Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 06:20 AM GMT

PDB ID	:	2WR7
Title	:	THE STRUCTURE OF INFLUENZA H2 HUMAN SINGAPORE HEMAGGLUTININ WITH HUMAN RECEPTOR
Authors	:	Liu, J.; Stevens, D.J.; Haire, L.F.; Walker, P.A.; Coombs, P.J.; Russell, R.J.; Gamblin, S.J.; Skehel, J.J.
Deposited on	:	2009-08-30
Resolution	:	2.50 Å(reported)

The following versions of software and data (see references ⓘ) 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	Percentile Ranks	Value
Rfree		0.286
Clashscore		17
Ramachandran outliers		2.6%
Sidechain outliers		6.8%
RSRZ outliers		6.3%

Worse　　　　　*Better*

■ Percentile relative to all X-ray structures

▯ Percentile relative to X-ray structures of similar resolution
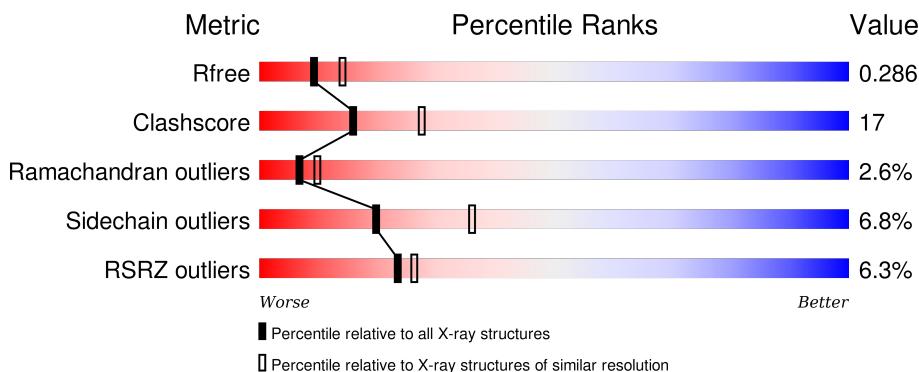
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	91344	3553 (2.50-2.50)
Clashscore	102246	4242 (2.50-2.50)
Ramachandran outliers	100387	4156 (2.50-2.50)
Sidechain outliers	100360	4158 (2.50-2.50)
RSRZ outliers	91569	3562 (2.50-2.50)

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	506	6% / 61% / 28% / • 7%
1	B	506	4% / 63% / 27% / • • •
1	C	506	8% / 61% / 27% / • 8%
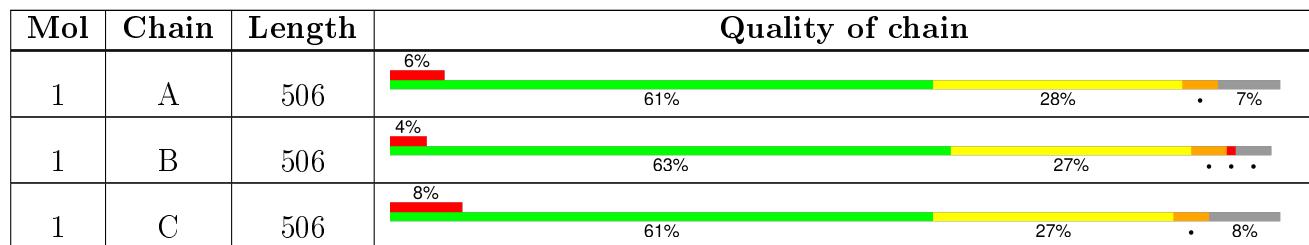
The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	GAL	A	1489	X	-	-	-

2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 11656 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 HEMAGGLUTININ.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	473	Total 3722	C 2336	N 640	O 723	S 23	0	0	0
1	B	486	Total 3842	C 2413	N 659	O 746	S 24	0	0	0
1	C	467	Total 3687	C 2318	N 635	O 710	S 24	0	0	0

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	155	GLU	LYS	CONFLICT	UNP B4UR26
A	347	ILE	VAL	CONFLICT	UNP B4UR26
B	155	GLU	LYS	CONFLICT	UNP B4UR26
B	347	ILE	VAL	CONFLICT	UNP B4UR26
C	155	GLU	LYS	CONFLICT	UNP B4UR26
C	347	ILE	VAL	CONFLICT	UNP B4UR26

- Molecule 2 is a polymer of unknown type called SUGAR (4-MER).

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	4	Total 57	C 31	N 2	O 24	0	0

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	86	Total 86	O 86	0	0
3	B	142	Total 142	O 142	0	0
3	C	120	Total 120	O 120	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: HEMAGGLUTININ

- Molecule 1: HEMAGGLUTININ

• Molecule 1: HEMAGGLUTININ

Chain C:
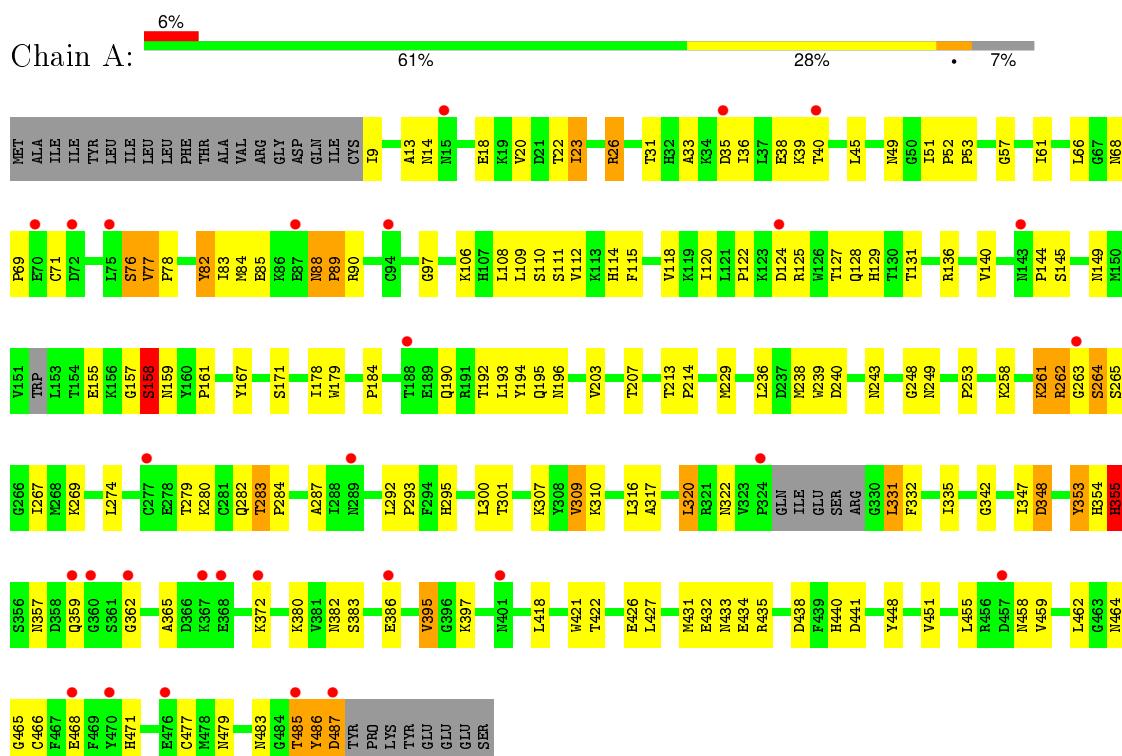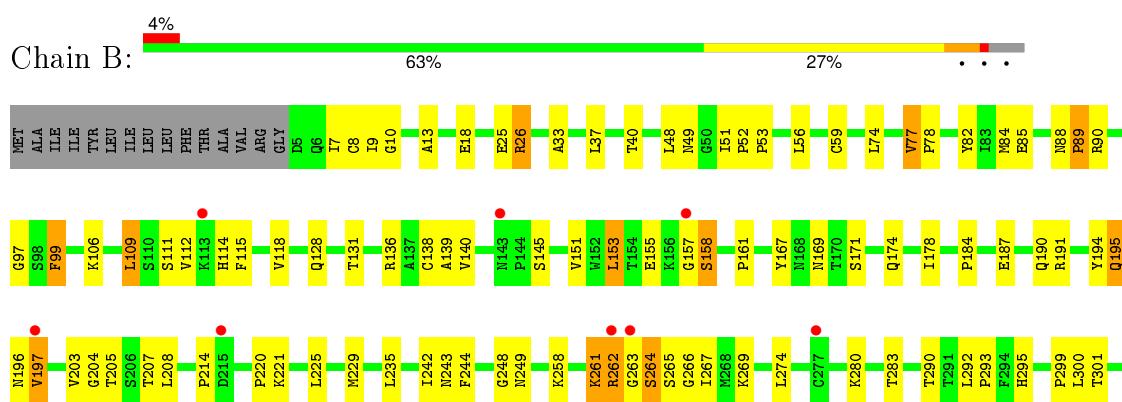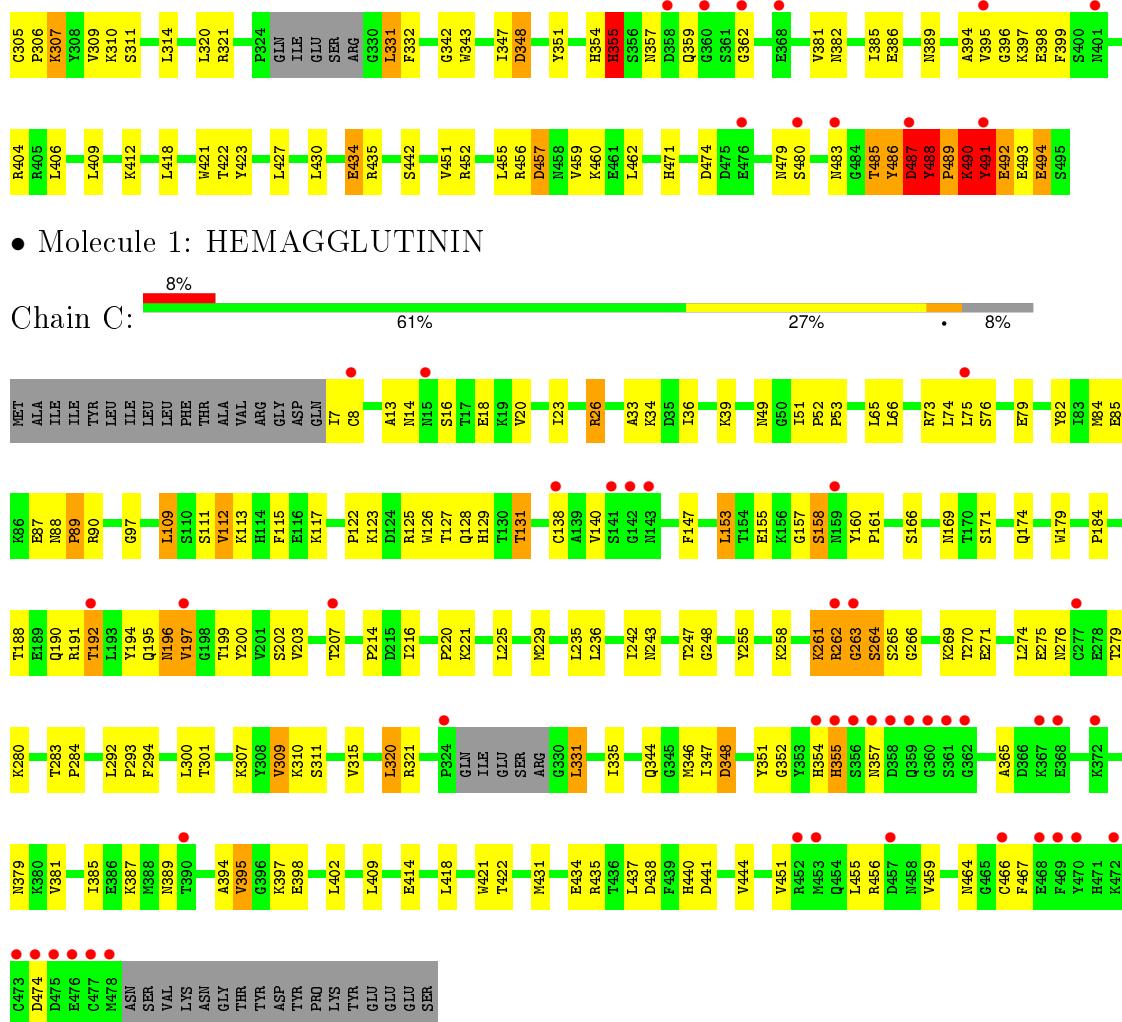
4 Data and refinement statistics (i)

| Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	80.17Å 123.68Å 222.16Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	8.00 – 2.50 8.00 – 2.50	Depositor EDS
% Data completeness (in resolution range)	99.7 (8.00-2.50) 99.7 (8.00-2.50)	Depositor EDS
R_{merge}	0.11	Depositor
R_{sym}	(Not available)	Depositor
$<I/\sigma(I)>$ [1]	1.76 (at 2.49Å)	Xtriage
Refinement program	PHENIX (PHENIX.REFINE)	Depositor
R, R_{free}	0.239 , 0.296 0.221 , 0.286	Depositor DCC
R_{free} test set	3734 reflections (5.03%)	DCC
Wilson B-factor (Å^2)	53.7	Xtriage
Anisotropy	0.978	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.36 , 63.9	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning[2]	$<|L|> = 0.50$, $<L^2> = 0.33$	Xtriage
Outliers	0 of 74386 reflections	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	11656	wwPDB-VP
Average B, all atoms (Å^2)	62.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.25% 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.

Full wwPDB X-ray Structure Validation Report

5 Model quality (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: SIA, GAL, NAG

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$\|Z\|$ >5	RMSZ	#$\|Z\|$ >5
1	A	0.46	0/3803	0.61	1/5143 (0.0%)
1	B	0.53	0/3929	0.69	2/5316 (0.0%)
1	C	0.46	0/3770	0.60	0/5100
All	All	0.49	0/11502	0.63	3/15559 (0.0%)

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
2	A	1	0

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	316	LEU	CA-CB-CG	6.14	129.43	115.30
1	B	488	TYR	N-CA-CB	5.85	121.13	110.60
1	B	488	TYR	CA-CB-CG	-5.08	103.75	113.40

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
2	A	1489	GAL	C1

There are no planarity outliers.

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	3722	0	3589	120	0
1	B	3842	0	3694	150	0
1	C	3687	0	3563	121	0
2	A	57	0	49	3	0
3	A	86	0	0	8	0
3	B	142	0	0	10	0
3	C	120	0	0	9	0
All	All	11656	0	10895	377	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 17.

All (377) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:283:THR:HG22	1:C:301:THR:HG22	1.48	0.91
1:C:8:CYS:HB2	1:C:354:HIS:HB3	1.50	0.91
1:B:490:LYS:HD2	1:B:490:LYS:O	1.72	0.88
1:C:155:GLU:OE1	1:C:195:GLN:HG2	1.74	0.87
1:B:111:SER:HB2	1:B:265:SER:HB3	1.54	0.86
1:C:138:CYS:SG	3:C:2050:HOH:O	2.33	0.86
1:C:261:LYS:HA	1:C:262:ARG:HB2	1.57	0.86
1:B:261:LYS:HA	1:B:262:ARG:HB2	1.58	0.85
1:A:36:ILE:HA	1:A:292:LEU:HD22	1.58	0.84
1:A:320:LEU:H	1:A:320:LEU:HD23	1.41	0.84
1:C:261:LYS:HB2	1:C:262:ARG:HB3	1.59	0.82
1:C:53:PRO:HG2	1:C:84:MET:HE2	1.61	0.82
1:B:493:GLU:HA	1:B:494:GLU:HB2	1.61	0.82
1:B:491:TYR:N	1:B:492:GLU:O	2.13	0.81
1:B:480:SER:HB2	1:B:486:TYR:H	1.45	0.81
1:B:493:GLU:HA	1:B:494:GLU:CB	2.11	0.80
1:C:261:LYS:HA	1:C:262:ARG:CB	2.12	0.80
1:B:53:PRO:HD2	1:B:274:LEU:HD22	1.63	0.79
1:A:380:LYS:HE2	1:A:432:GLU:OE2	1.81	0.79
1:B:112:VAL:HG11	1:B:115:PHE:HB2	1.65	0.79

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:112:VAL:HG11	1:A:115:PHE:HB2	1.65	0.78
1:A:261:LYS:HA	1:A:262:ARG:CB	2.14	0.78
1:B:261:LYS:HB2	1:B:262:ARG:HB3	1.65	0.78
1:C:111:SER:HB2	1:C:265:SER:HB3	1.66	0.78
1:C:320:LEU:HD23	1:C:320:LEU:H	1.48	0.78
1:A:348:ASP:HB2	1:A:365:ALA:HB3	1.64	0.77
1:B:53:PRO:HG2	1:B:84:MET:CE	2.14	0.77
1:B:452:ARG:HD2	3:B:2128:HOH:O	1.83	0.77
1:C:357:ASN:HD21	1:C:474:ASP:HA	1.49	0.77
1:B:155:GLU:OE1	1:B:195:GLN:HG2	1.86	0.75
1:B:310:LYS:HG3	1:B:418:LEU:HD21	1.69	0.74
1:C:53:PRO:HG2	1:C:84:MET:CE	2.16	0.74
1:B:485:THR:O	1:B:486:TYR:O	2.05	0.74
1:A:53:PRO:HG2	1:A:84:MET:CE	2.19	0.73
1:B:53:PRO:HG2	1:B:84:MET:HE2	1.70	0.73
1:B:487:ASP:HA	1:B:488:TYR:CB	2.19	0.72
1:A:53:PRO:HD2	1:A:274:LEU:HD22	1.69	0.72
1:A:455:LEU:HD13	1:A:459:VAL:HG11	1.72	0.72
1:B:357:ASN:HB3	1:B:359:GLN:H	1.54	0.72
1:C:184:PRO:HG2	1:C:190:GLN:HE21	1.55	0.72
1:B:471:HIS:CE1	1:B:490:LYS:HE3	2.25	0.72
1:B:397:LYS:HE2	3:B:2114:HOH:O	1.89	0.71
1:A:348:ASP:HB2	1:A:365:ALA:CB	2.21	0.71
1:C:184:PRO:HG2	1:C:190:GLN:NE2	2.06	0.70
1:A:127:THR:HA	3:A:2024:HOH:O	1.91	0.70
1:C:335:ILE:HD12	1:C:441:ASP:HA	1.73	0.70
1:B:487:ASP:HA	1:B:488:TYR:HB2	1.73	0.70
1:A:184:PRO:HG2	1:A:190:GLN:HE21	1.57	0.70
1:B:293:PRO:HG3	1:B:385:ILE:HA	1.76	0.69
1:C:309:VAL:HG13	1:C:311:SER:H	1.56	0.69
1:A:45:LEU:HB3	3:A:2018:HOH:O	1.92	0.68
1:A:171:SER:HB2	1:A:258:LYS:HD2	1.74	0.68
1:C:88:ASN:O	1:C:89:PRO:O	2.11	0.68
1:C:174:GLN:OE1	1:C:235:LEU:HD13	1.94	0.68
1:C:261:LYS:CA	1:C:262:ARG:CB	2.72	0.68
1:B:184:PRO:HG2	1:B:190:GLN:HE21	1.58	0.67
1:A:310:LYS:HE3	1:A:418:LEU:HD21	1.77	0.67
1:B:264:SER:HB3	3:B:2082:HOH:O	1.94	0.66
1:A:261:LYS:CA	1:A:262:ARG:CB	2.74	0.66
1:B:389:ASN:HD21	1:C:310:LYS:NZ	1.93	0.66
1:A:22:THR:HG22	1:A:433:ASN:HB3	1.77	0.66

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:261:LYS:CB	1:C:262:ARG:HB3	2.26	0.65
1:B:490:LYS:O	1:B:490:LYS:CD	2.45	0.65
1:B:106:LYS:HB3	1:B:267:ILE:HD11	1.79	0.64
1:A:53:PRO:HG2	1:A:84:MET:HE3	1.80	0.64
1:A:9:ILE:HD11	1:A:451:VAL:HG21	1.80	0.63
1:B:354:HIS:O	1:B:362:GLY:O	2.15	0.63
1:A:354:HIS:O	1:A:362:GLY:O	2.15	0.63
1:C:395:VAL:O	1:C:397:LYS:HG3	1.99	0.63
1:B:49:ASN:HD21	1:B:280:LYS:HG2	1.64	0.62
1:A:13:ALA:HB2	1:A:342:GLY:HA3	1.81	0.62
1:A:128:GLN:N	3:A:2024:HOH:O	2.33	0.62
1:A:127:THR:O	1:A:128:GLN:HB2	2.00	0.61
1:B:187:GLU:OE2	1:B:191:ARG:NH1	2.32	0.61
1:B:292:LEU:O	1:B:306:PRO:HB3	2.01	0.61
1:B:489:PRO:O	1:B:490:LYS:HB3	2.01	0.60
1:C:191:ARG:HD2	3:C:2066:HOH:O	2.00	0.60
1:B:487:ASP:CG	1:B:489:PRO:HD2	2.22	0.60
1:B:491:TYR:H	1:B:492:GLU:C	2.04	0.60
1:B:261:LYS:HA	1:B:262:ARG:CB	2.31	0.60
1:A:426:GLU:HB3	1:C:387:LYS:HD2	1.83	0.60
1:A:106:LYS:HB3	1:A:267:ILE:HD11	1.83	0.60
1:A:155:GLU:OE1	1:A:195:GLN:HG2	2.01	0.60
1:B:488:TYR:CD2	1:B:488:TYR:C	2.75	0.59
1:B:310:LYS:HE3	1:B:418:LEU:HD21	1.84	0.59
1:C:111:SER:HB2	1:C:265:SER:CB	2.31	0.59
1:C:320:LEU:HD23	1:C:320:LEU:N	2.16	0.59
1:A:395:VAL:O	1:A:397:LYS:HG3	2.02	0.59
1:A:178:ILE:O	1:A:253:PRO:HG3	2.02	0.59
1:B:493:GLU:CA	1:B:494:GLU:HB2	2.31	0.58
1:C:191:ARG:NH2	1:C:197:VAL:HG21	2.19	0.58
1:A:193:LEU:HD11	2:A:1488:SIA:H92	1.84	0.58
1:A:435:ARG:HH21	1:B:434:GLU:CD	2.06	0.58
1:A:49:ASN:HD21	1:A:280:LYS:HG2	1.69	0.58
1:B:261:LYS:HB2	1:B:262:ARG:CB	2.34	0.58
1:C:26:ARG:NH2	3:C:2009:HOH:O	2.36	0.58
1:C:455:LEU:HD13	1:C:459:VAL:HG11	1.86	0.58
1:B:26:ARG:NH2	3:B:2002:HOH:O	2.36	0.57
1:C:157:GLY:O	1:C:158:SER:CB	2.52	0.57
1:C:440:HIS:O	1:C:444:VAL:HG23	2.05	0.57
1:C:129:HIS:CE1	1:C:161:PRO:O	2.57	0.57
1:C:293:PRO:HB2	1:C:294:PHE:CD1	2.39	0.57

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:335:ILE:HD12	1:A:441:ASP:HA	1.87	0.57
1:B:492:GLU:HA	1:B:493:GLU:CB	2.35	0.56
1:B:264:SER:CB	3:B:2082:HOH:O	2.52	0.56
1:C:129:HIS:HE1	1:C:161:PRO:O	1.87	0.56
1:C:355:HIS:O	1:C:355:HIS:CG	2.58	0.56
1:C:7:ILE:HA	1:C:355:HIS:HA	1.87	0.56
1:A:53:PRO:HG2	1:A:84:MET:HE2	1.86	0.56
1:B:455:LEU:HD13	1:B:459:VAL:HG11	1.87	0.56
1:B:261:LYS:CA	1:B:262:ARG:HB2	2.33	0.56
1:C:464:ASN:OD1	1:C:466:CYS:HB2	2.06	0.56
1:C:97:GLY:HA3	1:C:229:MET:O	2.06	0.56
1:C:66:LEU:O	1:C:147:PHE:HB3	2.06	0.56
1:A:332:PHE:HB2	1:A:441:ASP:CG	2.27	0.55
1:A:136:ARG:HG3	1:A:144:PRO:HG3	1.88	0.55
1:B:494:GLU:HA	1:B:494:GLU:OE1	2.05	0.55
1:A:310:LYS:NZ	1:C:389:ASN:HD21	2.05	0.55
1:B:261:LYS:CA	1:B:262:ARG:CB	2.84	0.55
1:A:179:TRP:CE2	1:A:203:VAL:HG21	2.41	0.55
1:A:122:PRO:HG2	1:A:125:ARG:NH1	2.21	0.55
1:B:295:HIS:HB3	1:B:306:PRO:HG2	1.89	0.55
1:B:490:LYS:H	1:B:491:TYR:HB2	1.71	0.55
1:A:483:ASN:ND2	3:A:2083:HOH:O	2.39	0.55
1:B:136:ARG:HD2	3:B:2047:HOH:O	2.06	0.55
1:A:243:ASN:HD22	1:B:220:PRO:HD3	1.71	0.55
1:A:157:GLY:O	1:A:158:SER:HB2	2.06	0.54
1:B:248:GLY:C	1:B:249:ASN:HD22	2.11	0.54
1:A:485:THR:O	1:A:486:TYR:O	2.26	0.54
1:B:77:VAL:HG12	1:B:78:PRO:CD	2.37	0.54
1:C:127:THR:O	1:C:128:GLN:HB2	2.08	0.54
1:C:188:THR:O	1:C:192:THR:OG1	2.25	0.54
1:B:8:CYS:HB2	1:B:354:HIS:HB3	1.90	0.54
1:B:25:GLU:OE2	1:B:321:ARG:NH2	2.38	0.54
1:A:248:GLY:C	1:A:249:ASN:HD22	2.11	0.54
1:A:310:LYS:HE3	1:A:418:LEU:CD2	2.38	0.54
1:C:112:VAL:HG11	1:C:115:PHE:HB2	1.89	0.54
1:C:307:LYS:HG2	1:C:421:TRP:CE2	2.42	0.54
1:C:36:ILE:HA	1:C:292:LEU:HD22	1.90	0.54
1:A:479:ASN:O	1:A:483:ASN:HB2	2.08	0.53
1:C:301:THR:O	1:C:394:ALA:O	2.27	0.53
1:C:138:CYS:HB2	3:C:2050:HOH:O	2.09	0.53
1:C:122:PRO:HD2	1:C:125:ARG:HD2	1.90	0.53

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:310:LYS:HG3	1:C:418:LEU:HD21	1.90	0.53
1:A:284:PRO:HD3	1:A:300:LEU:O	2.08	0.52
1:C:346:MET:SD	1:C:352:GLY:HA3	2.49	0.52
1:B:491:TYR:HE2	1:B:494:GLU:OE2	1.92	0.52
1:B:494:GLU:OE1	1:B:494:GLU:CA	2.58	0.52
1:A:310:LYS:HG3	1:A:418:LEU:HD21	1.90	0.52
1:A:45:LEU:HD23	1:A:282:GLN:NE2	2.24	0.52
1:B:460:LYS:HE2	1:B:462:LEU:CD2	2.39	0.52
1:B:412:LYS:NZ	3:B:2113:HOH:O	2.43	0.52
1:B:490:LYS:O	1:B:490:LYS:CG	2.58	0.52
1:A:353:TYR:N	1:A:353:TYR:CD1	2.77	0.52
1:C:131:THR:HG23	1:C:131:THR:O	2.09	0.52
1:B:491:TYR:CE2	1:B:494:GLU:OE2	2.63	0.52
1:A:49:ASN:ND2	1:A:280:LYS:HG2	2.24	0.52
1:C:117:LYS:HD3	1:C:255:TYR:CD2	2.44	0.52
1:B:88:ASN:O	1:B:89:PRO:O	2.27	0.52
1:C:26:ARG:NH2	3:C:2008:HOH:O	2.42	0.52
1:A:26:ARG:HD2	1:C:379:ASN:OD1	2.08	0.52
1:C:53:PRO:HG3	1:C:82:TYR:CZ	2.45	0.52
1:C:117:LYS:HD3	1:C:255:TYR:CG	2.45	0.51
1:C:437:LEU:O	3:C:2117:HOH:O	2.18	0.51
1:A:36:ILE:HA	1:A:292:LEU:CD2	2.36	0.51
1:C:293:PRO:HB2	1:C:294:PHE:CE1	2.46	0.51
1:A:283:THR:HG22	1:A:301:THR:HG22	1.93	0.51
1:B:487:ASP:OD1	1:B:489:PRO:HD2	2.10	0.51
1:C:179:TRP:CE2	1:C:203:VAL:HG21	2.45	0.51
1:A:23:ILE:HD12	1:A:431:MET:HG2	1.93	0.51
1:B:10:GLY:HA3	1:B:343:TRP:CH2	2.46	0.51
1:C:309:VAL:HG22	1:C:422:THR:HA	1.94	0.50
1:B:348:ASP:OD1	1:B:348:ASP:N	2.43	0.50
1:A:108:LEU:HD13	1:B:404:ARG:NH1	2.26	0.50
1:A:61:ILE:HD12	1:A:106:LYS:HD2	1.91	0.50
1:A:435:ARG:HH12	1:B:435:ARG:HH11	1.59	0.50
1:B:77:VAL:HG12	1:B:78:PRO:HD3	1.94	0.50
1:C:23:ILE:HD12	1:C:431:MET:HG2	1.93	0.50
1:B:203:VAL:HG22	1:B:244:PHE:CD2	2.47	0.50
1:B:191:ARG:NH2	1:B:197:VAL:HG21	2.26	0.50
1:A:382:ASN:O	1:A:386:GLU:HG2	2.11	0.50
1:C:335:ILE:HD12	1:C:441:ASP:CA	2.40	0.50
1:A:140:VAL:HG12	1:A:145:SER:HB2	1.94	0.50
1:C:157:GLY:O	1:C:158:SER:HB2	2.11	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:111:SER:HB2	1:A:265:SER:HB3	1.94	0.50
1:A:157:GLY:O	1:A:158:SER:CB	2.60	0.50
1:A:77:VAL:HG12	1:A:78:PRO:CD	2.42	0.50
1:B:309:VAL:CG2	1:B:422:THR:HA	2.42	0.50
1:C:8:CYS:HB2	1:C:354:HIS:CB	2.31	0.49
1:A:77:VAL:HG12	1:A:78:PRO:HD2	1.94	0.49
1:A:464:ASN:OD1	1:A:466:CYS:HB2	2.11	0.49
1:A:53:PRO:HG3	1:A:82:TYR:CZ	2.47	0.49
1:A:20:VAL:HB	1:A:433:ASN:ND2	2.27	0.49
1:B:85:GLU:O	1:B:269:LYS:HA	2.12	0.49
1:B:399:PHE:CE1	1:B:406:LEU:HG	2.48	0.49
1:C:381:VAL:HG12	1:C:385:ILE:HD12	1.94	0.49
1:B:99:PHE:HZ	1:B:178:ILE:HD13	1.78	0.49
1:B:331:LEU:HD13	3:B:2126:HOH:O	2.11	0.49
1:C:321:ARG:CB	3:C:2091:HOH:O	2.60	0.49
1:C:196:ASN:N	1:C:196:ASN:ND2	2.60	0.49
1:C:200:TYR:CE2	1:C:247:THR:HG23	2.47	0.49
1:B:394:ALA:O	1:B:395:VAL:HB	2.11	0.49
1:A:38:GLU:O	1:A:295:HIS:HA	2.13	0.49
1:A:18:GLU:HG2	1:A:33:ALA:HB3	1.94	0.49
1:B:184:PRO:HG2	1:B:190:GLN:NE2	2.24	0.49
1:A:435:ARG:HH11	1:C:435:ARG:NH1	2.10	0.49
1:C:171:SER:HB2	1:C:258:LYS:HE3	1.94	0.49
1:C:85:GLU:O	1:C:269:LYS:HA	2.12	0.49
1:A:36:ILE:CA	1:A:292:LEU:HD22	2.38	0.49
1:B:460:LYS:HG2	1:B:462:LEU:HD23	1.95	0.49
1:A:111:SER:HB2	1:A:265:SER:CB	2.42	0.49
1:B:18:GLU:HG2	1:B:33:ALA:HB3	1.93	0.49
1:A:184:PRO:HG2	1:A:190:GLN:NE2	2.28	0.49
1:A:372:LYS:HE3	3:A:2027:HOH:O	2.11	0.49
1:B:37:LEU:HB2	1:B:314:LEU:HD12	1.95	0.49
1:B:194:TYR:O	1:B:196:ASN:N	2.37	0.49
1:A:236:LEU:CD1	1:A:240:ASP:HB3	2.43	0.49
1:C:331:LEU:HD22	1:C:438:ASP:OD2	2.13	0.48
1:C:348:ASP:HB2	1:C:365:ALA:HB3	1.94	0.48
1:C:261:LYS:CA	1:C:262:ARG:HB3	2.40	0.48
1:B:488:TYR:HD2	1:B:489:PRO:HD3	1.78	0.48
1:A:68:ASN:O	1:A:71:CYS:HB2	2.13	0.48
1:B:9:ILE:HD11	1:B:451:VAL:HG21	1.95	0.48
1:C:18:GLU:HG2	1:C:33:ALA:HB3	1.94	0.48
1:C:138:CYS:CB	3:C:2050:HOH:O	2.60	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:451:VAL:HG12	1:C:467:PHE:CE1	2.49	0.48
1:B:53:PRO:HG2	1:B:84:MET:HE3	1.91	0.48
1:C:123:LYS:HD3	1:C:131:THR:HG23	1.95	0.48
1:C:75:LEU:O	1:C:76:SER:HB2	2.12	0.48
1:C:51:ILE:HG23	1:C:52:PRO:HD2	1.96	0.48
1:B:265:SER:OG	1:B:266:GLY:N	2.45	0.47
1:A:320:LEU:H	1:A:320:LEU:CD2	2.21	0.47
1:C:265:SER:OG	1:C:266:GLY:N	2.47	0.47
1:B:389:ASN:HD21	1:C:310:LYS:HZ2	1.60	0.47
1:A:120:ILE:HG22	1:A:167:TYR:CZ	2.49	0.47
1:A:462:LEU:HD21	1:A:468:GLU:HB2	1.94	0.47
1:B:112:VAL:N	1:B:262:ARG:HD3	2.30	0.47
1:A:243:ASN:ND2	1:B:220:PRO:HD3	2.29	0.47
1:B:128:GLN:HB3	1:B:161:PRO:HG2	1.96	0.47
1:A:22:THR:HB	1:A:434:GLU:HB3	1.95	0.47
1:B:480:SER:HB2	1:B:486:TYR:N	2.22	0.47
1:A:435:ARG:NH1	1:B:435:ARG:HH11	2.12	0.47
1:A:434:GLU:HB2	3:A:2071:HOH:O	2.14	0.47
1:B:205:THR:HG22	1:B:242:ILE:HA	1.97	0.47
1:B:480:SER:HB2	1:B:485:THR:HB	1.96	0.46
1:A:108:LEU:HD12	1:A:261:LYS:HE2	1.97	0.46
1:A:14:ASN:OD1	1:A:322:ASN:ND2	2.48	0.46
1:C:53:PRO:HG3	1:C:82:TYR:CE2	2.50	0.46
1:C:155:GLU:OE1	1:C:195:GLN:CG	2.56	0.46
1:C:49:ASN:HD21	1:C:280:LYS:HG2	1.81	0.46
1:B:138:CYS:O	1:B:145:SER:HB3	2.15	0.46
1:B:483:ASN:HB3	1:B:485:THR:OG1	2.15	0.46
1:A:66:LEU:O	1:A:149:ASN:HB2	2.15	0.46
1:B:310:LYS:HE3	1:B:418:LEU:CD2	2.44	0.46
1:C:190:GLN:NE2	1:C:216:ILE:HD11	2.31	0.46
1:B:56:LEU:O	1:B:59:CYS:HB2	2.16	0.46
1:B:300:LEU:HD22	1:B:396:GLY:HA2	1.97	0.46
1:C:166:SER:HB3	1:C:243:ASN:OD1	2.16	0.46
1:A:309:VAL:HG22	1:A:422:THR:HA	1.97	0.46
3:B:2104:HOH:O	1:C:418:LEU:HD23	2.14	0.46
1:A:20:VAL:HG21	1:A:317:ALA:HB2	1.98	0.46
1:A:35:ASP:OD2	1:A:39:LYS:HE2	2.16	0.46
1:C:169:ASN:HB2	1:C:236:LEU:CD2	2.45	0.46
1:A:88:ASN:O	1:A:89:PRO:O	2.34	0.46
1:B:456:ARG:HB3	1:B:457:ASP:H	1.45	0.45
2:A:1491:GAL:H2	2:A:1491:GAL:H62	1.98	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:204:GLY:HA2	1:B:208:LEU:O	2.16	0.45
1:B:51:ILE:HD13	1:B:262:ARG:HH22	1.82	0.45
1:B:310:LYS:CG	1:B:418:LEU:HD21	2.44	0.45
1:B:381:VAL:HG12	1:B:385:ILE:HD12	1.98	0.45
1:A:236:LEU:HD12	1:A:240:ASP:HB3	1.98	0.45
1:A:448:TYR:CE1	1:A:465:GLY:HA2	2.52	0.45
1:B:395:VAL:O	1:B:397:LYS:HG3	2.16	0.45
1:C:160:TYR:CZ	1:C:248:GLY:HA2	2.51	0.45
1:B:479:ASN:O	1:B:483:ASN:HB2	2.17	0.44
1:A:194:TYR:O	1:A:196:ASN:N	2.46	0.44
1:B:389:ASN:HD21	1:C:310:LYS:HZ3	1.65	0.44
1:B:214:PRO:HG3	1:B:249:ASN:CG	2.37	0.44
1:C:200:TYR:CE2	1:C:247:THR:CG2	3.00	0.44
1:B:158:SER:O	1:B:195:GLN:HG3	2.18	0.44
1:B:332:PHE:CE1	1:B:442:SER:HB2	2.53	0.44
1:B:18:GLU:HG2	1:B:33:ALA:CB	2.48	0.44
1:B:7:ILE:HA	1:B:355:HIS:HA	1.99	0.44
1:C:221:LYS:HA	1:C:225:LEU:O	2.18	0.44
1:B:171:SER:HB2	1:B:258:LYS:HD2	1.98	0.44
1:A:83:ILE:HD12	1:A:110:SER:HA	1.99	0.44
1:C:79:GLU:HG3	1:C:113:LYS:O	2.18	0.44
1:C:199:THR:OG1	1:C:214:PRO:HG2	2.17	0.44
1:B:487:ASP:CA	1:B:488:TYR:CB	2.93	0.44
1:A:78:PRO:O	1:A:114:HIS:HA	2.18	0.44
1:A:155:GLU:OE2	1:A:192:THR:O	2.35	0.44
1:C:20:VAL:HG12	1:C:315:VAL:HG12	1.99	0.44
1:C:191:ARG:HH21	1:C:197:VAL:HG21	1.82	0.43
1:B:489:PRO:O	1:B:490:LYS:CB	2.64	0.43
1:B:203:VAL:HG22	1:B:244:PHE:HD2	1.83	0.43
1:A:129:HIS:CE1	1:A:161:PRO:HD2	2.53	0.43
1:C:284:PRO:HD3	1:C:300:LEU:O	2.17	0.43
1:B:136:ARG:HA	1:B:139:ALA:HB2	2.00	0.43
1:C:122:PRO:HG2	1:C:125:ARG:CZ	2.48	0.43
1:B:423:TYR:CE2	1:B:427:LEU:HD22	2.53	0.43
1:B:305:CYS:C	1:B:306:PRO:O	2.57	0.43
1:A:354:HIS:O	1:A:355:HIS:ND1	2.51	0.43
1:A:487:ASP:CG	1:A:487:ASP:O	2.56	0.43
1:A:97:GLY:HA3	1:A:229:MET:O	2.19	0.43
1:B:97:GLY:HA3	1:B:229:MET:O	2.19	0.43
1:A:279:THR:OG1	1:A:287:ALA:HB1	2.18	0.43
1:B:221:LYS:HA	1:B:225:LEU:O	2.19	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:213:THR:HA	1:A:214:PRO:HD3	1.88	0.43
1:C:394:ALA:O	1:C:395:VAL:HB	2.19	0.43
1:B:357:ASN:HD21	1:B:474:ASP:HA	1.84	0.43
1:B:299:PRO:O	1:B:395:VAL:HG11	2.19	0.43
1:C:65:LEU:HD11	1:C:109:LEU:HD21	2.00	0.43
1:B:109:LEU:HD12	1:B:109:LEU:HA	1.87	0.43
1:A:357:ASN:HB3	1:A:359:GLN:H	1.84	0.43
1:B:301:THR:O	1:B:394:ALA:O	2.36	0.43
1:C:307:LYS:HG2	1:C:421:TRP:CD2	2.54	0.43
2:A:1490:NAG:H83	3:A:2086:HOH:O	2.18	0.43
1:C:74:LEU:HA	1:C:74:LEU:HD23	1.79	0.43
1:C:194:TYR:O	1:C:195:GLN:HB2	2.19	0.43
1:B:13:ALA:HB2	1:B:342:GLY:HA3	2.01	0.43
1:A:458:ASN:ND2	1:A:458:ASN:N	2.66	0.42
1:C:270:THR:OG1	1:C:271:GLU:N	2.52	0.42
1:B:53:PRO:HG3	1:B:82:TYR:CZ	2.54	0.42
1:B:307:LYS:HG2	1:B:421:TRP:CG	2.54	0.42
1:C:262:ARG:HG3	1:C:263:GLY:N	2.34	0.42
1:C:263:GLY:O	1:C:264:SER:HB3	2.18	0.42
1:B:51:ILE:CD1	1:B:262:ARG:HH22	2.31	0.42
1:A:320:LEU:HB3	1:A:440:HIS:CG	2.54	0.42
1:B:78:PRO:O	1:B:114:HIS:HA	2.19	0.42
1:A:307:LYS:HG2	1:A:421:TRP:CE2	2.54	0.42
1:B:490:LYS:H	1:B:491:TYR:CB	2.31	0.42
1:A:426:GLU:CB	1:C:387:LYS:HD2	2.49	0.42
1:C:275:GLU:O	1:C:276:ASN:HB3	2.20	0.42
1:C:129:HIS:CE1	1:C:161:PRO:HD2	2.54	0.42
1:A:122:PRO:HG2	1:A:125:ARG:CZ	2.49	0.42
1:A:458:ASN:HB3	1:A:471:HIS:HD2	1.84	0.42
1:B:151:VAL:HG12	1:B:153:LEU:HD13	2.01	0.42
1:B:157:GLY:O	1:B:158:SER:CB	2.68	0.42
1:B:292:LEU:HA	1:B:293:PRO:HD3	1.98	0.42
1:A:179:TRP:CD2	1:A:203:VAL:HG21	2.54	0.42
1:A:69:PRO:C	1:A:71:CYS:H	2.23	0.42
1:A:331:LEU:HB2	1:A:438:ASP:OD1	2.20	0.42
1:C:402:LEU:HD23	1:C:402:LEU:HA	1.95	0.42
1:A:238:MET:O	1:A:239:TRP:CB	2.67	0.41
1:B:48:LEU:O	1:B:49:ASN:HB2	2.20	0.41
1:B:10:GLY:HA3	1:B:343:TRP:CZ3	2.55	0.41
1:B:309:VAL:HG22	1:B:422:THR:HA	2.02	0.41
1:B:307:LYS:HE2	3:B:2118:HOH:O	2.20	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:85:GLU:O	1:A:269:LYS:HA	2.20	0.41
1:C:310:LYS:HE3	1:C:418:LEU:HD21	2.02	0.41
1:C:87:GLU:O	3:C:2030:HOH:O	2.22	0.41
1:B:84:MET:HE1	1:B:274:LEU:HB2	2.02	0.41
1:B:307:LYS:HG2	1:B:421:TRP:CD2	2.55	0.41
1:B:74:LEU:HA	1:B:74:LEU:HD23	1.87	0.41
1:A:383:SER:HB3	1:B:430:LEU:CD1	2.50	0.41
1:C:14:ASN:OD1	1:C:16:SER:HB3	2.20	0.41
1:C:53:PRO:HD2	1:C:274:LEU:HD22	2.03	0.41
1:B:331:LEU:HD12	1:B:331:LEU:HA	1.75	0.41
1:B:56:LEU:HD23	1:B:56:LEU:HA	1.90	0.41
1:C:13:ALA:O	1:C:344:GLN:HA	2.21	0.41
1:A:292:LEU:HA	1:A:293:PRO:HD3	1.76	0.41
1:B:300:LEU:HD22	1:B:396:GLY:CA	2.51	0.41
1:C:348:ASP:HB2	1:C:365:ALA:CB	2.51	0.41
1:A:331:LEU:HD22	1:A:438:ASP:OD2	2.20	0.41
1:B:174:GLN:OE1	1:B:235:LEU:HD13	2.21	0.40
1:B:53:PRO:HD2	1:B:274:LEU:CD2	2.43	0.40
1:A:128:GLN:NE2	3:A:2032:HOH:O	2.54	0.40
1:B:243:ASN:HD22	1:C:220:PRO:HD3	1.87	0.40
1:A:120:ILE:HG22	1:A:167:TYR:CE1	2.56	0.40
1:C:166:SER:HA	1:C:242:ILE:O	2.21	0.40
1:C:113:LYS:O	1:C:113:LYS:HG2	2.21	0.40
1:C:126:TRP:CD2	1:C:153:LEU:HD21	2.57	0.40
1:A:51:ILE:HA	1:A:52:PRO:HD3	1.91	0.40
1:B:382:ASN:O	1:B:386:GLU:HG2	2.21	0.40
1:B:167:TYR:CE2	1:B:169:ASN:HA	2.56	0.40
1:A:348:ASP:HB2	1:A:365:ALA:HB2	2.02	0.40
1:B:300:LEU:HD23	1:B:395:VAL:HG12	2.02	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	467/506 (92%)	429 (92%)	25 (5%)	13 (3%)	6	9
1	B	482/506 (95%)	442 (92%)	24 (5%)	16 (3%)	5	6
1	C	463/506 (92%)	428 (92%)	27 (6%)	8 (2%)	11	19
All	All	1412/1518 (93%)	1299 (92%)	76 (5%)	37 (3%)	7	10

All (37) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	89	PRO
1	A	158	SER
1	A	262	ARG
1	A	485	THR
1	A	486	TYR
1	B	89	PRO
1	B	158	SER
1	B	262	ARG
1	B	486	TYR
1	B	488	TYR
1	B	490	LYS
1	B	491	TYR
1	C	89	PRO
1	C	158	SER
1	C	262	ARG
1	A	90	ARG
1	B	487	ASP
1	B	492	GLU
1	A	355	HIS
1	B	195	GLN
1	A	31	THR
1	A	76	SER
1	A	263	GLY
1	B	90	ARG
1	B	263	GLY
1	B	264	SER
1	C	90	ARG
1	C	395	VAL
1	B	355	HIS
1	B	485	THR
1	B	489	PRO
1	C	264	SER
1	C	456	ARG
1	A	264	SER

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	C	263	GLY
1	A	395	VAL
1	A	57	GLY

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	411/443 (93%)	384 (93%)	27 (7%)	21	38
1	B	424/443 (96%)	393 (93%)	31 (7%)	17	32
1	C	407/443 (92%)	380 (93%)	27 (7%)	21	38
All	All	1242/1329 (94%)	1157 (93%)	85 (7%)	20	36

All (85) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	23	ILE
1	A	26	ARG
1	A	40	THR
1	A	76	SER
1	A	77	VAL
1	A	82	TYR
1	A	88	ASN
1	A	109	LEU
1	A	118	VAL
1	A	124	ASP
1	A	131	THR
1	A	158	SER
1	A	159	ASN
1	A	207	THR
1	A	261	LYS
1	A	264	SER
1	A	283	THR
1	A	309	VAL
1	A	320	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	331	LEU
1	A	347	ILE
1	A	348	ASP
1	A	353	TYR
1	A	355	HIS
1	A	427	LEU
1	A	477	CYS
1	A	487	ASP
1	B	26	ARG
1	B	40	THR
1	B	52	PRO
1	B	77	VAL
1	B	99	PHE
1	B	109	LEU
1	B	118	VAL
1	B	131	THR
1	B	140	VAL
1	B	153	LEU
1	B	197	VAL
1	B	207	THR
1	B	261	LYS
1	B	283	THR
1	B	290	THR
1	B	307	LYS
1	B	311	SER
1	B	320	LEU
1	B	331	LEU
1	B	347	ILE
1	B	348	ASP
1	B	351	TYR
1	B	355	HIS
1	B	398	GLU
1	B	409	LEU
1	B	434	GLU
1	B	457	ASP
1	B	487	ASP
1	B	490	LYS
1	B	491	TYR
1	B	494	GLU
1	C	26	ARG
1	C	34	LYS
1	C	39	LYS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	C	73	ARG
1	C	109	LEU
1	C	112	VAL
1	C	131	THR
1	C	140	VAL
1	C	153	LEU
1	C	192	THR
1	C	196	ASN
1	C	197	VAL
1	C	202	SER
1	C	207	THR
1	C	261	LYS
1	C	279	THR
1	C	309	VAL
1	C	320	LEU
1	C	331	LEU
1	C	347	ILE
1	C	348	ASP
1	C	351	TYR
1	C	355	HIS
1	C	398	GLU
1	C	409	LEU
1	C	414	GLU
1	C	434	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (28) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	49	ASN
1	A	114	HIS
1	A	129	HIS
1	A	190	GLN
1	A	249	ASN
1	A	282	GLN
1	A	389	ASN
1	A	391	GLN
1	A	454	GLN
1	A	458	ASN
1	B	49	ASN
1	B	100	ASN
1	B	107	HIS
1	B	129	HIS

Continued from previous page...

Mol	Chain	Res	Type
1	B	190	GLN
1	B	249	ASN
1	B	357	ASN
1	B	389	ASN
1	B	454	GLN
1	B	458	ASN
1	C	49	ASN
1	C	129	HIS
1	C	190	GLN
1	C	196	ASN
1	C	249	ASN
1	C	357	ASN
1	C	389	ASN
1	C	458	ASN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

4 carbohydrates are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#|Z| > 2$	Counts	RMSZ	$\#|Z| > 2$
2	SIA	A	1488	2	16,20,21	0.56	0	18,28,31	1.11	1 (5%)
2	GAL	A	1489	2	11,11,12	0.47	0	14,15,17	2.76	3 (21%)
2	NAG	A	1490	2	14,14,15	0.40	0	15,19,21	1.79	3 (20%)
2	GAL	A	1491	2	12,12,12	0.58	0	17,17,17	1.26	1 (5%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	SIA	A	1488	2	-	0/14/34/38	0/1/1/1
2	GAL	A	1489	2	1/1/4/5	0/2/19/22	0/1/1/1
2	NAG	A	1490	2	-	0/6/23/26	0/1/1/1
2	GAL	A	1491	2	-	0/2/22/22	0/1/1/1

There are no bond length outliers.

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	1491	GAL	C4-C3-C2	-2.32	106.45	110.79
2	A	1490	NAG	C8-C7-N2	-2.09	112.10	116.11
2	A	1490	NAG	C1-O5-C5	2.12	114.94	112.25
2	A	1488	SIA	O6-C6-C5	2.84	113.13	108.48
2	A	1489	GAL	C1-C2-C3	3.11	113.22	109.54
2	A	1490	NAG	C2-N2-C7	5.36	129.92	123.04
2	A	1489	GAL	C1-O5-C5	6.18	120.09	112.25
2	A	1489	GAL	O5-C1-C2	6.97	122.17	110.86

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
2	A	1489	GAL	C1

There are no torsion outliers.

There are no ring outliers.

3 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	1488	SIA	1	0
2	A	1490	NAG	1	0
2	A	1491	GAL	1	0

5.6 Ligand geometry (i)

There are no ligands in this entry.

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data (i)

6.1 Protein, DNA and RNA chains (i)

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2		OWAB(Å²)	Q<0.9
1	A	473/506 (93%)	0.16	29 (6%)	25	27	31, 63, 103, 163	0
1	B	486/506 (96%)	-0.10	19 (3%)	43	48	30, 50, 83, 154	0
1	C	467/506 (92%)	0.21	42 (8%)	12	12	33, 57, 125, 263	0
All	All	1426/1518 (93%)	0.09	90 (6%)	23	26	30, 56, 104, 263	0

All (90) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	487	ASP	11.6
1	C	477	CYS	11.0
1	C	358	ASP	10.5
1	C	474	ASP	7.9
1	C	476	GLU	7.6
1	C	360	GLY	7.5
1	C	356	SER	6.1
1	A	487	ASP	5.9
1	C	362	GLY	5.8
1	C	457	ASP	5.4
1	A	277	CYS	4.6
1	C	359	GLN	4.6
1	C	473	CYS	4.5
1	C	468	GLU	4.4
1	C	368	GLU	4.2
1	C	357	ASN	4.2
1	A	401	ASN	4.1
1	C	472	LYS	4.0
1	A	362	GLY	3.9
1	C	324	PRO	3.9
1	C	143	ASN	3.8
1	C	361	SER	3.6
1	A	40	THR	3.5

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	368	GLU	3.5
1	A	457	ASP	3.5
1	A	289	ASN	3.4
1	C	390	THR	3.4
1	A	468	GLU	3.4
1	A	75	LEU	3.4
1	A	263	GLY	3.4
1	A	87	GLU	3.4
1	A	372	LYS	3.2
1	B	263	GLY	3.2
1	B	360	GLY	3.1
1	C	262	ARG	3.1
1	C	466	CYS	3.1
1	A	360	GLY	3.1
1	B	113	LYS	3.1
1	C	15	ASN	3.1
1	A	386	GLU	3.0
1	C	75	LEU	3.0
1	B	491	TYR	3.0
1	C	478	MET	2.9
1	C	141	SER	2.9
1	C	475	ASP	2.9
1	C	263	GLY	2.9
1	B	358	ASP	2.9
1	C	469	PHE	2.9
1	A	485	THR	2.8
1	C	354	HIS	2.8
1	C	470	TYR	2.8
1	C	138	CYS	2.7
1	A	35	ASP	2.7
1	B	401	ASN	2.7
1	C	453	MET	2.6
1	B	262	ARG	2.6
1	B	362	GLY	2.6
1	A	15	ASN	2.6
1	A	476	GLU	2.6
1	B	368	GLU	2.5
1	C	367	LYS	2.5
1	C	8	CYS	2.5
1	B	157	GLY	2.5
1	B	395	VAL	2.5
1	C	372	LYS	2.5

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	B	483	ASN	2.5
1	C	277	CYS	2.4
1	A	143	ASN	2.4
1	C	452	ARG	2.3
1	A	70	GLU	2.3
1	A	324	PRO	2.3
1	A	188	THR	2.3
1	C	355	HIS	2.3
1	B	215	ASP	2.3
1	B	143	ASN	2.3
1	B	277	CYS	2.2
1	A	124	ASP	2.2
1	A	94	CYS	2.2
1	C	207	THR	2.2
1	C	142	GLY	2.2
1	B	197	VAL	2.2
1	A	367	LYS	2.1
1	C	159	ASN	2.1
1	B	480	SER	2.1
1	B	476	GLU	2.1
1	A	72	ASP	2.1
1	C	197	VAL	2.1
1	A	470	TYR	2.0
1	C	192	THR	2.0
1	A	359	GLN	2.0

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

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

6.3 Carbohydrates (i)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors($Å^2$)	Q<0.9
2	SIA	A	1488	20/21	0.89	0.18	0.55	80,80,80,80	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors($Å^2$)	Q<0.9
2	NAG	A	1490	14/15	0.87	0.24	-	80,80,80,80	0
2	GAL	A	1489	11/12	0.87	0.20	-	80,80,80,80	0
2	GAL	A	1491	12/12	0.68	0.44	-	80,80,80,80	0

6.4 Ligands (i)

There are no ligands in this entry.

6.5 Other polymers (i)

There are no such residues in this entry.