	1.75	0.69
3:Z:294:LYS:O	3:Z:295:SER:CB	2.40	0.68
3:Y:256:PRO:O	5:Y:2041:HOH:O	2.10	0.68
3:Y:191:ASN:OD1	4:Y:1191:NAG:C1	2.40	0.68
3:Z:257:THR:HG22	3:Z:283:ARG:HH12	1.57	0.68
3:X:350:PRO:O	3:X:354:ASN:O	2.12	0.68
1:G:25:ILE:HD12	2:H:38:VAL:HG11	1.76	0.68
4:H:1007:NAG:C3	4:H:1007:NAG:O7	2.41	0.68
3:Y:342:VAL:O	3:Y:343:ASP:O	2.13	0.67
4:E:1024:NAG:O7	4:E:1024:NAG:C3	2.41	0.67
3:Y:18:CYS:SG	3:Y:19:HIS:N	2.67	0.67
1:A:47:MET:HE3	1:A:50:GLN:HA	1.76	0.67
3:X:101:ARG:CG	3:X:126:LEU:HD23	2.25	0.67

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:Z:355:PRO:C	3:Z:357:GLU:H	1.98	0.67
2:E:44:ARG:HB2	2:E:45:PRO:HA	1.75	0.67
1:D:12:LEU:O	1:D:13:GLN:HG2	1.95	0.67
3:X:354:ASN:OD1	5:X:2028:HOH:O	2.11	0.66
3:X:107:ASN:OD1	5:X:2007:HOH:O	2.12	0.66
3:Y:283:ARG:HG2	3:Y:284:GLN:H	1.60	0.66
3:X:177:LEU:O	3:X:180:ASN:ND2	2.28	0.66
3:X:285:ILE:CA	3:X:286:SER:HB2	2.26	0.66
3:Y:101:ARG:HG3	3:Y:126:LEU:HD23	1.76	0.66
1:G:38:PRO:HD3	2:H:27:TRP:CD1	2.30	0.66
3:Y:160:ILE:HD11	3:Y:182:ILE:HD13	1.76	0.66
2:H:41:ASP:OD1	2:H:42:PRO:HD2	1.95	0.66
2:H:13:GLU:HG3	2:H:20:CYS:SG	2.37	0.65
1:A:25:ILE:HD12	2:B:38:VAL:HG11	1.77	0.65
2:H:2:SER:O	2:H:2:SER:OG	2.13	0.65
3:Z:235:SER:HA	5:Z:2038:HOH:O	1.96	0.65
3:Y:342:VAL:HG23	3:Y:343:ASP:O	1.96	0.65
3:Z:272:PRO:O	5:Z:2042:HOH:O	2.15	0.65
2:H:14:LYS:NZ	2:H:72:SER:OG	2.30	0.65
3:Y:254:LYS:HG3	3:Y:255:LEU:N	2.08	0.65
1:G:45:LYS:NZ	2:H:15:GLU:OE1	2.24	0.65
3:Z:50:GLU:HG3	3:Z:74:LYS:HB2	1.79	0.65
1:D:86:THR:O	5:D:2016:HOH:O	2.14	0.65
3:X:50:GLU:HG3	3:X:74:LYS:HB2	1.78	0.65
1:D:18:PHE:CB	1:D:25:ILE:HD11	2.28	0.64
3:Z:354:ASN:ND2	3:Z:354:ASN:O	2.29	0.64
2:B:7:ASN:OD1	4:B:1007:NAG:O5	2.04	0.64
3:X:191:ASN:OD1	4:X:1191:NAG:C1	2.45	0.64
3:X:285:ILE:CA	3:X:286:SER:CB	2.75	0.64
3:Z:355:PRO:O	3:Z:357:GLU:HG3	1.97	0.64
3:Z:234:PRO:O	5:Z:2038:HOH:O	2.15	0.64
2:E:7:ASN:CG	4:E:1007:NAG:N2	2.51	0.64
3:Y:350:PRO:HG3	3:Y:356:CYS:SG	2.37	0.64
4:E:1024:NAG:O7	4:E:1024:NAG:H3	1.96	0.64
3:Z:282:ARG:HH11	3:Z:282:ARG:HG2	1.63	0.63
3:Z:282:ARG:HG2	3:Z:282:ARG:NH1	2.11	0.63
4:G:1052:NAG:O3	4:G:1052:NAG:O7	2.16	0.63
3:Y:293:ASN:O	3:Y:294:LYS:HB2	1.99	0.63
3:X:208:GLU:CD	3:Y:250:TYR:OH	2.37	0.63
3:Z:245:ARG:CG	3:Z:245:ARG:HH11	2.11	0.63
3:Z:18:CYS:SG	3:Z:19:HIS:N	2.72	0.63

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:38:PRO:HD3	2:H:27:TRP:NE1	2.14	0.63
2:E:72:SER:HB2	5:E:2014:HOH:O	1.99	0.63
3:Y:40:ILE:HD11	3:Y:61:ILE:HG23	1.80	0.63
3:Z:335:TYS:C	3:Z:336:ASP:OD1	2.46	0.62
3:X:226:SER:CA	5:X:2018:HOH:O	2.35	0.62
3:Z:215:HIS:CE1	5:Z:2033:HOH:O	2.51	0.62
1:D:18:PHE:HB2	1:D:25:ILE:HD11	1.80	0.62
1:D:10:CYS:HA	1:D:30:GLY:HA3	1.80	0.62
2:E:44:ARG:CD	2:E:45:PRO:HA	2.29	0.62
3:X:193:THR:CG2	3:X:195:LEU:HG	2.29	0.62
2:E:7:ASN:CG	4:E:1007:NAG:HN2	2.03	0.62
1:A:49:VAL:HA	5:A:2012:HOH:O	1.99	0.62
1:D:76:VAL:HB	2:E:38:VAL:CG1	2.30	0.62
1:G:47:MET:HE3	1:G:50:GLN:HA	1.80	0.62
3:Z:284:GLN:HG2	3:Z:284:GLN:O	1.98	0.62
3:Y:208:GLU:OE1	3:Z:250:TYR:OH	2.14	0.62
2:B:95:THR:OG1	2:B:96:VAL:N	2.31	0.62
3:X:40:ILE:HD11	3:X:61:ILE:HG23	1.82	0.62
3:Y:193:THR:CG2	3:Y:195:LEU:HG	2.30	0.62
2:B:4:GLU:O	2:B:6:THR:HG23	1.99	0.62
2:E:41:ASP:OD1	2:E:42:PRO:CD	2.48	0.62
3:X:214:PHE:HB2	5:X:2016:HOH:O	1.99	0.62
1:A:7:CYS:SG	2:B:1:ASN:HB2	2.40	0.62
3:Y:207:GLU:N	5:Y:2026:HOH:O	2.23	0.61
3:X:18:CYS:SG	3:X:19:HIS:N	2.74	0.61
1:D:76:VAL:HB	2:E:38:VAL:HG12	1.82	0.61
3:Y:291:ILE:HD11	3:Y:293:ASN:ND2	2.16	0.61
3:Z:258:LEU:HD13	3:Z:283:ARG:HB2	1.82	0.61
3:Z:355:PRO:C	3:Z:357:GLU:N	2.54	0.61
3:Y:184:GLU:HA	5:Y:2025:HOH:O	2.00	0.61
3:X:208:GLU:CD	3:Y:250:TYR:HH	2.04	0.61
3:Z:193:THR:CG2	3:Z:195:LEU:HG	2.31	0.60
3:Y:287:GLU:O	3:Y:288:LEU:HG	2.01	0.60
4:H:1024:NAG:H5	4:H:1024:NAG:O7	2.01	0.60
3:Z:254:LYS:O	3:Z:255:LEU:HG	2.01	0.60
3:Y:342:VAL:C	3:Y:343:ASP:O	2.39	0.60
2:E:4:GLU:O	2:E:6:THR:HG23	2.02	0.60
4:D:1052:NAG:O7	4:D:1052:NAG:C3	2.50	0.60
3:X:229:ARG:O	3:X:251:ASN:OD1	2.19	0.60
3:Y:101:ARG:CG	3:Y:126:LEU:HD23	2.31	0.60
3:X:350:PRO:O	3:X:355:PRO:HA	2.02	0.60

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:Y:56:THR:OG1	3:Y:58:LEU:HB2	2.02	0.59
3:X:285:ILE:CB	3:X:286:SER:HB2	2.32	0.59
3:X:285:ILE:HA	3:X:286:SER:HB2	1.84	0.59
3:X:249:THR:HG23	5:X:2018:HOH:O	2.01	0.59
3:X:353:PHE:O	3:X:354:ASN:OD1	2.21	0.59
3:Z:276:CYS:CB	5:Z:2042:HOH:O	2.24	0.59
3:Z:40:ILE:HD11	3:Z:61:ILE:HG23	1.84	0.59
3:X:338:CYS:HB2	3:X:340:GLU:HG2	1.85	0.59
3:X:185:ILE:O	3:X:210:PRO:HG2	2.02	0.59
3:Z:276:CYS:SG	3:Z:350:PRO:HG3	2.43	0.58
3:X:49:ILE:O	3:X:72:LEU:HD12	2.03	0.58
3:Y:81:ASP:OD1	3:Y:81:ASP:N	2.29	0.58
3:Z:28:ARG:NH2	3:Z:49:ILE:HD11	2.17	0.58
3:Z:185:ILE:O	3:Z:210:PRO:HG2	2.02	0.58
3:Z:190:PHE:N	5:Z:2031:HOH:O	2.29	0.58
3:X:175:LEU:HD12	3:X:195:LEU:HD21	1.86	0.58
2:H:44:ARG:HB3	2:H:45:PRO:C	2.24	0.58
3:Z:101:ARG:CG	3:Z:126:LEU:HD23	2.34	0.58
3:Z:60:VAL:HG13	3:Z:85:VAL:CG2	2.31	0.58
3:Z:156:ASN:HA	5:Z:2020:HOH:O	2.04	0.58
1:A:12:LEU:O	1:A:13:GLN:HG2	2.03	0.58
3:X:81:ASP:N	3:X:81:ASP:OD1	2.28	0.58
1:G:91:LYS:O	1:G:92:SER:C	2.42	0.58
4:A:1052:NAG:O7	4:A:1052:NAG:O3	2.21	0.57
2:B:41:ASP:OD1	2:B:42:PRO:CD	2.51	0.57
2:E:95:THR:OG1	2:E:96:VAL:N	2.37	0.57
3:X:160:ILE:HD11	3:X:182:ILE:HD13	1.86	0.57
2:E:54:LYS:HE3	2:E:83:HIS:CD2	2.40	0.57
1:G:27:GLN:HA	1:G:79:HIS:ND1	2.20	0.57
3:Y:40:ILE:HG13	3:Y:62:GLN:HE21	1.70	0.57
1:A:27:GLN:HA	1:A:79:HIS:ND1	2.20	0.57
3:Y:85:VAL:HG12	3:Y:110:TYR:HD2	1.70	0.57
2:B:44:ARG:HD2	2:B:46:LYS:HD2	1.86	0.57
3:Y:294:LYS:O	3:Y:295:SER:C	2.43	0.56
3:Y:33:GLN:HG2	3:Y:34:GLU:H	1.71	0.56
3:Y:342:VAL:O	3:Y:343:ASP:C	2.42	0.56
1:G:15:ASN:O	1:G:19:SER:HB2	2.05	0.56
3:X:254:LYS:O	3:X:255:LEU:HG	2.05	0.56
3:Z:243:LYS:HG2	3:Z:266:GLU:HB3	1.87	0.56
3:Z:168:LEU:HD23	3:Z:173:VAL:HG21	1.86	0.56
1:D:56:GLU:HG2	2:E:97:ARG:HA	1.88	0.56

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:Y:254:LYS:O	3:Y:255:LEU:HG	2.06	0.56
3:X:294:LYS:C	3:X:294:LYS:HD2	2.26	0.56
3:X:336:ASP:OD1	3:X:336:ASP:N	2.36	0.56
3:Z:85:VAL:HG12	3:Z:110:TYR:HD2	1.71	0.56
3:Z:56:THR:OG1	3:Z:58:LEU:HB2	2.06	0.56
3:Y:168:LEU:HD23	3:Y:173:VAL:HG21	1.86	0.56
3:Y:209:LEU:N	5:Y:2032:HOH:O	2.13	0.56
2:B:17:CYS:SG	2:B:66:CYS:N	2.79	0.56
3:Y:185:ILE:O	3:Y:210:PRO:HG2	2.06	0.56
3:Y:341:VAL:O	3:Y:341:VAL:HG12	2.06	0.55
1:A:77:GLU:O	2:B:38:VAL:HG13	2.06	0.55
3:Z:283:ARG:O	3:Z:284:GLN:HB3	2.05	0.55
4:H:1007:NAG:O3	4:H:1007:NAG:O7	2.24	0.55
4:H:1024:NAG:C1	4:H:1024:NAG:O7	2.53	0.55
3:X:282:ARG:HG2	3:X:282:ARG:HH11	1.69	0.55
3:X:352:ALA:C	3:X:353:PHE:HD1	2.08	0.55
3:Y:356:CYS:O	3:Y:357:GLU:CG	2.51	0.55
1:G:47:MET:CE	1:G:50:GLN:HA	2.35	0.55
1:D:70:VAL:O	1:D:72:GLY:N	2.39	0.55
3:Z:33:GLN:HG2	3:Z:34:GLU:H	1.71	0.55
3:Z:207:GLU:OE1	3:Z:231:HIS:NE2	2.37	0.55
1:G:33:PHE:O	1:G:58:THR:HG22	2.06	0.55
1:G:18:PHE:HB3	1:G:25:ILE:CD1	2.36	0.55
3:Y:245:ARG:CG	3:Y:245:ARG:NH1	2.67	0.55
2:H:41:ASP:OD1	2:H:42:PRO:CD	2.54	0.55
2:E:7:ASN:OD1	4:E:1007:NAG:N2	2.39	0.55
3:X:92:SER:HB3	3:X:117:GLN:HB2	1.88	0.55
3:Y:40:ILE:HD12	3:Y:65:ALA:HB1	1.88	0.54
3:Z:294:LYS:O	3:Z:295:SER:HB3	2.07	0.54
4:H:1007:NAG:H3	4:H:1007:NAG:O7	2.08	0.54
3:Y:191:ASN:OD1	4:Y:1191:NAG:H2	2.07	0.54
3:Z:135:LEU:HD11	3:Z:160:ILE:HG12	1.90	0.54
1:A:14:GLU:CD	5:A:2003:HOH:O	2.44	0.54
1:A:76:VAL:HB	2:B:38:VAL:HG12	1.90	0.54
3:X:283:ARG:CZ	3:X:283:ARG:HB3	2.37	0.54
3:Y:50:GLU:HG3	3:Y:74:LYS:HB2	1.90	0.54
2:H:54:LYS:HE3	2:H:83:HIS:CD2	2.42	0.54
1:A:14:GLU:CG	5:A:2003:HOH:O	2.52	0.54
1:D:47:MET:HE3	1:D:50:GLN:HA	1.89	0.54
3:Y:18:CYS:N	5:Y:2001:HOH:O	2.41	0.54
3:X:38:THR:HA	3:X:57:LYS:O	2.08	0.54

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:Y:292:CYS:O	3:Y:294:LYS:HD2	2.08	0.54
2:H:17:CYS:SG	2:H:66:CYS:N	2.80	0.53
3:X:85:VAL:HG12	3:X:110:TYR:HD2	1.74	0.53
2:E:17:CYS:SG	2:E:66:CYS:N	2.81	0.53
2:B:14:LYS:NZ	2:B:72:SER:OG	2.41	0.53
3:X:245:ARG:NH1	3:X:245:ARG:HG2	2.20	0.53
2:E:44:ARG:NH2	3:Y:197:GLU:OE1	2.42	0.53
1:G:6:ASP:CG	1:G:7:CYS:H	2.12	0.53
3:X:88:ALA:HB1	3:X:114:GLU:HB2	1.89	0.53
2:B:44:ARG:HB3	2:B:45:PRO:C	2.28	0.53
3:X:245:ARG:CG	3:X:245:ARG:HH11	2.16	0.53
2:E:44:ARG:NH1	5:E:2009:HOH:O	2.42	0.53
3:Y:98:HIS:HA	3:Y:121:ASN:O	2.09	0.53
1:D:15:ASN:O	1:D:19:SER:HB2	2.08	0.53
3:Y:191:ASN:OD1	4:Y:1191:NAG:C2	2.57	0.53
3:X:258:LEU:HD22	3:X:284:GLN:NE2	2.24	0.53
3:X:191:ASN:OD1	4:X:1191:NAG:H2	2.09	0.52
3:X:285:ILE:HG12	3:X:286:SER:N	2.24	0.52
1:D:72:GLY:C	5:D:2012:HOH:O	2.45	0.52
3:Z:245:ARG:CG	3:Z:245:ARG:NH1	2.72	0.52
3:Z:160:ILE:HD11	3:Z:182:ILE:HD13	1.92	0.52
3:Y:22:ILE:HG23	3:Y:36:LYS:HD3	1.90	0.52
2:B:44:ARG:HD2	2:B:46:LYS:CG	2.38	0.52
3:Y:287:GLU:O	3:Y:288:LEU:CB	2.57	0.52
3:X:88:ALA:CB	3:X:114:GLU:HB2	2.39	0.52
3:X:243:LYS:HG2	3:X:266:GLU:HB3	1.91	0.52
2:B:2:SER:O	2:B:2:SER:OG	2.27	0.52
3:X:22:ILE:HG23	3:X:36:LYS:HD3	1.90	0.52
3:Y:135:LEU:HD11	3:Y:160:ILE:HG12	1.91	0.52
3:X:33:GLN:HG2	3:X:34:GLU:H	1.75	0.52
2:E:73:LEU:HD12	3:X:84:GLU:OE1	2.10	0.52
4:A:1052:NAG:O7	4:A:1052:NAG:H3	2.10	0.52
2:B:67:ALA:O	2:B:68:HIS:HB2	2.10	0.52
3:Y:285:ILE:O	3:Y:287:GLU:N	2.43	0.52
3:X:28:ARG:NH2	3:X:49:ILE:HD11	2.25	0.52
3:X:135:LEU:HD11	3:X:160:ILE:HG12	1.93	0.51
3:Z:257:THR:CG2	3:Z:283:ARG:HH12	2.22	0.51
3:Y:193:THR:HG21	3:Y:195:LEU:HG	1.92	0.51
1:D:12:LEU:HD22	1:D:26:LEU:HB3	1.93	0.51
1:G:47:MET:HE3	1:G:51:LYS:H	1.72	0.51
3:Z:291:ILE:HG12	3:Z:292:CYS:H	1.75	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:Z:40:ILE:HG13	3:Z:62:GLN:NE2	2.25	0.51
1:G:28:CYS:SG	1:G:62:ALA:HA	2.51	0.51
3:Z:92:SER:HB3	3:Z:117:GLN:HB2	1.92	0.51
4:G:1052:NAG:H3	4:G:1052:NAG:O7	2.10	0.51
3:X:207:GLU:OE1	3:X:231:HIS:NE2	2.44	0.51
2:H:44:ARG:HD2	2:H:46:LYS:HD2	1.92	0.51
1:A:47:MET:CE	1:A:50:GLN:HA	2.40	0.51
2:B:54:LYS:HE3	2:B:83:HIS:CD2	2.46	0.51
2:E:43:ALA:O	2:E:44:ARG:C	2.49	0.51
1:G:18:PHE:HB3	1:G:25:ILE:HD11	1.91	0.51
1:A:38:PRO:HD3	2:B:27:TRP:CD1	2.46	0.51
1:D:17:LEU:CD1	3:Y:335:TYS:CB	2.89	0.50
1:G:41:LEU:HD11	2:H:74:TYR:CE1	2.46	0.50
3:Z:81:ASP:N	3:Z:81:ASP:OD1	2.31	0.50
1:A:18:PHE:CB	1:A:25:ILE:HD11	2.32	0.50
3:Z:245:ARG:HG2	3:Z:245:ARG:NH1	2.15	0.50
1:D:70:VAL:HG23	1:D:71:MET:HG3	1.93	0.50
3:Z:177:LEU:O	3:Z:180:ASN:ND2	2.41	0.50
1:G:70:VAL:HG23	1:G:71:MET:HG3	1.91	0.50
1:A:15:ASN:O	1:A:19:SER:HB2	2.10	0.50
3:X:282:ARG:HG2	3:X:282:ARG:NH1	2.26	0.50
2:H:17:CYS:HB3	2:H:19:PHE:CE2	2.46	0.50
3:Y:288:LEU:HD13	3:Y:339:ASN:ND2	2.24	0.50
1:A:76:VAL:HB	2:B:38:VAL:CG1	2.42	0.50
3:Z:258:LEU:N	3:Z:283:ARG:NH1	2.60	0.50
3:Y:175:LEU:HD12	3:Y:195:LEU:HD21	1.94	0.50
1:D:27:GLN:HA	1:D:79:HIS:ND1	2.27	0.50
3:Y:288:LEU:CD1	3:Y:339:ASN:HD22	2.23	0.50
3:Y:257:THR:CA	5:Y:2041:HOH:O	2.52	0.50
1:D:25:ILE:HD12	2:E:38:VAL:HG11	1.93	0.50
3:Y:53:PHE:HE2	3:Y:66:PHE:CE1	2.30	0.50
2:B:19:PHE:CD1	2:B:19:PHE:C	2.84	0.50
1:A:65:TYR:CD2	1:A:77:GLU:HB3	2.47	0.50
3:Y:282:ARG:HG2	3:Y:282:ARG:HH11	1.77	0.50
3:X:291:ILE:O	3:X:291:ILE:HG22	2.11	0.50
3:Y:187:ASN:OD1	3:Y:212:ASP:CB	2.45	0.49
3:Y:205:ASN:ND2	5:Y:2031:HOH:O	2.42	0.49
3:Z:335:TYS:O	3:Z:336:ASP:C	2.51	0.49
3:X:285:ILE:HG12	3:X:286:SER:HB2	1.86	0.49
3:Y:207:GLU:OE1	3:Y:231:HIS:NE2	2.43	0.49
3:X:288:LEU:O	3:X:289:HIS:HB2	2.12	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:Z:250:TYR:HB2	5:Z:2036:HOH:O	2.12	0.49
3:Y:282:ARG:HG2	3:Y:282:ARG:NH1	2.28	0.49
1:G:12:LEU:O	1:G:13:GLN:HG2	2.12	0.49
3:Z:40:ILE:HD12	3:Z:65:ALA:HB1	1.93	0.49
1:D:38:PRO:HD3	2:E:27:TRP:CD1	2.48	0.49
3:X:247:ARG:NH2	3:X:347:SER:OG	2.44	0.49
3:Z:258:LEU:H	3:Z:283:ARG:NH1	2.11	0.49
3:X:239:GLU:H	3:X:239:GLU:CD	2.16	0.49
3:Y:193:THR:N	5:Y:2029:HOH:O	2.46	0.49
3:Z:193:THR:HG21	3:Z:195:LEU:HG	1.95	0.49
2:E:67:ALA:O	2:E:68:HIS:HB2	2.13	0.49
3:X:191:ASN:OD1	4:X:1191:NAG:C2	2.61	0.49
3:Z:284:GLN:CG	3:Z:284:GLN:O	2.60	0.49
3:X:255:LEU:HA	5:X:2025:HOH:O	2.13	0.49
3:X:287:GLU:HG3	3:X:288:LEU:HD22	1.95	0.49
3:Y:28:ARG:NH2	3:Y:49:ILE:HD11	2.28	0.49
1:D:28:CYS:SG	1:D:62:ALA:HA	2.53	0.49
3:X:353:PHE:CB	5:X:2028:HOH:O	2.54	0.49
1:G:47:MET:CE	1:G:51:LYS:N	2.67	0.49
3:X:193:THR:HG21	3:X:195:LEU:HG	1.94	0.49
3:Z:355:PRO:O	3:Z:357:GLU:CG	2.61	0.49
3:X:40:ILE:HD12	3:X:65:ALA:HB1	1.95	0.48
3:Y:19:HIS:CG	3:Y:20:HIS:N	2.81	0.48
2:E:44:ARG:HD3	2:E:45:PRO:HA	1.94	0.48
1:D:33:PHE:O	1:D:58:THR:HG22	2.13	0.48
2:E:24:ASN:OD1	4:E:1024:NAG:C2	2.60	0.48
1:D:38:PRO:HD3	2:E:27:TRP:NE1	2.28	0.48
3:X:53:PHE:HE2	3:X:66:PHE:CE1	2.30	0.48
1:G:76:VAL:HB	2:H:38:VAL:CG1	2.43	0.48
3:Z:19:HIS:CG	3:Z:20:HIS:N	2.81	0.48
3:X:19:HIS:CG	3:X:20:HIS:N	2.81	0.48
3:X:56:THR:OG1	3:X:58:LEU:HB2	2.14	0.48
3:Y:247:ARG:NH2	3:Y:347:SER:OG	2.46	0.48
3:X:69:PHE:C	5:X:2002:HOH:O	2.47	0.48
3:X:245:ARG:NH1	3:X:245:ARG:CG	2.75	0.48
1:A:56:GLU:HG2	2:B:97:ARG:HA	1.95	0.48
3:Z:38:THR:HA	3:Z:57:LYS:O	2.14	0.48
3:X:69:PHE:HA	5:X:2002:HOH:O	1.97	0.48
1:G:9:GLU:HG2	1:G:10:CYS:N	2.29	0.48
2:H:95:THR:OG1	2:H:96:VAL:N	2.47	0.48
3:Y:62:GLN:O	3:Y:65:ALA:HB2	2.13	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:Y:38:THR:HA	3:Y:57:LYS:O	2.14	0.48
1:A:70:VAL:HG23	1:A:71:MET:HG3	1.96	0.48
3:X:356:CYS:SG	3:X:357:GLU:N	2.87	0.48
3:Z:34:GLU:HA	3:Z:34:GLU:OE1	2.14	0.48
3:Z:25:CYS:SG	3:Z:26:SER:N	2.86	0.48
2:E:56:LEU:HD12	2:E:56:LEU:C	2.34	0.48
1:D:17:LEU:HD11	3:Y:335:TYS:CB	2.43	0.48
3:Y:91:PHE:CD2	3:Y:116:PHE:CE1	3.02	0.47
3:X:91:PHE:CD2	3:X:116:PHE:CE1	3.02	0.47
1:D:47:MET:HE3	1:D:51:LYS:H	1.76	0.47
3:X:57:LYS:HA	3:X:82:VAL:CG2	2.44	0.47
2:H:44:ARG:HB3	2:H:46:LYS:N	2.30	0.47
3:Y:349:LYS:HB3	3:Y:349:LYS:HE3	1.65	0.47
1:D:77:GLU:O	2:E:38:VAL:HG13	2.14	0.47
2:E:44:ARG:HD2	2:E:45:PRO:HA	1.96	0.47
3:Y:349:LYS:O	3:Y:351:ASP:N	2.35	0.47
3:Z:284:GLN:HG3	3:Z:287:GLU:HB2	1.96	0.47
3:X:101:ARG:HG3	3:X:126:LEU:HB3	1.96	0.47
1:G:45:LYS:HZ1	2:H:15:GLU:CD	2.12	0.47
3:X:191:ASN:ND2	4:X:1191:NAG:O5	2.40	0.47
1:D:18:PHE:HB3	1:D:25:ILE:CD1	2.44	0.47
3:X:62:GLN:O	3:X:65:ALA:HB2	2.15	0.47
3:Z:281:TRP:O	3:Z:282:ARG:C	2.53	0.47
1:A:33:PHE:O	1:A:58:THR:HG22	2.14	0.47
3:Y:26:SER:O	3:Y:29:VAL:HB	2.15	0.47
3:Y:92:SER:HB3	3:Y:117:GLN:HB2	1.97	0.47
3:Y:341:VAL:HG11	3:Y:342:VAL:HG22	1.86	0.47
3:Z:191:ASN:N	5:Z:2031:HOH:O	2.46	0.47
2:B:42:PRO:O	5:B:2009:HOH:O	2.20	0.47
2:B:44:ARG:HB3	2:B:46:LYS:N	2.30	0.47
2:B:44:ARG:HD2	2:B:46:LYS:CD	2.45	0.47
3:Y:293:ASN:OD1	3:Y:293:ASN:N	2.48	0.47
3:Z:175:LEU:HD12	3:Z:195:LEU:HD21	1.96	0.47
3:X:40:ILE:HG23	3:X:53:PHE:CZ	2.50	0.46
3:Y:285:ILE:O	3:Y:286:SER:C	2.54	0.46
1:A:18:PHE:CB	1:A:25:ILE:CD1	2.92	0.46
2:E:44:ARG:HB2	2:E:46:LYS:N	2.29	0.46
3:Z:239:GLU:CD	3:Z:239:GLU:H	2.19	0.46
3:X:168:LEU:HD23	3:X:173:VAL:HG21	1.96	0.46
3:Z:335:TYS:O3	3:Z:335:TYS:HE1	2.14	0.46
3:Y:282:ARG:O	3:Y:283:ARG:CB	2.64	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:Z:22:ILE:HG23	3:Z:36:LYS:HD3	1.97	0.46
3:Y:243:LYS:HG2	3:Y:266:GLU:HB3	1.97	0.46
3:Z:193:THR:HG22	3:Z:193:THR:O	2.15	0.46
3:X:210:PRO:O	3:X:213:VAL:HG22	2.16	0.46
1:A:70:VAL:O	1:A:72:GLY:N	2.49	0.46
3:X:357:GLU:HA	3:X:357:GLU:OE1	2.15	0.46
3:Y:64:GLY:HA2	3:Y:89:ASP:O	2.16	0.46
3:Z:254:LYS:HG3	3:Z:255:LEU:N	2.31	0.46
3:Y:254:LYS:O	3:Y:255:LEU:CG	2.63	0.46
2:H:25:THR:OG1	2:H:26:THR:N	2.48	0.46
3:Y:341:VAL:CG1	3:Y:341:VAL:O	2.59	0.45
2:E:71:ASP:OD1	3:X:59:ARG:NH2	2.49	0.45
3:Y:334:ASP:O	3:Y:335:TYS:C	2.64	0.45
1:D:17:LEU:HD13	3:Y:335:TYS:HD2	1.97	0.45
3:X:98:HIS:HB2	3:X:123:GLN:HG2	1.95	0.45
3:Y:53:PHE:HE2	3:Y:66:PHE:HE1	1.63	0.45
3:Y:49:ILE:O	3:Y:72:LEU:HD12	2.16	0.45
3:Y:351:ASP:OD1	3:Y:351:ASP:C	2.55	0.45
1:D:92:SER:O	2:E:86:LYS:HD2	2.16	0.45
3:X:50:GLU:O	3:X:51:LEU:HD23	2.17	0.45
1:A:12:LEU:HD22	1:A:26:LEU:HB3	1.97	0.45
1:A:42:ARG:NH2	3:X:55:LEU:HD22	2.32	0.45
3:X:258:LEU:HD22	3:X:284:GLN:HE21	1.81	0.45
1:D:32:CYS:HB3	1:D:58:THR:CG2	2.39	0.45
1:G:25:ILE:CD1	2:H:38:VAL:HG11	2.45	0.45
3:Y:18:CYS:CA	5:Y:2001:HOH:O	2.64	0.45
3:Z:94:LEU:HD13	3:Z:97:LEU:HD22	1.97	0.45
3:Z:352:ALA:HB1	3:Z:353:PHE:CE1	2.51	0.45
2:B:17:CYS:HB3	2:B:19:PHE:CE2	2.52	0.45
3:Y:88:ALA:HB1	3:Y:114:GLU:HB2	1.97	0.45
3:Z:349:LYS:HE3	3:Z:349:LYS:HB3	1.67	0.45
1:D:65:TYR:CD2	1:D:77:GLU:HB3	2.52	0.45
1:D:17:LEU:CD1	3:Y:335:TYS:HB3	2.47	0.45
3:Y:98:HIS:HB2	3:Y:123:GLN:HG2	1.97	0.45
3:Z:40:ILE:HG23	3:Z:53:PHE:CZ	2.51	0.45
2:E:56:LEU:O	2:E:56:LEU:HD12	2.17	0.45
1:D:17:LEU:C	1:D:19:SER:H	2.08	0.45
1:G:6:ASP:N	5:G:2001:HOH:O	2.46	0.45
1:G:12:LEU:HD22	1:G:26:LEU:HB3	1.99	0.45
1:G:27:GLN:NE2	3:Z:335:TYS:O1	2.50	0.45
1:G:18:PHE:CE2	2:H:39:TYR:HB2	2.52	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:44:ARG:CB	2:E:45:PRO:CA	2.85	0.45
3:X:53:PHE:HE2	3:X:66:PHE:HE1	1.65	0.45
3:Z:294:LYS:O	3:Z:295:SER:HB2	2.15	0.45
1:D:17:LEU:HD13	3:Y:335:TYS:CD2	2.46	0.44
2:E:14:LYS:NZ	2:E:72:SER:OG	2.50	0.44
3:X:40:ILE:HG13	3:X:62:GLN:NE2	2.32	0.44
1:D:47:MET:CE	1:D:50:GLN:HA	2.46	0.44
3:X:129:ASN:HA	3:X:153:ASP:O	2.17	0.44
3:Z:353:PHE:N	5:Z:2043:HOH:O	2.47	0.44
3:Z:154:ASN:HB2	3:Z:157:ILE:HD12	1.99	0.44
3:X:284:GLN:O	3:X:285:ILE:HB	2.18	0.44
3:X:255:LEU:N	5:X:2025:HOH:O	2.50	0.44
3:Y:140:LYS:HB2	5:Y:2010:HOH:O	2.17	0.44
3:Y:356:CYS:C	3:Y:357:GLU:HG2	2.37	0.44
3:Y:291:ILE:CG2	3:Y:291:ILE:O	2.63	0.44
3:Z:64:GLY:HA2	3:Z:89:ASP:O	2.18	0.44
1:D:6:ASP:O	1:D:6:ASP:OD1	2.36	0.44
3:X:73:GLU:HB3	3:X:98:HIS:CE1	2.53	0.44
3:X:352:ALA:C	3:X:353:PHE:CD1	2.91	0.44
3:X:289:HIS:O	3:X:291:ILE:N	2.42	0.44
1:A:28:CYS:SG	1:A:62:ALA:HA	2.58	0.44
3:Y:88:ALA:CB	3:Y:114:GLU:HB2	2.49	0.43
3:Z:353:PHE:O	3:Z:354:ASN:C	2.57	0.43
2:H:19:PHE:C	2:H:19:PHE:CD1	2.91	0.43
3:Y:57:LYS:HA	3:Y:82:VAL:CG2	2.48	0.43
3:X:128:SER:HA	3:X:152:GLN:O	2.18	0.43
3:Y:187:ASN:CG	3:Y:212:ASP:HB2	2.33	0.43
1:A:45:LYS:NZ	2:B:15:GLU:OE1	2.49	0.43
1:G:26:LEU:O	1:G:79:HIS:HB2	2.19	0.43
3:X:78:SER:HA	3:X:103:GLU:O	2.18	0.43
3:Y:294:LYS:O	3:Y:295:SER:O	2.36	0.43
3:X:185:ILE:O	3:X:210:PRO:CG	2.66	0.43
3:Y:229:ARG:O	3:Y:251:ASN:OD1	2.36	0.43
3:X:332:GLU:HB3	3:X:333:PHE:H	1.69	0.43
2:B:2:SER:O	2:B:31:TYR:N	2.40	0.43
3:Z:53:PHE:HE2	3:Z:66:PHE:CE1	2.37	0.43
3:X:158:HIS:NE2	5:X:2010:HOH:O	2.36	0.43
5:Y:2033:HOH:O	3:Z:229:ARG:NE	2.43	0.43
3:Y:286:SER:O	3:Y:287:GLU:C	2.57	0.43
4:B:1007:NAG:H61	5:B:2003:HOH:O	2.19	0.43
1:G:70:VAL:HG23	1:G:71:MET:N	2.33	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:41:ASP:HA	2:H:42:PRO:HD3	1.90	0.43
3:Z:34:GLU:O	3:Z:56:THR:HA	2.18	0.43
3:X:357:GLU:CA	3:X:357:GLU:OE1	2.67	0.43
3:Y:338:CYS:HB2	3:Y:340:GLU:HG2	2.00	0.43
3:Z:352:ALA:C	3:Z:353:PHE:CD1	2.93	0.43
3:X:101:ARG:NH1	3:X:103:GLU:OE2	2.52	0.43
3:Z:57:LYS:HA	3:Z:82:VAL:CG2	2.48	0.43
3:Y:25:CYS:SG	3:Y:26:SER:N	2.92	0.43
1:A:42:ARG:CZ	3:X:55:LEU:HD22	2.48	0.43
3:Z:247:ARG:NH2	3:Z:347:SER:OG	2.52	0.43
3:Y:287:GLU:O	3:Y:288:LEU:CG	2.65	0.42
1:D:5:GLN:HB2	2:E:2:SER:HB2	2.00	0.42
1:G:90:HIS:HA	2:H:48:GLN:O	2.19	0.42
3:Y:131:GLY:O	3:Y:132:ILE:C	2.58	0.42
3:Z:49:ILE:O	3:Z:72:LEU:HD12	2.19	0.42
2:E:17:CYS:HB3	2:E:19:PHE:CE2	2.54	0.42
3:Z:88:ALA:HB1	3:Z:114:GLU:HB2	2.01	0.42
2:B:44:ARG:CB	2:B:45:PRO:C	2.87	0.42
3:X:254:LYS:HG3	3:X:255:LEU:N	2.34	0.42
3:Y:66:PHE:O	3:Y:69:PHE:HD1	2.01	0.42
3:X:247:ARG:O	3:X:248:SER:C	2.57	0.42
3:X:25:CYS:SG	3:X:26:SER:N	2.92	0.42
2:B:44:ARG:NH1	3:X:197:GLU:OE1	2.53	0.42
3:X:353:PHE:CD1	3:X:353:PHE:N	2.86	0.42
3:Y:287:GLU:HB3	3:Y:288:LEU:H	1.58	0.42
3:Z:254:LYS:O	3:Z:255:LEU:CG	2.67	0.42
1:G:91:LYS:HD3	2:H:94:CYS:HB2	2.02	0.42
3:Z:249:THR:HG22	5:Z:2037:HOH:O	2.18	0.42
1:G:17:LEU:C	1:G:19:SER:H	2.08	0.42
3:Z:187:ASN:CG	3:Z:212:ASP:HB2	2.37	0.42
3:Y:53:PHE:CE2	3:Y:66:PHE:HE1	2.37	0.42
3:Z:128:SER:HA	3:Z:152:GLN:O	2.18	0.42
3:Z:62:GLN:O	3:Z:65:ALA:HB2	2.19	0.42
5:Y:2033:HOH:O	3:Z:229:ARG:NH2	2.35	0.42
2:H:4:GLU:O	2:H:6:THR:HG23	2.20	0.42
3:X:349:LYS:HB3	3:X:349:LYS:HE3	1.65	0.42
1:D:18:PHE:CB	1:D:25:ILE:CD1	2.98	0.42
3:Z:87:GLU:O	3:Z:90:VAL:HG23	2.20	0.42
3:X:226:SER:C	5:X:2018:HOH:O	2.47	0.42
3:Z:352:ALA:HB1	3:Z:353:PHE:CD1	2.54	0.42
3:Z:353:PHE:CD1	3:Z:353:PHE:N	2.88	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:12:LEU:O	1:A:13:GLN:CG	2.66	0.42
3:X:79:GLN:HE21	3:X:104:LYS:HE3	1.84	0.42
3:X:193:THR:O	3:X:193:THR:HG22	2.19	0.42
3:X:356:CYS:O	3:X:357:GLU:C	2.57	0.42
3:Y:353:PHE:CD1	3:Y:353:PHE:N	2.87	0.42
3:Z:335:TYS:O	3:Z:337:LEU:HD12	2.19	0.42
3:Y:285:ILE:CG2	3:Y:286:SER:H	2.10	0.42
1:A:77:GLU:OE2	2:B:40:LYS:HE2	2.20	0.42
3:Z:352:ALA:O	3:Z:353:PHE:C	2.58	0.42
3:Y:336:ASP:HB2	3:Y:340:GLU:OE2	2.20	0.42
2:H:67:ALA:O	2:H:68:HIS:HB2	2.19	0.42
4:G:1052:NAG:C7	4:G:1052:NAG:O3	2.68	0.41
3:X:26:SER:O	3:X:29:VAL:HB	2.19	0.41
1:A:31:CYS:HA	2:B:32:CYS:O	2.20	0.41
3:X:292:CYS:SG	3:X:337:LEU:C	2.99	0.41
3:X:159:THR:HB	3:X:184:GLU:HB2	2.01	0.41
1:D:17:LEU:CD1	3:Y:335:TYS:HD2	2.50	0.41
3:Y:287:GLU:O	3:Y:288:LEU:HB2	2.19	0.41
1:A:33:PHE:HB3	5:A:2006:HOH:O	2.20	0.41
3:Y:35:SER:HA	3:Y:57:LYS:HG2	2.02	0.41
1:D:17:LEU:HD11	3:Y:335:TYS:HB3	2.02	0.41
3:X:53:PHE:CE2	3:X:66:PHE:HE1	2.38	0.41
3:Y:285:ILE:C	3:Y:287:GLU:N	2.73	0.41
3:X:204:ASN:O	3:X:229:ARG:HG3	2.19	0.41
3:X:92:SER:CB	3:X:117:GLN:HB2	2.50	0.41
3:X:35:SER:HA	3:X:57:LYS:HG2	2.00	0.41
3:X:207:GLU:O	3:X:230:ILE:HA	2.21	0.41
2:E:23:ILE:HD11	2:E:61:VAL:HG11	2.02	0.41
3:Y:128:SER:HA	3:Y:152:GLN:O	2.21	0.41
3:X:353:PHE:HD1	3:X:353:PHE:N	2.18	0.41
2:B:7:ASN:ND2	4:B:1007:NAG:C7	2.83	0.41
2:E:41:ASP:OD1	2:E:42:PRO:N	2.53	0.41
3:Z:358:ASP:O	3:Z:359:ILE:C	2.59	0.41
3:Y:349:LYS:HG2	3:Y:349:LYS:H	1.73	0.41
3:Z:98:HIS:HB2	3:Z:123:GLN:HG2	2.00	0.41
2:B:56:LEU:HD12	2:B:56:LEU:C	2.41	0.41
3:Z:88:ALA:CB	3:Z:114:GLU:HB2	2.51	0.41
3:X:112:ASN:HA	3:X:113:PRO:HD3	1.94	0.41
1:D:17:LEU:HD11	3:Y:335:TYS:HB2	2.02	0.41
1:D:18:PHE:HB3	1:D:25:ILE:HD11	2.03	0.41
3:X:73:GLU:HB3	3:X:98:HIS:HE1	1.86	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:24:ASN:OD1	4:E:1024:NAG:H2	2.21	0.41
3:Z:26:SER:O	3:Z:29:VAL:HB	2.20	0.41
3:Y:204:ASN:O	3:Y:229:ARG:HG3	2.20	0.41
2:H:23:ILE:HD11	2:H:61:VAL:HG11	2.03	0.41
3:Y:78:SER:HA	3:Y:103:GLU:O	2.21	0.41
3:Y:214:PHE:HE2	3:Y:238:LEU:HD21	1.85	0.41
1:D:41:LEU:HD11	2:E:74:TYR:CE1	2.56	0.41
3:X:66:PHE:O	3:X:69:PHE:HD1	2.04	0.41
3:X:64:GLY:HA2	3:X:89:ASP:O	2.21	0.41
1:G:65:TYR:CD2	1:G:77:GLU:HB3	2.56	0.41
1:A:20:GLN:HA	1:A:20:GLN:OE1	2.21	0.41
3:Z:258:LEU:HB3	3:Z:283:ARG:CD	2.44	0.40
1:G:42:ARG:CZ	3:Z:55:LEU:HD22	2.52	0.40
3:Y:73:GLU:HB3	3:Y:98:HIS:CE1	2.56	0.40
3:Z:191:ASN:OD1	4:Z:1191:NAG:H2	2.21	0.40
3:Z:235:SER:CA	5:Z:2038:HOH:O	2.61	0.40
1:D:87:CYS:HA	5:D:2016:HOH:O	2.22	0.40
3:Z:30:PHE:CZ	3:Z:45:PRO:HG2	2.56	0.40
2:H:44:ARG:CB	2:H:45:PRO:C	2.87	0.40
3:Z:129:ASN:HA	3:Z:153:ASP:O	2.22	0.40
1:G:6:ASP:CG	1:G:7:CYS:N	2.75	0.40
3:Z:353:PHE:C	5:Z:2043:HOH:O	2.57	0.40
2:E:41:ASP:C	2:E:41:ASP:OD1	2.60	0.40
3:Z:204:ASN:O	3:Z:229:ARG:HG3	2.22	0.40

There are no symmetry-related clashes.

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	86/92 (94%)	82 (95%)	1 (1%)	3 (4%)	4 6

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	D	87/92 (95%)	80 (92%)	4 (5%)	3 (3%)	5 6
1	G	86/92 (94%)	81 (94%)	0	5 (6%)	2 2
2	B	105/111 (95%)	103 (98%)	1 (1%)	1 (1%)	19 34
2	E	105/111 (95%)	102 (97%)	1 (1%)	2 (2%)	10 16
2	H	105/111 (95%)	101 (96%)	3 (3%)	1 (1%)	19 34
3	X	302/350 (86%)	269 (89%)	26 (9%)	7 (2%)	8 12
3	Y	302/350 (86%)	266 (88%)	23 (8%)	13 (4%)	3 4
3	Z	302/350 (86%)	274 (91%)	18 (6%)	10 (3%)	5 6
All	All	1480/1659 (89%)	1358 (92%)	77 (5%)	45 (3%)	5 7

All (45) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	17	LEU
1	A	18	PHE
2	B	44	ARG
1	D	18	PHE
2	E	44	ARG
1	G	18	PHE
2	H	44	ARG
3	X	282	ARG
3	X	285	ILE
3	Y	255	LEU
3	Y	282	ARG
3	Y	286	SER
3	Y	342	VAL
3	Y	343	ASP
3	Z	336	ASP
1	D	71	MET
3	X	286	SER
3	Y	283	ARG
3	Z	356	CYS
1	A	71	MET
2	E	2	SER
1	G	71	MET
3	Y	284	GLN
3	Z	282	ARG
1	D	17	LEU
1	G	17	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	G	73	GLY
3	Y	254	LYS
3	Y	288	LEU
3	Y	352	ALA
3	Z	283	ARG
3	Z	284	GLN
3	X	254	LYS
3	X	255	LEU
3	Y	294	LYS
3	Z	254	LYS
3	Z	255	LEU
3	X	287	GLU
3	Y	285	ILE
3	Y	291	ILE
3	Z	354	ASN
3	Z	355	PRO
3	X	291	ILE
1	G	72	GLY
3	Z	342	VAL

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.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	80/83 (96%)	71 (89%)	9 (11%)	7 13
1	D	81/83 (98%)	75 (93%)	6 (7%)	17 31
1	G	80/83 (96%)	73 (91%)	7 (9%)	12 23
2	B	95/99 (96%)	88 (93%)	7 (7%)	17 31
2	E	95/99 (96%)	86 (90%)	9 (10%)	11 20
2	H	95/99 (96%)	88 (93%)	7 (7%)	17 31
3	X	283/320 (88%)	245 (87%)	38 (13%)	5 9
3	Y	283/320 (88%)	253 (89%)	30 (11%)	8 16
3	Z	283/320 (88%)	248 (88%)	35 (12%)	6 11

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
All	All	1375/1506 (91%)	1227 (89%)	148 (11%)	8 15

All (148) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	5	GLN
1	A	6	ASP
1	A	11	THR
1	A	17	LEU
1	A	19	SER
1	A	41	LEU
1	A	77	GLU
1	A	83	HIS
1	A	92	SER
2	B	16	GLU
2	B	47	ILE
2	B	61	VAL
2	B	62	ARG
2	B	75	THR
2	B	83	HIS
2	B	95	THR
1	D	4	VAL
1	D	17	LEU
1	D	41	LEU
1	D	55	SER
1	D	77	GLU
1	D	83	HIS
2	E	2	SER
2	E	16	GLU
2	E	44	ARG
2	E	47	ILE
2	E	61	VAL
2	E	62	ARG
2	E	75	THR
2	E	83	HIS
2	E	95	THR
1	G	11	THR
1	G	17	LEU
1	G	41	LEU
1	G	67	ARG
1	G	77	GLU
1	G	83	HIS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	G	90	HIS
2	H	16	GLU
2	H	47	ILE
2	H	61	VAL
2	H	62	ARG
2	H	75	THR
2	H	83	HIS
2	H	95	THR
3	X	31	LEU
3	X	40	ILE
3	X	58	LEU
3	X	62	GLN
3	X	81	ASP
3	X	85	VAL
3	X	86	ILE
3	X	101	ARG
3	X	109	LEU
3	X	121	ASN
3	X	123	GLN
3	X	128	SER
3	X	159	THR
3	X	173	VAL
3	X	191	ASN
3	X	193	THR
3	X	213	VAL
3	X	247	ARG
3	X	249	THR
3	X	257	THR
3	X	259	GLU
3	X	262	VAL
3	X	265	MET
3	X	282	ARG
3	X	285	ILE
3	X	286	SER
3	X	287	GLU
3	X	288	LEU
3	X	292	CYS
3	X	294	LYS
3	X	331	THR
3	X	332	GLU
3	X	334	ASP
3	X	336	ASP

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
3	X	340	GLU
3	X	349	LYS
3	X	357	GLU
3	X	359	ILE
3	Y	40	ILE
3	Y	58	LEU
3	Y	62	GLN
3	Y	81	ASP
3	Y	85	VAL
3	Y	101	ARG
3	Y	109	LEU
3	Y	121	ASN
3	Y	123	GLN
3	Y	128	SER
3	Y	159	THR
3	Y	191	ASN
3	Y	193	THR
3	Y	213	VAL
3	Y	247	ARG
3	Y	249	THR
3	Y	257	THR
3	Y	259	GLU
3	Y	262	VAL
3	Y	265	MET
3	Y	282	ARG
3	Y	284	GLN
3	Y	287	GLU
3	Y	289	HIS
3	Y	294	LYS
3	Y	334	ASP
3	Y	337	LEU
3	Y	340	GLU
3	Y	342	VAL
3	Y	349	LYS
3	Z	25	CYS
3	Z	40	ILE
3	Z	58	LEU
3	Z	62	GLN
3	Z	81	ASP
3	Z	85	VAL
3	Z	101	ARG
3	Z	109	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
3	Z	121	ASN
3	Z	123	GLN
3	Z	128	SER
3	Z	159	THR
3	Z	173	VAL
3	Z	191	ASN
3	Z	193	THR
3	Z	213	VAL
3	Z	247	ARG
3	Z	249	THR
3	Z	257	THR
3	Z	259	GLU
3	Z	262	VAL
3	Z	265	MET
3	Z	276	CYS
3	Z	282	ARG
3	Z	292	CYS
3	Z	294	LYS
3	Z	331	THR
3	Z	332	GLU
3	Z	340	GLU
3	Z	341	VAL
3	Z	342	VAL
3	Z	349	LYS
3	Z	353	PHE
3	Z	357	GLU
3	Z	359	ILE

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
3	X	284	GLN
3	Y	62	GLN
3	Y	163	ASN
3	Y	191	ASN
3	Y	339	ASN

5.3.3 RNA

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains (i)

3 non-standard protein/DNA/RNA residues 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	TYS	X	335	3	15,16,17	1.20	1 (6%)	16,22,24	1.57	1 (6%)
3	TYS	Y	335	3	15,16,17	2.48	3 (20%)	16,22,24	1.94	3 (18%)
3	TYS	Z	335	3	15,16,17	1.19	1 (6%)	16,22,24	1.96	2 (12%)

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	TYS	X	335	3	-	0/9/11/13	0/1/1/1
3	TYS	Y	335	3	-	0/9/11/13	0/1/1/1
3	TYS	Z	335	3	-	0/9/11/13	0/1/1/1

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	Y	335	TYS	OH-S	-6.04	1.52	1.63
3	Y	335	TYS	OH-CZ	-4.75	1.35	1.42
3	Y	335	TYS	CE2-CD2	-4.35	1.30	1.38
3	Z	335	TYS	OH-CZ	-3.25	1.37	1.42
3	X	335	TYS	OH-CZ	-3.17	1.37	1.42

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	Z	335	TYS	CZ-OH-S	-7.44	105.84	118.52
3	X	335	TYS	CZ-OH-S	-5.95	108.39	118.52
3	Y	335	TYS	CZ-OH-S	-5.82	108.61	118.52
3	Y	335	TYS	OH-CZ-CE2	-2.53	113.75	118.74

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	Z	335	TYS	O-C-CA	-2.06	120.13	125.49
3	Y	335	TYS	OH-CZ-CE1	2.81	124.28	118.74

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

3 monomers are involved in 21 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	X	335	TYS	1	0
3	Y	335	TYS	12	0
3	Z	335	TYS	8	0

5.5 Carbohydrates (i)

There are no carbohydrates in this entry.

5.6 Ligand geometry (i)

15 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	A	1052	1	14,14,15	0.97	0	15,19,21	2.56	5 (33%)
4	NAG	A	1078	1	14,14,15	0.67	0	15,19,21	1.79	3 (20%)
4	NAG	B	1007	2	14,14,15	0.72	0	15,19,21	2.16	4 (26%)
4	NAG	B	1024	2	14,14,15	0.46	0	15,19,21	1.88	3 (20%)
4	NAG	D	1052	1	14,14,15	0.71	0	15,19,21	2.20	4 (26%)
4	NAG	D	1078	1	14,14,15	0.71	0	15,19,21	1.30	2 (13%)
4	NAG	E	1007	2	14,14,15	0.46	0	15,19,21	1.34	2 (13%)
4	NAG	E	1024	-	14,14,15	0.82	0	15,19,21	2.26	3 (20%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
4	NAG	G	1052	1	14,14,15	0.71	0	15,19,21	2.47	5 (33%)
4	NAG	G	1078	1	14,14,15	0.64	0	15,19,21	1.44	2 (13%)
4	NAG	H	1007	2	14,14,15	0.64	0	15,19,21	1.60	2 (13%)
4	NAG	H	1024	2	14,14,15	0.75	0	15,19,21	2.22	5 (33%)
4	NAG	X	1191	3	14,14,15	0.54	0	15,19,21	1.30	1 (6%)
4	NAG	Y	1191	3	14,14,15	0.55	0	15,19,21	1.24	1 (6%)
4	NAG	Z	1191	3	14,14,15	0.53	0	15,19,21	1.22	1 (6%)

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	A	1052	1	-	0/6/23/26	0/1/1/1
4	NAG	A	1078	1	-	0/6/23/26	0/1/1/1
4	NAG	B	1007	2	-	0/6/23/26	0/1/1/1
4	NAG	B	1024	2	-	0/6/23/26	0/1/1/1
4	NAG	D	1052	1	-	0/6/23/26	0/1/1/1
4	NAG	D	1078	1	-	0/6/23/26	0/1/1/1
4	NAG	E	1007	2	-	0/6/23/26	0/1/1/1
4	NAG	E	1024	-	-	0/6/23/26	0/1/1/1
4	NAG	G	1052	1	-	0/6/23/26	0/1/1/1
4	NAG	G	1078	1	-	0/6/23/26	0/1/1/1
4	NAG	H	1007	2	-	0/6/23/26	0/1/1/1
4	NAG	H	1024	2	-	0/6/23/26	0/1/1/1
4	NAG	X	1191	3	-	0/6/23/26	0/1/1/1
4	NAG	Y	1191	3	-	0/6/23/26	0/1/1/1
4	NAG	Z	1191	3	-	0/6/23/26	0/1/1/1

There are no bond length outliers.

All (43) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	G	1052	NAG	C4-C3-C2	-7.32	99.85	111.23
4	A	1052	NAG	C4-C3-C2	-7.02	100.31	111.23
4	E	1024	NAG	C1-O5-C5	-6.76	103.67	112.25
4	D	1052	NAG	C4-C3-C2	-6.41	101.27	111.23
4	B	1007	NAG	C1-O5-C5	-5.38	105.42	112.25
4	H	1024	NAG	C2-N2-C7	-4.72	116.97	123.04

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	A	1078	NAG	C6-C5-C4	-4.54	101.83	113.02
4	B	1024	NAG	C2-N2-C7	-4.13	117.73	123.04
4	B	1024	NAG	C4-C3-C2	-3.83	105.27	111.23
4	H	1024	NAG	C3-C2-N2	-3.80	101.46	110.56
4	A	1052	NAG	C2-N2-C7	-3.61	118.41	123.04
4	X	1191	NAG	C4-C3-C2	-3.54	105.72	111.23
4	G	1052	NAG	C2-N2-C7	-3.54	118.50	123.04
4	D	1052	NAG	C1-O5-C5	-3.46	107.86	112.25
4	B	1024	NAG	C3-C4-C5	-3.43	104.22	110.20
4	Y	1191	NAG	C4-C3-C2	-3.26	106.16	111.23
4	G	1078	NAG	C1-O5-C5	-3.20	108.19	112.25
4	A	1052	NAG	C1-O5-C5	-3.13	108.28	112.25
4	H	1024	NAG	C1-O5-C5	-3.12	108.28	112.25
4	G	1052	NAG	C1-O5-C5	-2.76	108.74	112.25
4	A	1078	NAG	O6-C6-C5	-2.70	102.42	111.33
4	H	1007	NAG	C6-C5-C4	-2.58	106.66	113.02
4	D	1078	NAG	C6-C5-C4	-2.54	106.74	113.02
4	A	1052	NAG	C6-C5-C4	-2.53	106.78	113.02
4	Z	1191	NAG	C4-C3-C2	-2.48	107.38	111.23
4	A	1078	NAG	C2-N2-C7	-2.34	120.04	123.04
4	B	1007	NAG	C6-C5-C4	-2.32	107.28	113.02
4	D	1052	NAG	C6-C5-C4	-2.26	107.44	113.02
4	G	1052	NAG	C6-C5-C4	-2.21	107.56	113.02
4	E	1024	NAG	C2-N2-C7	-2.20	120.21	123.04
4	E	1007	NAG	C6-C5-C4	-2.18	107.64	113.02
4	G	1078	NAG	O6-C6-C5	-2.12	104.33	111.33
4	D	1078	NAG	C3-C2-N2	-2.06	105.63	110.56
4	G	1052	NAG	C3-C2-N2	2.30	116.06	110.56
4	E	1007	NAG	O5-C5-C6	2.54	112.86	107.35
4	D	1052	NAG	C3-C2-N2	2.61	116.82	110.56
4	B	1007	NAG	C4-C3-C2	2.61	115.29	111.23
4	H	1024	NAG	C3-C4-C5	2.62	114.77	110.20
4	A	1052	NAG	C3-C2-N2	2.74	117.11	110.56
4	H	1024	NAG	C4-C3-C2	3.67	116.94	111.23
4	E	1024	NAG	C3-C4-C5	3.91	117.01	110.20
4	B	1007	NAG	O5-C5-C6	4.14	116.31	107.35
4	H	1007	NAG	C3-C4-C5	4.84	118.64	110.20

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

12 monomers are involved in 45 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	1052	NAG	3	0
4	B	1007	NAG	5	0
4	B	1024	NAG	4	0
4	D	1052	NAG	1	0
4	E	1007	NAG	8	0
4	E	1024	NAG	4	0
4	G	1052	NAG	4	0
4	H	1007	NAG	3	0
4	H	1024	NAG	2	0
4	X	1191	NAG	5	0
4	Y	1191	NAG	5	0
4	Z	1191	NAG	1	0

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95^{th} percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled 'Q< 0.9' lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
1	A	88/92 (95%)	0.51	4 (4%)	37	42	38, 50, 81, 100	0
1	D	89/92 (96%)	0.70	6 (6%)	21	23	36, 48, 82, 112	0
1	G	88/92 (95%)	0.56	4 (4%)	37	42	38, 48, 82, 100	0
2	B	107/111 (96%)	0.66	4 (3%)	45	50	40, 56, 89, 101	0
2	E	107/111 (96%)	0.56	8 (7%)	17	19	40, 56, 88, 100	0
2	H	107/111 (96%)	0.62	9 (8%)	14	14	39, 56, 88, 103	0
3	X	306/350 (87%)	1.04	50 (16%)	2	2	27, 64, 155, 165	0
3	Y	306/350 (87%)	1.19	44 (14%)	3	3	24, 63, 154, 187	0
3	Z	306/350 (87%)	0.89	34 (11%)	7	7	27, 62, 149, 179	0
All	All	1504/1659 (90%)	0.87	163 (10%)	8	8	24, 58, 139, 187	0

All (163) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	Y	285	ILE	22.1
3	X	331	THR	13.7
3	X	285	ILE	13.7
3	Y	333	PHE	13.7
3	Y	284	GLN	12.3
3	X	281	TRP	11.8
3	Y	332	GLU	11.7
3	Y	281	TRP	11.4
3	Z	332	GLU	11.3
3	Y	282	ARG	10.2
3	Y	331	THR	9.6
3	X	333	PHE	9.2
3	X	295	SER	9.1
3	X	287	GLU	9.0
3	Y	280	ASN	8.7

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
3	Z	285	ILE	8.2
1	D	4	VAL	8.1
3	X	282	ARG	8.0
3	Z	292	CYS	7.6
3	Y	295	SER	7.4
3	X	288	LEU	7.3
3	X	286	SER	7.1
3	Z	356	CYS	6.9
3	Y	286	SER	6.8
3	Y	292	CYS	6.8
3	X	293	ASN	6.7
3	Y	283	ARG	6.5
3	Y	36	LYS	6.4
3	X	357	GLU	6.3
3	Z	293	ASN	6.2
3	Z	291	ILE	6.2
3	Z	288	LEU	6.2
3	Z	289	HIS	6.1
3	X	30	PHE	6.0
3	Z	286	SER	6.0
3	Z	333	PHE	5.7
3	Y	18	CYS	5.7
3	Z	235	SER	5.6
3	Z	359	ILE	5.4
3	X	342	VAL	5.4
3	X	284	GLN	5.4
3	Z	294	LYS	5.1
3	Z	341	VAL	5.1
3	Y	289	HIS	5.1
3	Y	359	ILE	5.0
3	Z	295	SER	4.9
3	Z	331	THR	4.9
3	X	355	PRO	4.9
3	Z	281	TRP	4.9
2	H	107	GLY	4.8
3	Z	339	ASN	4.8
3	Z	337	LEU	4.8
3	Y	338	CYS	4.8
3	Y	290	PRO	4.7
3	X	283	ARG	4.6
3	Z	340	GLU	4.5
3	Y	344	VAL	4.4

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
3	Y	21	ARG	4.4
3	Y	340	GLU	4.4
3	Z	290	PRO	4.4
3	Y	235	SER	4.4
3	X	353	PHE	4.3
3	X	62	GLN	4.2
3	X	332	GLU	4.2
3	X	338	CYS	4.2
3	Z	338	CYS	4.1
3	Y	19	HIS	4.0
3	X	280	ASN	4.0
3	X	110	TYR	4.0
3	Y	341	VAL	4.0
3	Y	343	ASP	4.0
1	A	5	GLN	3.9
1	G	5	GLN	3.9
2	B	35	ARG	3.9
3	X	294	LYS	3.9
3	X	352	ALA	3.8
2	H	68	HIS	3.7
3	X	31	LEU	3.7
3	Z	19	HIS	3.6
3	Z	259	GLU	3.5
3	Y	257	THR	3.5
1	A	7	CYS	3.5
3	X	339	ASN	3.4
3	X	356	CYS	3.4
3	Y	288	LEU	3.3
3	X	19	HIS	3.3
3	X	24	HIS	3.3
3	X	289	HIS	3.3
3	X	292	CYS	3.3
3	X	358	ASP	3.2
3	Z	351	ASP	3.2
3	Z	283	ARG	3.1
3	Y	287	GLU	3.1
2	B	18	ARG	3.1
1	G	71	MET	3.0
1	D	5	GLN	3.0
1	A	71	MET	2.9
3	Y	353	PHE	2.9
3	X	336	ASP	2.8

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
3	Y	339	ASN	2.8
2	B	107	GLY	2.8
2	E	23	ILE	2.8
3	X	340	GLU	2.7
3	Z	260	LYS	2.7
2	E	102	SER	2.7
3	Y	25	CYS	2.7
3	Y	43	ASP	2.7
3	Y	44	LEU	2.6
3	X	231	HIS	2.6
1	D	45	LYS	2.6
1	D	33	PHE	2.6
3	X	23	CYS	2.6
3	X	90	VAL	2.6
3	X	359	ILE	2.5
3	X	36	LYS	2.5
3	X	60	VAL	2.5
3	Z	60	VAL	2.5
3	X	54	VAL	2.5
3	Y	41	PRO	2.5
2	H	62	ARG	2.4
3	X	208	GLU	2.4
3	Y	358	ASP	2.4
3	Z	336	ASP	2.4
3	X	55	LEU	2.4
2	H	5	LEU	2.4
2	E	63	VAL	2.4
3	Y	337	LEU	2.4
3	Y	351	ASP	2.4
1	D	41	LEU	2.4
2	E	10	ILE	2.4
3	Z	54	VAL	2.3
2	E	107	GLY	2.3
3	X	254	LYS	2.3
3	X	111	ILE	2.3
3	X	182	ILE	2.3
1	G	20	GLN	2.3
3	X	51	LEU	2.3
3	X	351	ASP	2.2
3	Y	22	ILE	2.2
3	Y	262	VAL	2.2
2	E	35	ARG	2.2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
2	H	47	ILE	2.2
3	Y	93	ASN	2.2
3	Z	110	TYR	2.2
3	Z	276	CYS	2.2
2	H	35	ARG	2.1
3	Y	263	ALA	2.1
1	G	21	PRO	2.1
2	E	62	ARG	2.1
1	A	41	LEU	2.1
3	Y	97	LEU	2.1
2	H	26	THR	2.1
3	Z	254	LYS	2.1
2	B	74	TYR	2.1
2	E	33	TYR	2.1
2	H	23	ILE	2.0
3	Y	134	HIS	2.0
1	D	25	ILE	2.0
2	H	45	PRO	2.0
3	X	337	LEU	2.0
3	X	350	PRO	2.0
3	Y	336	ASP	2.0
3	Z	236	TYR	2.0

6.2 Non-standard residues in protein, DNA, RNA chains (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
3	TYS	X	335	16/17	0.79	0.31	-	103,127,146,146	0
3	TYS	Y	335	16/17	0.63	0.36	-	104,127,145,145	0
3	TYS	Z	335	16/17	0.71	0.36	-	101,124,144,144	0

6.3 Carbohydrates (i)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
4	NAG	Y	1191	14/15	0.90	0.33	6.84	10,11,12,12	0
4	NAG	X	1191	14/15	0.88	0.23	1.94	14,15,16,17	0
4	NAG	Z	1191	14/15	0.92	0.21	1.44	9,10,11,12	0
4	NAG	A	1078	14/15	0.95	0.14	-1.06	22,24,25,25	0
4	NAG	A	1052	14/15	0.94	0.11	-1.14	19,20,24,26	0
4	NAG	G	1078	14/15	0.92	0.13	-1.23	22,23,24,26	0
4	NAG	D	1052	14/15	0.92	0.12	-1.39	17,21,24,26	0
4	NAG	D	1078	14/15	0.90	0.11	-1.77	23,25,27,27	0
4	NAG	G	1052	14/15	0.94	0.10	-3.83	20,22,26,29	0
4	NAG	B	1007	14/15	0.91	0.31	-	28,30,32,33	0
4	NAG	E	1007	14/15	0.87	0.39	-	24,26,29,29	0
4	NAG	H	1024	14/15	0.89	0.39	-	32,32,35,36	0
4	NAG	B	1024	14/15	0.88	0.34	-	27,32,34,34	0
4	NAG	E	1024	14/15	0.83	0.35	-	23,24,26,27	0
4	NAG	H	1007	14/15	0.88	0.34	-	26,29,30,33	0

6.5 Other polymers

There are no such residues in this entry.