Full wwPDB X-ray Structure Validation Report (i)

Feb 1, 2016 – 06:21 AM GMT

PDB ID	:	2WRC
Title	:	THE STRUCTURE OF INFLUENZA H2 HUMAN SINGAPORE HEMAGGLUTININ
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	:	2009-09-01
Resolution	:	2.71 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:

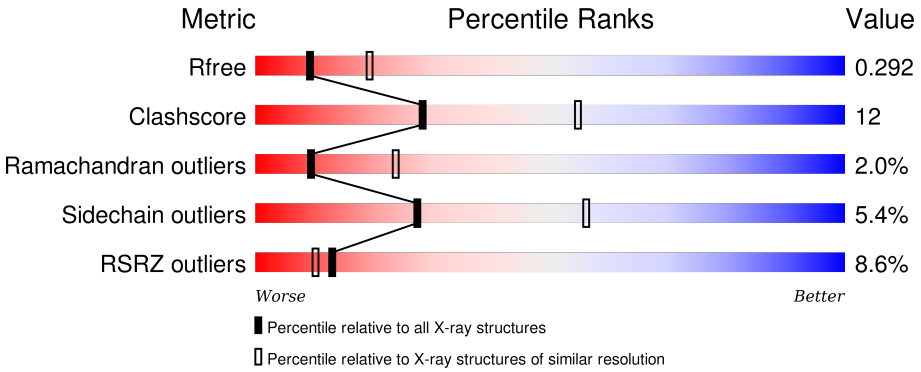
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	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 2.71 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	2103 (2.70-2.70)
Clashscore	102246	2422 (2.70-2.70)
Ramachandran outliers	100387	2382 (2.70-2.70)
Sidechain outliers	100360	2382 (2.70-2.70)
RSRZ outliers	91569	2107 (2.70-2.70)

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	9% 71% 20% 6%
1	B	506	6% 71% 21%
1	C	506	9% 68% 22% 8%

2 Entry composition (i)

There is only 1 type of molecule in this entry. The entry contains 11265 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.

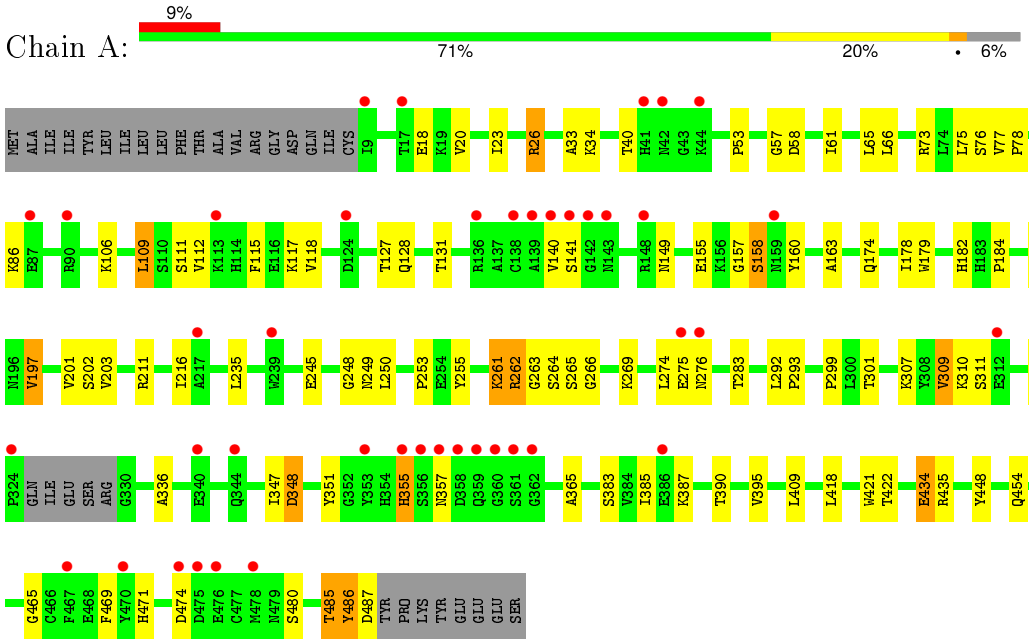
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	474	Total	C	N	O	S	0	0	0
			3736	2347	642	724	23			
1	B	486	Total	C	N	O	S	0	0	0
			3842	2413	659	746	24			
1	C	467	Total	C	N	O	S	0	0	0
			3687	2318	635	710	24			

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.

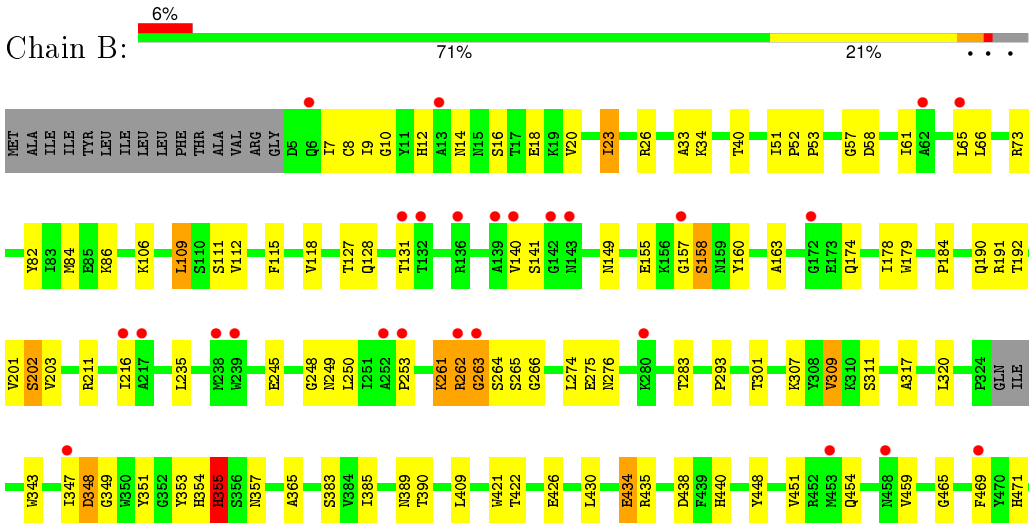
- Molecule 1: HEMAGGLUTININ

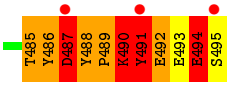
Chain A:



- Molecule 1: HEMAGGLUTININ

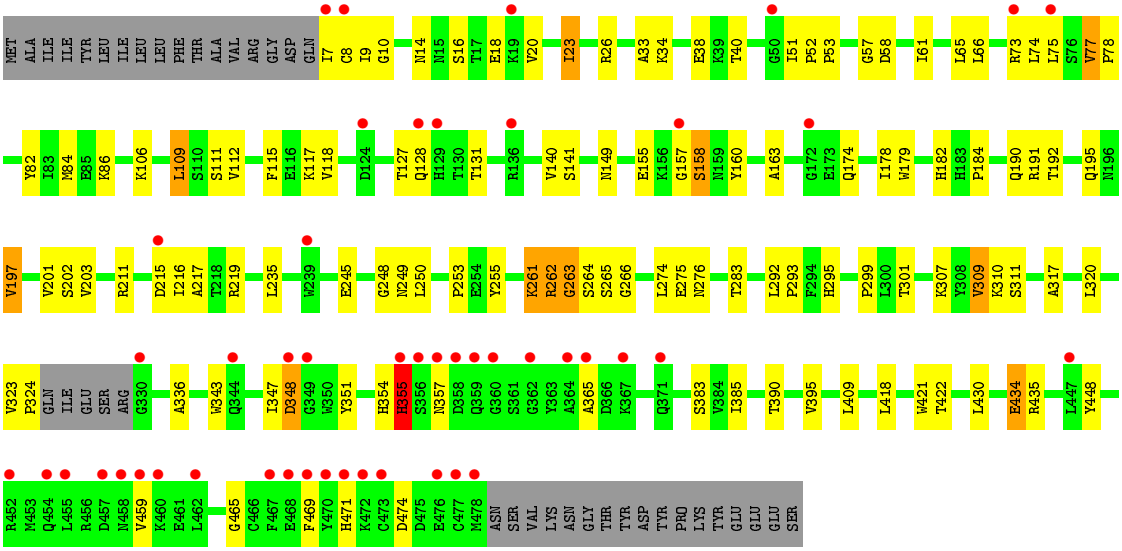
Chain B:





• 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	79.95Å 122.46Å 222.91Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	29.52 – 2.71 29.58 – 2.71	Depositor EDS
% Data completeness (in resolution range)	76.8 (29.52-2.71) 76.8 (29.58-2.71)	Depositor EDS
R_{merge}	0.16	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	7.28 (at 2.72Å)	Xtriage
Refinement program	PHENIX (PHENIX.REFINE)	Depositor
R, R_{free}	0.267 , 0.301 0.259 , 0.292	Depositor DCC
R_{free} test set	2336 reflections (5.03%)	DCC
Wilson B-factor (Å^2)	78.1	Xtriage
Anisotropy	0.005	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.30 , 51.4	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.53$, $< L^2 > = 0.37$	Xtriage
Outliers	0 of 46476 reflections	Xtriage
F_o,F_c correlation	0.91	EDS
Total number of atoms	11265	wwPDB-VP
Average B, all atoms (Å^2)	99.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.54% 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

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	0.31	0/3820	0.48	0/5169
1	B	0.35	0/3929	0.52	0/5316
1	C	0.32	0/3770	0.47	0/5100
All	All	0.33	0/11519	0.49	0/15585

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3736	0	3600	76	0
1	B	3842	0	3694	108	0
1	C	3687	0	3563	87	0
All	All	11265	0	10857	256	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 12.

All (256) 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:B:490:LYS:H	1:B:491:TYR:HB2	1.29	0.96

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:471:HIS:CE1	1:B:490:LYS:HE3	2.03	0.94
1:B:490:LYS:N	1:B:491:TYR:HB2	1.94	0.83
1:A:112:VAL:HG11	1:A:115:PHE:HB2	1.61	0.82
1:B:261:LYS:HA	1:B:262:ARG:HB2	1.59	0.82
1:C:261:LYS:HA	1:C:262:ARG:HB2	1.59	0.82
1:C:112:VAL:HG11	1:C:115:PHE:HB2	1.61	0.80
1:B:487:ASP:HA	1:B:488:TYR:HB2	1.64	0.79
1:C:261:LYS:HB2	1:C:262:ARG:HB3	1.66	0.78
1:C:8:CYS:HB2	1:C:354:HIS:HB3	1.66	0.77
1:B:157:GLY:O	1:B:158:SER:HB2	1.85	0.77
1:B:112:VAL:HG11	1:B:115:PHE:HB2	1.65	0.76
1:A:157:GLY:O	1:A:158:SER:HB2	1.86	0.76
1:A:184:PRO:HG2	1:A:190:GLN:HE21	1.51	0.76
1:A:261:LYS:HA	1:A:262:ARG:CB	2.16	0.76
1:C:184:PRO:HG2	1:C:190:GLN:HE21	1.52	0.74
1:C:261:LYS:HA	1:C:262:ARG:CB	2.16	0.74
1:A:348:ASP:HB2	1:A:365:ALA:HB3	1.68	0.74
1:B:184:PRO:HG2	1:B:190:GLN:HE21	1.51	0.73
1:C:348:ASP:HB2	1:C:365:ALA:HB3	1.69	0.73
1:B:348:ASP:HB2	1:B:365:ALA:HB3	1.69	0.73
1:B:487:ASP:CG	1:B:489:PRO:HD2	2.08	0.72
1:C:157:GLY:O	1:C:158:SER:HB2	1.85	0.72
1:B:261:LYS:HA	1:B:262:ARG:CB	2.20	0.72
1:B:111:SER:HB2	1:B:265:SER:HB3	1.71	0.72
1:B:487:ASP:OD2	1:B:489:PRO:HD2	1.89	0.71
1:B:261:LYS:HB2	1:B:262:ARG:HB3	1.74	0.70
1:A:111:SER:HB2	1:A:265:SER:HB3	1.74	0.70
1:B:491:TYR:H	1:B:492:GLU:C	1.95	0.69
1:B:493:GLU:HA	1:B:494:GLU:CB	2.23	0.68
1:B:459:VAL:HG12	1:B:469:PHE:HA	1.76	0.68
1:B:491:TYR:N	1:B:492:GLU:O	2.26	0.68
1:B:53:PRO:HG2	1:B:84:MET:HE2	1.77	0.67
1:B:8:CYS:HB2	1:B:354:HIS:HB3	1.77	0.67
1:A:53:PRO:HG2	1:A:84:MET:HE2	1.75	0.66
1:A:155:GLU:OE1	1:A:158:SER:HA	1.96	0.66
1:C:155:GLU:OE1	1:C:158:SER:HA	1.96	0.66
1:C:459:VAL:HG12	1:C:469:PHE:HA	1.77	0.66
1:A:459:VAL:HG12	1:A:469:PHE:HA	1.76	0.66
1:B:448:TYR:CE1	1:B:465:GLY:HA2	2.32	0.65
1:B:127:THR:O	1:B:128:GLN:HB2	1.95	0.65
1:A:448:TYR:CE1	1:A:465:GLY:HA2	2.30	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:7:ILE:HA	1:C:355:HIS:HA	1.79	0.65
1:C:309:VAL:HG22	1:C:422:THR:HA	1.78	0.65
1:C:111:SER:HB2	1:C:265:SER:HB3	1.76	0.65
1:C:127:THR:O	1:C:128:GLN:HB2	1.97	0.65
1:C:61:ILE:HD12	1:C:106:LYS:HD2	1.79	0.65
1:A:61:ILE:HD12	1:A:106:LYS:HD2	1.78	0.64
1:B:61:ILE:HD12	1:B:106:LYS:HD2	1.78	0.64
1:C:448:TYR:CE1	1:C:465:GLY:HA2	2.32	0.64
1:B:155:GLU:OE1	1:B:158:SER:HA	1.96	0.64
1:A:127:THR:O	1:A:128:GLN:HB2	1.97	0.64
1:B:293:PRO:HG3	1:B:385:ILE:HA	1.78	0.64
1:B:184:PRO:HG2	1:B:190:GLN:NE2	2.13	0.64
1:A:309:VAL:HG22	1:A:422:THR:HA	1.81	0.63
1:A:283:THR:HG22	1:A:301:THR:HG22	1.81	0.62
1:C:261:LYS:CA	1:C:262:ARG:CB	2.77	0.62
1:B:53:PRO:HD2	1:B:274:LEU:HD22	1.82	0.62
1:C:184:PRO:HG2	1:C:190:GLN:NE2	2.15	0.62
1:A:184:PRO:HG2	1:A:190:GLN:NE2	2.13	0.62
1:A:261:LYS:CA	1:A:262:ARG:CB	2.77	0.62
1:C:53:PRO:HD2	1:C:274:LEU:HD22	1.81	0.62
1:B:487:ASP:HA	1:B:488:TYR:CB	2.29	0.62
1:A:323:VAL:HG21	1:A:336:ALA:HB2	1.81	0.61
1:A:77:VAL:HG12	1:A:78:PRO:HD2	1.83	0.60
1:B:53:PRO:HG2	1:B:84:MET:CE	2.30	0.60
1:B:490:LYS:CA	1:B:491:TYR:HB2	2.31	0.60
1:A:53:PRO:HD2	1:A:274:LEU:HD22	1.82	0.60
1:C:283:THR:HG22	1:C:301:THR:HG22	1.83	0.60
1:A:178:ILE:O	1:A:253:PRO:HG3	2.01	0.60
1:C:53:PRO:HG2	1:C:84:MET:HE2	1.84	0.60
1:C:261:LYS:CB	1:C:262:ARG:HB3	2.31	0.60
1:C:77:VAL:HG12	1:C:78:PRO:HD2	1.82	0.60
1:C:262:ARG:HG3	1:C:263:GLY:N	2.17	0.59
1:C:293:PRO:HG3	1:C:385:ILE:HA	1.85	0.59
1:A:293:PRO:HG3	1:A:385:ILE:HA	1.83	0.59
1:C:178:ILE:O	1:C:253:PRO:HG3	2.03	0.59
1:A:53:PRO:HG2	1:A:84:MET:CE	2.33	0.58
1:A:320:LEU:H	1:A:320:LEU:HD23	1.68	0.58
1:B:261:LYS:CA	1:B:262:ARG:CB	2.81	0.58
1:C:320:LEU:HD23	1:C:320:LEU:H	1.69	0.58
1:B:309:VAL:HG22	1:B:422:THR:HA	1.85	0.58
1:B:178:ILE:O	1:B:253:PRO:HG3	2.04	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:283:THR:HG22	1:B:301:THR:HG22	1.86	0.57
1:B:77:VAL:HG12	1:B:78:PRO:HD2	1.85	0.57
1:A:435:ARG:NH1	1:B:435:ARG:HH11	2.02	0.57
1:A:309:VAL:HG13	1:A:311:SER:H	1.70	0.57
1:B:320:LEU:HD23	1:B:320:LEU:H	1.70	0.56
1:C:309:VAL:HG13	1:C:311:SER:H	1.71	0.56
1:C:53:PRO:HG2	1:C:84:MET:CE	2.36	0.56
1:B:7:ILE:HA	1:B:355:HIS:HA	1.88	0.56
1:B:348:ASP:HB2	1:B:365:ALA:CB	2.36	0.56
1:B:493:GLU:HA	1:B:494:GLU:HB2	1.87	0.56
1:B:211:ARG:NH1	1:C:216:ILE:O	2.39	0.55
1:A:480:SER:HB2	1:A:485:THR:HB	1.89	0.55
1:B:84:MET:HE1	1:B:274:LEU:HB2	1.88	0.55
1:A:84:MET:HE1	1:A:274:LEU:HB2	1.90	0.54
1:B:8:CYS:O	1:B:353:TYR:HA	2.07	0.54
1:C:309:VAL:CG2	1:C:422:THR:HA	2.38	0.54
1:A:191:ARG:NH2	1:A:197:VAL:HG21	2.23	0.54
1:B:309:VAL:HG13	1:B:311:SER:H	1.71	0.54
1:C:84:MET:HE1	1:C:274:LEU:HB2	1.89	0.54
1:C:348:ASP:HB2	1:C:365:ALA:CB	2.38	0.54
1:B:265:SER:OG	1:B:266:GLY:N	2.42	0.53
1:B:480:SER:HB2	1:B:485:THR:HB	1.90	0.53
1:A:434:GLU:CD	1:C:435:ARG:HH21	2.10	0.53
1:A:480:SER:HB2	1:A:486:TYR:H	1.74	0.53
1:B:480:SER:HB2	1:B:486:TYR:H	1.73	0.53
1:B:488:TYR:HB3	1:B:489:PRO:CD	2.39	0.53
1:B:9:ILE:HD11	1:B:451:VAL:HG21	1.92	0.52
1:C:53:PRO:HG3	1:C:82:TYR:CZ	2.44	0.52
1:B:191:ARG:NH2	1:B:197:VAL:HG21	2.25	0.52
1:C:310:LYS:HG3	1:C:418:LEU:HD21	1.91	0.52
1:C:323:VAL:HG21	1:C:336:ALA:HB2	1.91	0.52
1:A:348:ASP:HB2	1:A:365:ALA:CB	2.36	0.51
1:C:191:ARG:NH2	1:C:197:VAL:HG21	2.24	0.51
1:B:12:HIS:HB2	1:B:349:GLY:O	2.10	0.51
1:A:18:GLU:HG2	1:A:33:ALA:HB3	1.93	0.51
1:A:53:PRO:HG3	1:A:82:TYR:CZ	2.45	0.51
1:B:489:PRO:O	1:B:490:LYS:CB	2.58	0.51
1:C:201:VAL:HG22	1:C:250:LEU:HB2	1.93	0.51
1:C:179:TRP:CE2	1:C:203:VAL:HG21	2.46	0.51
1:B:490:LYS:CA	1:B:491:TYR:CB	2.89	0.50
1:B:53:PRO:HG3	1:B:82:TYR:CZ	2.46	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:265:SER:OG	1:C:266:GLY:N	2.45	0.50
1:A:448:TYR:HE1	1:A:465:GLY:HA2	1.76	0.50
1:A:309:VAL:CG2	1:A:422:THR:HA	2.41	0.50
1:A:211:ARG:NH1	1:B:216:ILE:O	2.44	0.50
1:A:216:ILE:O	1:C:211:ARG:NH1	2.44	0.50
1:B:10:GLY:HA3	1:B:343:TRP:CH2	2.46	0.50
1:B:435:ARG:NH1	1:C:435:ARG:HH11	2.09	0.50
1:B:174:GLN:OE1	1:B:235:LEU:HD13	2.11	0.49
1:B:51:ILE:CD1	1:B:262:ARG:HH22	2.25	0.49
1:A:65:LEU:HD11	1:A:109:LEU:HD21	1.95	0.49
1:B:489:PRO:O	1:B:490:LYS:HB3	2.12	0.49
1:B:261:LYS:CB	1:B:262:ARG:HB3	2.41	0.49
1:A:111:SER:HB2	1:A:265:SER:CB	2.41	0.49
1:A:265:SER:OG	1:A:266:GLY:N	2.44	0.49
1:B:201:VAL:HG22	1:B:250:LEU:HB2	1.94	0.49
1:A:179:TRP:CE2	1:A:203:VAL:HG21	2.48	0.49
1:C:307:LYS:HG2	1:C:421:TRP:CE2	2.48	0.49
1:B:111:SER:HB2	1:B:265:SER:CB	2.41	0.49
1:C:65:LEU:HD11	1:C:109:LEU:HD21	1.93	0.49
1:B:65:LEU:HD11	1:B:109:LEU:HD21	1.94	0.49
1:B:140:VAL:O	1:B:141:SER:HB2	2.13	0.48
1:C:357:ASN:HD21	1:C:474:ASP:HA	1.78	0.48
1:B:66:LEU:O	1:B:149:ASN:HB2	2.14	0.48
1:B:23:ILE:HG12	1:B:430:LEU:HB3	1.96	0.48
1:B:320:LEU:HB3	1:B:440:HIS:CG	2.48	0.48
1:A:174:GLN:OE1	1:A:235:LEU:HD13	2.14	0.48
1:A:435:ARG:HH11	1:C:435:ARG:NH1	2.12	0.48
1:B:179:TRP:CE2	1:B:203:VAL:HG21	2.48	0.48
1:B:448:TYR:HE1	1:B:465:GLY:HA2	1.77	0.47
1:A:357:ASN:HD21	1:A:474:ASP:HA	1.79	0.47
1:A:310:LYS:HG3	1:A:418:LEU:HD21	1.97	0.47
1:A:248:GLY:C	1:A:249:ASN:HD22	2.18	0.47
1:C:248:GLY:C	1:C:249:ASN:HD22	2.17	0.47
1:C:174:GLN:OE1	1:C:235:LEU:HD13	2.14	0.47
1:C:20:VAL:HG21	1:C:317:ALA:HB2	1.97	0.47
1:C:111:SER:HB2	1:C:265:SER:CB	2.42	0.47
1:C:18:GLU:HG2	1:C:33:ALA:HB3	1.97	0.47
1:B:18:GLU:HG2	1:B:33:ALA:HB3	1.97	0.46
1:B:435:ARG:HH21	1:C:434:GLU:CD	2.18	0.46
1:B:409:LEU:HD23	1:B:409:LEU:O	2.15	0.46
1:B:163:ALA:O	1:B:245:GLU:HA	2.14	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:299:PRO:O	1:C:395:VAL:HG11	2.14	0.46
1:A:435:ARG:HH21	1:B:434:GLU:CD	2.18	0.46
1:B:357:ASN:HD21	1:B:474:ASP:HA	1.79	0.46
1:B:20:VAL:HG21	1:B:317:ALA:HB2	1.97	0.46
1:A:163:ALA:O	1:A:245:GLU:HA	2.14	0.46
1:B:248:GLY:O	1:B:249:ASN:HB2	2.16	0.46
1:B:383:SER:OG	1:C:26:ARG:NH2	2.48	0.46
1:A:20:VAL:HG21	1:A:317:ALA:HB2	1.96	0.46
1:B:51:ILE:HD13	1:B:262:ARG:HH22	1.82	0.45
1:C:182:HIS:O	1:C:184:PRO:HD3	2.16	0.45
1:C:66:LEU:O	1:C:149:ASN:HB2	2.15	0.45
1:B:488:TYR:O	1:B:490:LYS:N	2.49	0.45
1:C:23:ILE:HG12	1:C:430:LEU:HB3	1.98	0.45
1:C:57:GLY:O	1:C:86:LYS:HG3	2.17	0.45
1:C:155:GLU:OE1	1:C:195:GLN:HG2	2.16	0.45
1:A:201:VAL:HG22	1:A:250:LEU:HB2	1.99	0.45
1:C:163:ALA:O	1:C:245:GLU:HA	2.15	0.45
1:B:490:LYS:HD2	1:B:490:LYS:O	2.16	0.45
1:B:491:TYR:N	1:B:492:GLU:C	2.65	0.45
1:C:248:GLY:O	1:C:249:ASN:HB2	2.16	0.45
1:A:140:VAL:O	1:A:141:SER:HB2	2.16	0.45
1:B:275:GLU:O	1:B:276:ASN:HB3	2.17	0.44
1:B:74:LEU:HA	1:B:74:LEU:HD23	1.86	0.44
1:A:157:GLY:O	1:A:158:SER:CB	2.61	0.44
1:B:454:GLN:NE2	1:B:486:TYR:HB3	2.31	0.44
1:B:262:ARG:CG	1:B:263:GLY:N	2.80	0.44
1:B:160:TYR:CZ	1:B:248:GLY:HA2	2.51	0.44
1:A:57:GLY:O	1:A:86:LYS:HG3	2.18	0.44
1:A:292:LEU:HA	1:A:293:PRO:HD3	1.87	0.44
1:B:248:GLY:C	1:B:249:ASN:HD22	2.20	0.44
1:C:8:CYS:C	1:C:9:ILE:HD12	2.38	0.44
1:A:307:LYS:HG2	1:A:421:TRP:CE2	2.53	0.44
1:A:155:GLU:OE1	1:A:195:GLN:HG2	2.18	0.43
1:C:160:TYR:CZ	1:C:248:GLY:HA2	2.53	0.43
1:A:387:LYS:HD2	1:B:426:GLU:HB3	1.99	0.43
1:A:276:ASN:CG	1:A:276:ASN:O	2.57	0.43
1:B:487:ASP:OD1	1:B:487:ASP:C	2.56	0.43
1:A:182:HIS:O	1:A:184:PRO:HD3	2.18	0.43
1:C:77:VAL:HG12	1:C:78:PRO:CD	2.49	0.43
1:C:292:LEU:HA	1:C:293:PRO:HD3	1.86	0.43
1:A:275:GLU:O	1:A:276:ASN:HB3	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:307:LYS:HG2	1:B:421:TRP:CE2	2.54	0.43
1:B:487:ASP:CA	1:B:488:TYR:CB	2.96	0.43
1:C:14:ASN:OD1	1:C:16:SER:HB3	2.19	0.42
1:A:409:LEU:HD23	1:A:409:LEU:O	2.19	0.42
1:B:14:ASN:OD1	1:B:16:SER:HB3	2.19	0.42
1:B:488:TYR:HB3	1:B:489:PRO:HD2	2.00	0.42
1:C:307:LYS:HG2	1:C:421:TRP:CD2	2.54	0.42
1:C:140:VAL:O	1:C:141:SER:HB2	2.19	0.42
1:C:53:PRO:HG3	1:C:82:TYR:CE2	2.54	0.42
1:B:235:LEU:HA	1:B:235:LEU:HD23	1.90	0.42
1:A:160:TYR:CZ	1:A:248:GLY:HA2	2.54	0.42
1:C:157:GLY:O	1:C:158:SER:CB	2.61	0.42
1:A:307:LYS:HG2	1:A:421:TRP:CD2	2.55	0.42
1:C:74:LEU:HA	1:C:74:LEU:HD23	1.85	0.42
1:A:66:LEU:O	1:A:149:ASN:HB2	2.19	0.42
1:B:51:ILE:HA	1:B:52:PRO:HD3	1.83	0.42
1:A:26:ARG:NH2	1:C:383:SER:OG	2.53	0.42
1:B:276:ASN:CG	1:B:276:ASN:O	2.59	0.42
1:C:38:GLU:O	1:C:295:HIS:HA	2.20	0.42
1:C:51:ILE:HA	1:C:52:PRO:HD3	1.82	0.41
1:B:490:LYS:N	1:B:491:TYR:CB	2.75	0.41
1:C:261:LYS:CA	1:C:262:ARG:HB3	2.48	0.41
1:B:155:GLU:OE1	1:B:195:GLN:HG2	2.20	0.41
1:A:320:LEU:HD23	1:A:320:LEU:N	2.35	0.41
1:A:53:PRO:HG3	1:A:82:TYR:CE2	2.55	0.41
1:A:383:SER:OG	1:B:26:ARG:NH2	2.52	0.41
1:B:493:GLU:CB	1:B:495:SER:O	2.68	0.41
1:C:215:ASP:O	1:C:219:ARG:NH2	2.53	0.41
1:A:117:LYS:HD3	1:A:255:TYR:CD2	2.55	0.41
1:C:275:GLU:O	1:C:276:ASN:HB3	2.20	0.41
1:A:77:VAL:HG12	1:A:78:PRO:CD	2.49	0.41
1:A:248:GLY:O	1:A:249:ASN:HB2	2.21	0.41
1:B:202:SER:OG	1:C:217:ALA:HB2	2.21	0.41
1:C:323:VAL:HA	1:C:324:PRO:HD3	1.84	0.41
1:B:65:LEU:HD11	1:B:109:LEU:CD2	2.51	0.41
1:C:409:LEU:O	1:C:409:LEU:HD23	2.21	0.41
1:B:487:ASP:OD2	1:B:489:PRO:CD	2.64	0.41
1:C:469:PHE:HB3	1:C:471:HIS:O	2.20	0.41
1:A:469:PHE:HB3	1:A:471:HIS:O	2.21	0.41
1:C:448:TYR:HE1	1:C:465:GLY:HA2	1.78	0.41
1:B:389:ASN:HD21	1:C:310:LYS:NZ	2.18	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:117:LYS:HD3	1:A:255:TYR:CG	2.56	0.40
1:B:57:GLY:O	1:B:86:LYS:HG3	2.21	0.40
1:C:276:ASN:CG	1:C:276:ASN:O	2.59	0.40
1:A:454:GLN:NE2	1:A:486:TYR:HB3	2.36	0.40
1:A:299:PRO:O	1:A:395:VAL:HG11	2.21	0.40
1:B:331:LEU:HD22	1:B:438:ASP:OD2	2.21	0.40
1:C:117:LYS:HD3	1:C:255:TYR:CD2	2.56	0.40
1:A:85:GLU:O	1:A:269:LYS:HA	2.21	0.40
1:C:10:GLY:N	1:C:343:TRP:CH2	2.89	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	470/506 (93%)	439 (93%)	23 (5%)	8 (2%)	11 29
1	B	482/506 (95%)	444 (92%)	23 (5%)	15 (3%)	5 12
1	C	463/506 (92%)	434 (94%)	24 (5%)	5 (1%)	17 42
All	All	1415/1518 (93%)	1317 (93%)	70 (5%)	28 (2%)	9 24

All (28) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	262	ARG
1	A	485	THR
1	A	486	TYR
1	B	262	ARG
1	B	485	THR
1	B	486	TYR
1	B	488	TYR
1	B	490	LYS

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Mol	Chain	Res	Type
1	B	491	TYR
1	C	262	ARG
1	A	158	SER
1	B	158	SER
1	B	487	ASP
1	B	492	GLU
1	C	158	SER
1	A	263	GLY
1	B	263	GLY
1	B	489	PRO
1	C	263	GLY
1	C	264	SER
1	A	264	SER
1	B	264	SER
1	A	355	HIS
1	B	355	HIS
1	C	355	HIS
1	A	76	SER
1	B	76	SER
1	B	494	GLU

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	412/443 (93%)	390 (95%)	22 (5%)	28 57
1	B	424/443 (96%)	400 (94%)	24 (6%)	25 53
1	C	407/443 (92%)	386 (95%)	21 (5%)	29 58
All	All	1243/1329 (94%)	1176 (95%)	67 (5%)	27 56

All (67) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	23	ILE
1	A	26	ARG

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Mol	Chain	Res	Type
1	A	34	LYS
1	A	40	THR
1	A	58	ASP
1	A	73	ARG
1	A	75	LEU
1	A	109	LEU
1	A	118	VAL
1	A	131	THR
1	A	192	THR
1	A	197	VAL
1	A	202	SER
1	A	261	LYS
1	A	309	VAL
1	A	347	ILE
1	A	348	ASP
1	A	351	TYR
1	A	355	HIS
1	A	390	THR
1	A	434	GLU
1	A	487	ASP
1	B	23	ILE
1	B	34	LYS
1	B	40	THR
1	B	58	ASP
1	B	73	ARG
1	B	75	LEU
1	B	109	LEU
1	B	118	VAL
1	B	131	THR
1	B	192	THR
1	B	197	VAL
1	B	202	SER
1	B	261	LYS
1	B	309	VAL
1	B	347	ILE
1	B	348	ASP
1	B	351	TYR
1	B	355	HIS
1	B	390	THR
1	B	434	GLU
1	B	487	ASP
1	B	490	LYS

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Mol	Chain	Res	Type
1	B	491	TYR
1	B	494	GLU
1	C	23	ILE
1	C	34	LYS
1	C	40	THR
1	C	58	ASP
1	C	73	ARG
1	C	75	LEU
1	C	77	VAL
1	C	109	LEU
1	C	118	VAL
1	C	131	THR
1	C	192	THR
1	C	197	VAL
1	C	202	SER
1	C	261	LYS
1	C	309	VAL
1	C	347	ILE
1	C	348	ASP
1	C	351	TYR
1	C	355	HIS
1	C	390	THR
1	C	434	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (22) such sidechains are listed below:

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

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Mol	Chain	Res	Type
1	C	49	ASN
1	C	129	HIS
1	C	190	GLN
1	C	249	ASN
1	C	389	ASN
1	C	391	GLN
1	C	458	ASN

5.3.3 RNA

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains

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

5.5 Carbohydrates

There are no carbohydrates in this entry.

5.6 Ligand geometry

There are no ligands in this entry.

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
1	A	474/506 (93%)	0.57	45 (9%) 10 8	53, 102, 156, 202	0
1	B	486/506 (96%)	0.37	30 (6%) 24 23	48, 81, 126, 181	0
1	C	467/506 (92%)	0.60	48 (10%) 9 6	54, 100, 178, 279	0
All	All	1427/1518 (94%)	0.51	123 (8%) 13 10	48, 94, 156, 279	0

All (123) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	470	TYR	6.7
1	C	470	TYR	6.6
1	C	362	GLY	6.6
1	A	136	ARG	5.7
1	C	367	LYS	5.6
1	C	360	GLY	5.4
1	A	44	LYS	5.2
1	C	349	GLY	5.2
1	A	359	GLN	5.1
1	C	356	SER	4.9
1	C	469	PHE	4.6
1	A	361	SER	4.5
1	A	358	ASP	4.4
1	C	7	ILE	4.4
1	C	458	ASN	4.3
1	C	239	TRP	4.3
1	B	458	ASN	4.2
1	A	143	ASN	4.2
1	C	478	MET	4.2
1	A	360	GLY	4.1
1	C	471	HIS	4.0
1	C	355	HIS	4.0
1	A	113	LYS	4.0

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Mol	Chain	Res	Type	RSRZ
1	B	491	TYR	4.0
1	C	472	LYS	4.0
1	C	477	CYS	4.0
1	A	17	THR	3.9
1	A	276	ASN	3.9
1	B	453	MET	3.8
1	C	473	CYS	3.7
1	A	9	ILE	3.7
1	C	364	ALA	3.7
1	B	157	GLY	3.6
1	C	73	ARG	3.6
1	C	365	ALA	3.5
1	B	252	ALA	3.5
1	A	386	GLU	3.5
1	A	140	VAL	3.4
1	B	469	PHE	3.4
1	C	124	ASP	3.4
1	A	159	ASN	3.4
1	C	457	ASP	3.4
1	C	462	LEU	3.4
1	A	142	GLY	3.4
1	C	75	LEU	3.4
1	A	195	GLN	3.3
1	C	359	GLN	3.3
1	A	90	ARG	3.2
1	A	139	ALA	3.2
1	A	239	TRP	3.2
1	C	460	LYS	3.2
1	A	340	GLU	3.2
1	A	344	GLN	3.2
1	C	172	GLY	3.2
1	B	216	ILE	3.2
1	A	138	CYS	3.1
1	A	217	ALA	3.0
1	C	136	ARG	3.0
1	A	124	ASP	3.0
1	C	459	VAL	3.0
1	C	330	GLY	2.9
1	B	487	ASP	2.9
1	B	136	ARG	2.9
1	A	148	ARG	2.9
1	A	467	PHE	2.8

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Mol	Chain	Res	Type	RSRZ
1	A	324	PRO	2.8
1	C	468	GLU	2.8
1	A	462	LEU	2.8
1	A	362	GLY	2.8
1	A	353	TYR	2.7
1	B	495	SER	2.7
1	C	467	PHE	2.7
1	C	454	GLN	2.6
1	C	50	GLY	2.6
1	C	476	GLU	2.6
1	C	358	ASP	2.6
1	A	312	GLU	2.5
1	B	65	LEU	2.5
1	C	344	GLN	2.5
1	C	455	LEU	2.4
1	B	280	LYS	2.4
1	C	215	ASP	2.4
1	A	41	HIS	2.4
1	C	129	HIS	2.4
1	A	356	SER	2.4
1	A	475	ASP	2.4
1	C	128	GLN	2.4
1	A	460	LYS	2.3
1	B	131	THR	2.3
1	B	6	GLN	2.3
1	C	348	ASP	2.3
1	B	62	ALA	2.3
1	B	139	ALA	2.3
1	B	13	ALA	2.3
1	B	239	TRP	2.3
1	C	19	LYS	2.2
1	B	253	PRO	2.2
1	A	141	SER	2.2
1	B	143	ASN	2.2
1	B	238	MET	2.2
1	C	452	ARG	2.2
1	A	275	GLU	2.2
1	C	157	GLY	2.2
1	A	355	HIS	2.2
1	B	347	ILE	2.1
1	B	132	THR	2.1
1	A	357	ASN	2.1

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Mol	Chain	Res	Type	RSRZ
1	B	140	VAL	2.1
1	B	217	ALA	2.1
1	B	142	GLY	2.1
1	C	371	GLN	2.1
1	A	474	ASP	2.1
1	C	357	ASN	2.1
1	B	262	ARG	2.1
1	A	476	GLU	2.1
1	C	8	CYS	2.1
1	C	447	LEU	2.0
1	B	263	GLY	2.0
1	A	478	MET	2.0
1	B	479	ASN	2.0
1	B	172	GLY	2.0
1	A	42	ASN	2.0
1	A	87	GLU	2.0

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

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

6.3 Carbohydrates (i)

There are no carbohydrates in this entry.

6.4 Ligands (i)

There are no ligands in this entry.

6.5 Other polymers (i)

There are no such residues in this entry.