Full wwPDB X-ray Structure Validation Report ⓘ

Jan 31, 2016 – 07:50 PM GMT

PDB ID	:	1HIN
Title	:	STRUCTURAL EVIDENCE FOR INDUCED FIT AS A MECHANISM FOR ANTIBODY-ANTIGEN RECOGNITION
Authors	:	Rini, J.M.; Wilson, I.A.
Deposited on	:	1992-07-08
Resolution	:	3.10 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 ⓘ symbol.

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

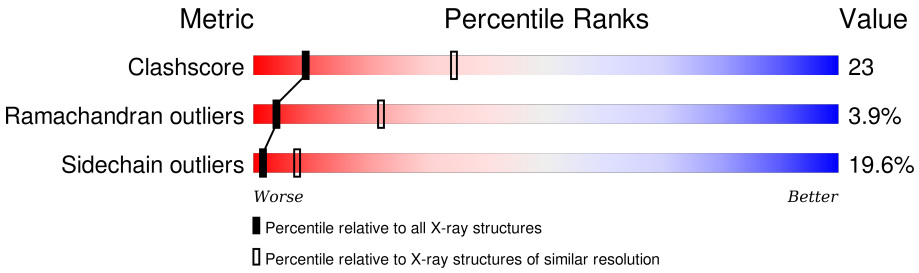
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
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 3.10 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))
Clashscore	102246	1222 (3.14-3.06)
Ramachandran outliers	100387	1174 (3.14-3.06)
Sidechain outliers	100360	1174 (3.14-3.06)

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.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	L	217	43% 43% 11% ·
2	H	220	40% 44% 13% ·
3	P	8	50% 13% 25% 13%

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 3432 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 IGG2A-KAPPA 17/9 FAB (LIGHT CHAIN).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	L	217	Total	C	N	O	S	0	0	0
			1680	1047	279	347	7			

- Molecule 2 is a protein called IGG2A-KAPPA 17/9 FAB (HEAVY CHAIN).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	H	220	Total	C	N	O	S	0	0	0
			1664	1047	276	333	8			

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
H	227	PRO	-	INSERTION	GB 533229

- Molecule 3 is a protein called INFLUENZA HEMAGGLUTININ HA1 (STRAIN X47) (RESIDUES 100-107).

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
3	P	8	Total	C	N	O	0	0	0
			66	42	8	16			

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	H	11	Total	O	0	0
			11	11		
4	L	11	Total	O	0	0
			11	11		

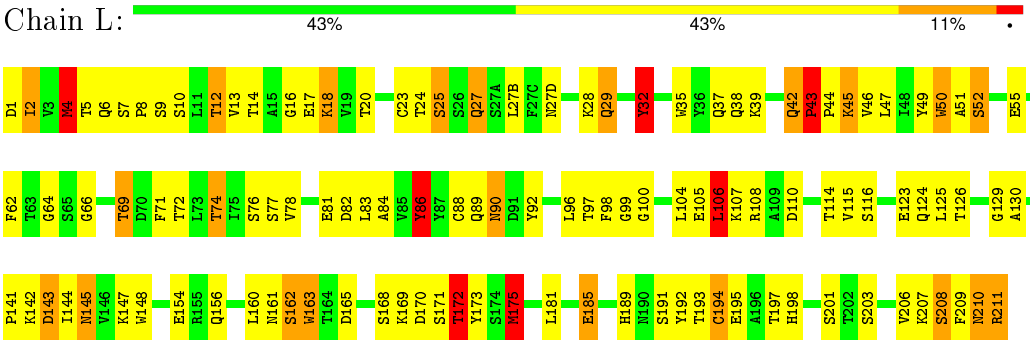
3 Residue-property plots (i)

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.

Note EDS was not executed.

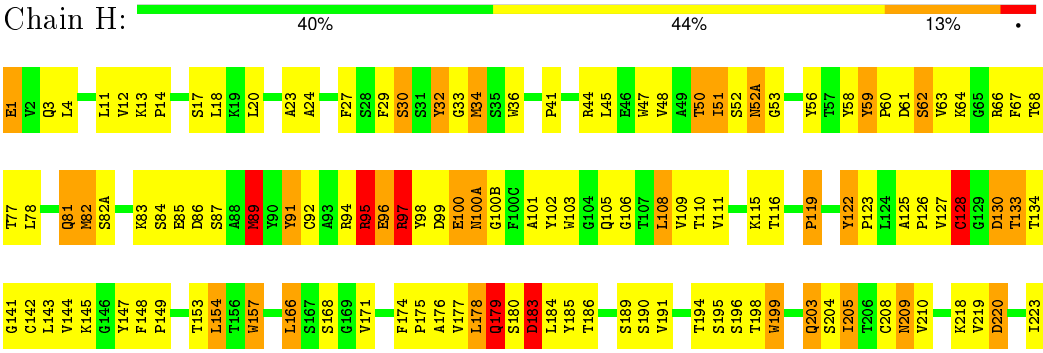
- Molecule 1: IGG2A-KAPPA 17/9 FAB (LIGHT CHAIN)

Chain L:



- Molecule 2: IGG2A-KAPPA 17/9 FAB (HEAVY CHAIN)

Chain H:



- Molecule 3: INFLUENZA HEMAGGLUTININ HA1 (STRAIN X47) (RESIDUES 100-107)

Chain P:

4 Data and refinement statistics (i)

Xtriage (Phenix) and EDS were not executed - this section will therefore be incomplete.

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	63.50Å 73.40Å 62.70Å 90.00° 117.10° 90.00°	Depositor
Resolution (Å)	8.00 – 3.10	Depositor
% Data completeness (in resolution range)	(Not available) (8.00-3.10)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	X-PLOR	Depositor
R, R_{free}	0.220 , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	3432	wwPDB-VP
Average B, all atoms (Å^2)	11.0	wwPDB-VP

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	L	1.02	2/1718 (0.1%)	1.84	41/2334 (1.8%)
2	H	1.07	2/1705 (0.1%)	1.98	48/2322 (2.1%)
3	P	1.20	0/68	2.27	4/92 (4.3%)
All	All	1.05	4/3491 (0.1%)	1.92	93/4748 (2.0%)

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
1	L	0	2
2	H	0	1
All	All	0	3

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	H	100	GLU	CD-OE2	-6.93	1.18	1.25
1	L	81	GLU	CB-CG	5.99	1.63	1.52
2	H	100	GLU	CD-OE1	-5.63	1.19	1.25
1	L	27	GLN	CA-CB	-5.05	1.42	1.53

All (93) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	L	211	ARG	NE-CZ-NH1	12.81	126.71	120.30
2	H	97	ARG	NE-CZ-NH1	12.48	126.54	120.30
3	P	101	ASP	CB-CG-OD1	-10.94	108.46	118.30
2	H	102	TYR	CB-CG-CD2	-9.89	115.06	121.00
2	H	157	TRP	CD1-CG-CD2	9.76	114.11	106.30
3	P	101	ASP	CB-CG-OD2	9.76	127.08	118.30
2	H	32	TYR	CB-CG-CD1	-9.76	115.15	121.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	H	59	TYR	CB-CG-CD1	-9.23	115.46	121.00
1	L	50	TRP	CD1-CG-CD2	8.90	113.42	106.30
1	L	175	MET	CG-SD-CE	-8.83	86.08	100.20
2	H	95	ARG	CD-NE-CZ	-8.76	111.34	123.60
2	H	199	TRP	CD1-CG-CD2	8.70	113.26	106.30
2	H	122	TYR	CB-CG-CD2	-8.45	115.93	121.00
1	L	148	TRP	CD1-CG-CD2	8.43	113.04	106.30
1	L	45	LYS	CA-CB-CG	8.02	131.05	113.40
2	H	178	LEU	CA-CB-CG	7.96	133.62	115.30
1	L	148	TRP	CE2-CD2-CG	-7.93	100.95	107.30
2	H	97	ARG	NE-CZ-NH2	-7.93	116.34	120.30
1	L	50	TRP	CE2-CD2-CG	-7.88	101.00	107.30
2	H	228	ARG	NE-CZ-NH1	7.86	124.23	120.30
2	H	157	TRP	CE2-CD2-CG	-7.68	101.16	107.30
1	L	163	TRP	CD1-CG-CD2	7.68	112.44	106.30
2	H	94	ARG	NE-CZ-NH1	-7.60	116.50	120.30
1	L	106	LEU	CA-CB-CG	7.50	132.54	115.30
1	L	211	ARG	NE-CZ-NH2	-7.49	116.56	120.30
2	H	47	TRP	CD1-CG-CD2	7.44	112.25	106.30
2	H	228	ARG	CA-CB-CG	7.39	129.65	113.40
2	H	199	TRP	CE2-CD2-CG	-7.35	101.42	107.30
3	P	101	ASP	CA-CB-CG	-7.26	97.44	113.40
1	L	50	TRP	CG-CD1-NE1	-7.07	103.03	110.10
1	L	69	THR	N-CA-CB	-7.06	96.89	110.30
2	H	44	ARG	NE-CZ-NH2	-6.98	116.81	120.30
2	H	179	GLN	CA-CB-CG	6.98	128.76	113.40
2	H	103	TRP	CD1-CG-CD2	6.93	111.85	106.30
2	H	91	TYR	CB-CG-CD1	-6.88	116.87	121.00
2	H	32	TYR	CB-CG-CD2	6.80	125.08	121.00
1	L	145	ASN	CB-CG-ND2	6.71	132.80	116.70
2	H	95	ARG	NH1-CZ-NH2	-6.71	112.02	119.40
1	L	35	TRP	CD1-CG-CD2	6.67	111.64	106.30
2	H	47	TRP	CE2-CD2-CG	-6.63	101.99	107.30
1	L	192	TYR	CB-CG-CD1	-6.62	117.03	121.00
2	H	36	TRP	CD1-CG-CD2	6.62	111.59	106.30
1	L	52	SER	N-CA-CB	-6.59	100.62	110.50
1	L	25	SER	N-CA-CB	-6.55	100.67	110.50
2	H	71	ARG	NE-CZ-NH2	-6.42	117.09	120.30
2	H	157	TRP	CG-CD1-NE1	-6.34	103.76	110.10
2	H	142	CYS	CA-CB-SG	6.33	125.39	114.00
1	L	173	TYR	CB-CG-CD1	-6.30	117.22	121.00
1	L	208	SER	CA-CB-OG	6.29	128.17	111.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	H	34	MET	CG-SD-CE	-6.23	90.24	100.20
2	H	127	VAL	CA-C-N	-6.16	103.64	117.20
2	H	103	TRP	CE2-CD2-CG	-6.13	102.40	107.30
1	L	4	MET	CG-SD-CE	-6.04	90.54	100.20
1	L	145	ASN	OD1-CG-ND2	-6.03	108.03	121.90
1	L	43	PRO	CA-N-CD	-5.99	103.11	111.50
2	H	228	ARG	CG-CD-NE	5.97	124.34	111.80
1	L	163	TRP	CE2-CD2-CG	-5.97	102.52	107.30
1	L	32	TYR	CB-CG-CD1	-5.97	117.42	121.00
2	H	127	VAL	C-N-CA	5.92	136.51	121.70
2	H	96	GLU	CA-C-N	-5.89	104.24	117.20
2	H	47	TRP	CG-CD1-NE1	-5.86	104.24	110.10
1	L	147	LYS	CB-CG-CD	-5.84	96.42	111.60
2	H	178	LEU	CB-CG-CD2	-5.83	101.08	111.00
2	H	100	GLU	CA-CB-CG	-5.81	100.62	113.40
2	H	220	ASP	CB-CG-OD1	5.80	123.52	118.30
2	H	36	TRP	CE2-CD2-CG	-5.77	102.68	107.30
1	L	35	TRP	CE2-CD2-CG	-5.76	102.69	107.30
1	L	14	THR	O-C-N	-5.75	113.49	122.70
2	H	50	THR	CA-CB-CG2	5.75	120.45	112.40
2	H	128	CYS	N-CA-CB	-5.74	100.26	110.60
2	H	203	GLN	CA-CB-CG	5.70	125.93	113.40
2	H	226	GLU	CA-CB-CG	5.64	125.81	113.40
1	L	194	CYS	CA-CB-SG	5.61	124.09	114.00
1	L	35	TRP	CG-CD1-NE1	-5.58	104.52	110.10
1	L	148	TRP	CG-CD1-NE1	-5.51	104.59	110.10
1	L	143	ASP	CA-CB-CG	5.48	125.45	113.40
1	L	172	THR	OG1-CB-CG2	5.47	122.59	110.00
1	L	81	GLU	CB-CG-CD	5.47	128.97	114.20
1	L	50	TRP	CG-CD2-CE3	5.45	138.81	133.90
1	L	81	GLU	CA-CB-CG	5.42	125.31	113.40
1	L	86	TYR	CB-CG-CD2	-5.34	117.80	121.00
2	H	199	TRP	CG-CD1-NE1	-5.33	104.77	110.10
1	L	163	TRP	CG-CD1-NE1	-5.24	104.86	110.10
1	L	172	THR	N-CA-CB	-5.20	100.41	110.30
2	H	183	ASP	CA-CB-CG	5.17	124.78	113.40
2	H	89	MET	CG-SD-CE	5.12	108.39	100.20
1	L	148	TRP	CB-CG-CD1	-5.09	120.38	127.00
1	L	156	GLN	CB-CG-CD	5.08	124.82	111.60
2	H	58	TYR	CB-CG-CD1	-5.04	117.97	121.00
3	P	105	TYR	CA-CB-CG	5.02	122.94	113.40
2	H	100(B)	GLY	CA-C-N	-5.02	106.17	117.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	H	82	MET	CG-SD-CE	-5.01	92.19	100.20
1	L	58	VAL	CA-CB-CG2	-5.00	103.40	110.90

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	H	95	ARG	Sidechain
1	L	32	TYR	Sidechain
1	L	86	TYR	Sidechain

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	L	1680	0	1612	69	0
2	H	1664	0	1616	95	0
3	P	66	0	51	4	0
4	H	11	0	0	0	0
4	L	11	0	0	0	0
All	All	3432	0	3279	156	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 23.

All (156) 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)
2:H:11:LEU:HD13	2:H:110:THR:HG22	1.56	0.87
1:L:181:LEU:HD22	1:L:185:GLU:HG2	1.56	0.86
2:H:126:PRO:HG2	2:H:128:CYS:HA	1.60	0.84
2:H:166:LEU:HD13	2:H:191:VAL:HG21	1.61	0.83
1:L:83:LEU:HD11	1:L:106:LEU:HB3	1.58	0.83
1:L:66:GLY:HA3	1:L:71:PHE:HA	1.61	0.81
2:H:137:SER:HA	2:H:194:THR:HA	1.63	0.80

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:37:GLN:HB2	1:L:47:LEU:HD11	1.66	0.78
2:H:4:LEU:HA	2:H:23:ALA:O	1.87	0.74
1:L:47:LEU:HA	1:L:58:VAL:HG21	1.69	0.74
1:L:38:GLN:O	1:L:84:ALA:HB1	1.89	0.73
1:L:20:THR:HG23	1:L:72:THR:HG23	1.75	0.69
2:H:154:LEU:HD12	2:H:210:VAL:HG22	1.75	0.68
2:H:130:ASP:HA	2:H:137:SER:O	1.94	0.68
2:H:84:SER:HA	2:H:111:VAL:HG13	1.75	0.67
1:L:49:TYR:CD2	2:H:100(A):ASN:HB2	2.29	0.67
1:L:160:LEU:HD11	2:H:177:VAL:HG11	1.77	0.66
2:H:140:LEU:HD22	2:H:223:ILE:HG21	1.77	0.66
2:H:228:ARG:HB2	2:H:228:ARG:HH11	1.59	0.66
2:H:34:MET:HB2	2:H:78:LEU:HD13	1.77	0.65
1:L:162:SER:HB2	2:H:174:PHE:HB3	1.77	0.65
2:H:63:VAL:HG13	2:H:67:PHE:CD2	2.31	0.65
1:L:138:ASN:HA	1:L:172:THR:HG23	1.80	0.64
1:L:20:THR:OG1	1:L:74:THR:HG23	1.97	0.64
1:L:25:SER:OG	1:L:69:THR:HA	1.97	0.64
2:H:119:PRO:HB2	2:H:144:VAL:HG13	1.78	0.64
1:L:12:THR:HG23	1:L:107:LYS:HG2	1.79	0.64
1:L:28:LYS:O	1:L:29:GLN:HB2	1.98	0.64
1:L:193:THR:HG23	1:L:206:VAL:HG13	1.81	0.63
2:H:100(A):ASN:N	2:H:100(A):ASN:HD22	1.97	0.61
2:H:100:GLU:HG2	3:P:105:TYR:CD2	2.36	0.61
2:H:11:LEU:HA	2:H:110:THR:O	2.01	0.60
1:L:17:GLU:O	1:L:78:VAL:HG12	2.02	0.60
1:L:108:ARG:HG3	1:L:171:SER:HB2	1.83	0.59
1:L:38:GLN:NE2	1:L:44:PRO:HD3	2.18	0.59
2:H:60:PRO:O	2:H:64:LYS:HG3	2.02	0.59
2:H:1:GLU:OE1	2:H:3:GLN:HB2	2.03	0.59
2:H:4:LEU:HB3	2:H:92:CYS:SG	2.42	0.58
1:L:38:GLN:HA	1:L:42:GLN:OE1	2.04	0.58
2:H:82:MET:HE1	2:H:109:VAL:HG21	1.84	0.58
1:L:13:VAL:CG2	1:L:78:VAL:HG11	2.33	0.58
2:H:51:ILE:HG12	2:H:52:SER:H	1.68	0.58
2:H:171:VAL:HA	2:H:190:SER:O	2.03	0.58
2:H:27:PHE:HE2	2:H:32:TYR:HB2	1.69	0.57
2:H:24:ALA:HB1	2:H:27:PHE:HE1	1.69	0.57
2:H:52(A):ASN:HD21	3:P:102:VAL:HG22	1.68	0.57
1:L:47:LEU:O	1:L:55:GLU:HB2	2.05	0.56
2:H:24:ALA:HB1	2:H:27:PHE:CE1	2.40	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:66:ARG:HB3	2:H:82(A):SER:O	2.06	0.55
2:H:14:PRO:HG3	2:H:111:VAL:HG22	1.88	0.55
2:H:33:GLY:HA2	2:H:71:ARG:HH12	1.70	0.55
1:L:89:GLN:HE21	1:L:96:LEU:HB3	1.71	0.55
1:L:18:LYS:HG2	1:L:76:SER:HA	1.88	0.55
1:L:43:PRO:HD2	2:H:105:GLN:HE21	1.72	0.54
1:L:25:SER:HB2	1:L:27:GLN:O	2.07	0.54
2:H:144:VAL:O	2:H:186:THR:HA	2.07	0.54
2:H:134:THR:N	2:H:137:SER:OG	2.41	0.54
2:H:140:LEU:HD22	2:H:223:ILE:CG2	2.37	0.53
1:L:193:THR:CG2	1:L:206:VAL:HG13	2.38	0.53
1:L:12:THR:HA	1:L:105:GLU:O	2.08	0.53
2:H:52(A):ASN:HA	2:H:71:ARG:NH1	2.23	0.53
2:H:83:LYS:HE2	2:H:86:ASP:OD1	2.09	0.52
1:L:2:ILE:HD13	1:L:90:ASN:ND2	2.24	0.52
2:H:29:PHE:HB2	2:H:76:ASN:HD21	1.74	0.52
2:H:179:GLN:O	2:H:183:ASP:N	2.43	0.52
2:H:85:GLU:H	2:H:85:GLU:CD	2.13	0.51
2:H:63:VAL:HG13	2:H:67:PHE:HB2	1.93	0.51
2:H:119:PRO:HB3	2:H:147:TYR:HB3	1.92	0.51
1:L:2:ILE:HG23	1:L:27:GLN:HB2	1.92	0.51
2:H:199:TRP:HB2	2:H:205:ILE:HD13	1.92	0.51
2:H:134:THR:N	2:H:137:SER:HG	2.09	0.51
2:H:178:LEU:HD13	2:H:185:TYR:CZ	2.46	0.51
1:L:46:VAL:HG23	2:H:101:ALA:HA	1.93	0.50
2:H:33:GLY:O	2:H:95:ARG:HB2	2.12	0.50
2:H:116:THR:HA	2:H:148:PHE:O	2.12	0.50
1:L:82:ASP:O	1:L:104:LEU:HD12	2.12	0.50
1:L:115:VAL:HG22	1:L:136:LEU:HG	1.94	0.49
1:L:185:GLU:O	1:L:189:HIS:HD2	1.95	0.49
1:L:124:GLN:HG2	1:L:129:GLY:O	2.11	0.49
1:L:27(D):ASN:HB3	1:L:92:TYR:HE1	1.77	0.49
2:H:52(A):ASN:ND2	2:H:97:ARG:HH21	2.11	0.49
2:H:209:ASN:HA	2:H:220:ASP:HA	1.93	0.49
1:L:8:PRO:HB2	1:L:10:SER:O	2.12	0.49
1:L:5:THR:O	1:L:23:CYS:HA	2.12	0.49
1:L:51:ALA:HB2	1:L:71:PHE:HE2	1.78	0.48
2:H:97:ARG:HD2	2:H:98:TYR:CE1	2.47	0.48
2:H:12:VAL:O	2:H:111:VAL:HA	2.13	0.48
3:P:100:TYR:O	3:P:100:TYR:CD1	2.67	0.48
2:H:48:VAL:O	2:H:63:VAL:HG11	2.14	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:83:LYS:HG2	2:H:86:ASP:OD2	2.13	0.47
1:L:32:TYR:HE2	2:H:100:GLU:HB3	1.79	0.47
2:H:27:PHE:CE2	2:H:29:PHE:HA	2.50	0.47
1:L:4:MET:HB3	1:L:99:GLY:HA2	1.96	0.47
1:L:61:ARG:HA	1:L:76:SER:OG	2.13	0.47
1:L:16:GLY:HA2	1:L:77:SER:OG	2.15	0.47
2:H:140:LEU:HB3	2:H:223:ILE:HD13	1.96	0.47
2:H:3:GLN:O	2:H:24:ALA:HA	2.15	0.47
1:L:142:LYS:HG2	1:L:163:TRP:CZ2	2.50	0.47
2:H:92:CYS:O	2:H:92:CYS:SG	2.73	0.46
2:H:157:TRP:CZ3	2:H:208:CYS:HB2	2.50	0.46
2:H:96:GLU:HG3	2:H:100(A):ASN:HD21	1.80	0.46
2:H:143:LEU:HG	2:H:145:LYS:HG2	1.96	0.46
1:L:160:LEU:HD12	1:L:161:ASN:H	1.81	0.46
2:H:179:GLN:OE1	2:H:184:LEU:HB2	2.16	0.46
2:H:176:ALA:HA	2:H:186:THR:O	2.16	0.46
2:H:27:PHE:CE2	2:H:32:TYR:HB2	2.50	0.46
1:L:2:ILE:O	1:L:97:THR:HG21	2.17	0.45
2:H:145:LYS:NZ	2:H:179:GLN:HE21	2.13	0.45
1:L:59:PRO:HD2	1:L:62:PHE:HE2	1.81	0.45
1:L:37:GLN:HG2	1:L:38:GLN:N	2.30	0.45
2:H:34:MET:HB3	2:H:78:LEU:HD22	1.98	0.45
1:L:110:ASP:OD1	1:L:141:PRO:HD3	2.17	0.45
2:H:18:LEU:HD23	2:H:109:VAL:HG13	1.98	0.45
1:L:52:SER:HA	1:L:64:GLY:HA3	1.97	0.45
2:H:89:MET:HA	2:H:108:LEU:HA	1.98	0.45
1:L:144:ILE:HD12	1:L:198:HIS:HD2	1.82	0.45
1:L:13:VAL:HG22	1:L:78:VAL:HG11	1.98	0.45
1:L:160:LEU:HD11	2:H:177:VAL:CG1	2.46	0.44
2:H:148:PHE:HB2	2:H:184:LEU:CD2	2.48	0.44
1:L:161:ASN:HB3	1:L:175:MET:HE2	2.00	0.44
1:L:27(B):LEU:HD22	1:L:92:TYR:HB3	1.98	0.44
1:L:50:TRP:NE1	2:H:100:GLU:O	2.50	0.44
1:L:66:GLY:CA	1:L:71:PHE:HA	2.38	0.44
2:H:18:LEU:CD2	2:H:109:VAL:HG13	2.48	0.43
2:H:148:PHE:HB2	2:H:184:LEU:HD22	2.01	0.43
1:L:59:PRO:HD2	1:L:62:PHE:CE2	2.53	0.43
2:H:134:THR:O	2:H:137:SER:N	2.52	0.43
1:L:88:CYS:SG	1:L:99:GLY:HA3	2.58	0.43
2:H:81:GLN:HE22	2:H:82(A):SER:HB2	1.83	0.43
1:L:114:THR:HG22	2:H:133:THR:HG22	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:87:SER:HA	2:H:109:VAL:O	2.19	0.43
2:H:154:LEU:CD1	2:H:210:VAL:HG22	2.47	0.42
1:L:170:ASP:OD1	1:L:172:THR:HB	2.19	0.42
2:H:30:SER:O	2:H:52(A):ASN:HB2	2.20	0.42
1:L:185:GLU:HG3	1:L:185:GLU:O	2.15	0.42
2:H:100(A):ASN:N	2:H:100(A):ASN:ND2	2.67	0.42
2:H:174:PHE:HA	2:H:175:PRO:HD2	1.84	0.42
2:H:59:TYR:OH	2:H:68:THR:HA	2.20	0.42
1:L:125:LEU:HD21	1:L:130:ALA:HB2	2.02	0.41
2:H:34:MET:CB	2:H:78:LEU:HD13	2.45	0.41
1:L:2:ILE:HD12	1:L:2:ILE:N	2.35	0.41
1:L:42:GLN:HA	1:L:43:PRO:HD2	1.97	0.41
1:L:18:LYS:NZ	1:L:20:THR:OG1	2.52	0.41
2:H:96:GLU:CB	2:H:100(A):ASN:ND2	2.83	0.41
2:H:62:SER:O	2:H:66:ARG:NH2	2.47	0.41
1:L:37:GLN:HG3	1:L:86:TYR:CE2	2.55	0.41
2:H:125:ALA:HB2	2:H:223:ILE:HG23	2.03	0.41
2:H:20:LEU:HD21	2:H:82:MET:HE1	2.03	0.41
2:H:52:SER:HB2	3:P:101:ASP:OD1	2.21	0.41
2:H:178:LEU:HA	2:H:185:TYR:HA	2.03	0.41
2:H:141:GLY:HA2	2:H:189:SER:O	2.21	0.41
2:H:89:MET:HG2	2:H:91:TYR:CE2	2.56	0.40
2:H:122:TYR:HA	2:H:123:PRO:HD2	1.97	0.40
1:L:209:PHE:O	1:L:210:ASN:HB2	2.21	0.40
1:L:90:ASN:HB3	1:L:97:THR:OG1	2.22	0.40
2:H:95:ARG:HD3	2:H:95:ARG:HA	1.70	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	L	215/217 (99%)	188 (87%)	22 (10%)	5 (2%)	8 35
2	H	218/220 (99%)	187 (86%)	19 (9%)	12 (6%)	2 13
3	P	6/8 (75%)	6 (100%)	0	0	100 100
All	All	439/445 (99%)	381 (87%)	41 (9%)	17 (4%)	4 22

All (17) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	L	29	GLN
2	H	149	PRO
2	H	180	SER
2	H	183	ASP
2	H	195	SER
2	H	196	SER
2	H	227	PRO
1	L	201	SER
2	H	106	GLY
2	H	128	CYS
2	H	179	GLN
1	L	60	ASP
1	L	210	ASN
2	H	30	SER
2	H	56	TYR
1	L	100	GLY
2	H	53	GLY

5.3.2 Protein sidechains

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	L	194/194 (100%)	155 (80%)	39 (20%)	1 7
2	H	187/187 (100%)	152 (81%)	35 (19%)	2 8
3	P	7/7 (100%)	5 (71%)	2 (29%)	0 1
All	All	388/388 (100%)	312 (80%)	76 (20%)	1 7

All (76) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	L	1	ASP
1	L	2	ILE
1	L	4	MET
1	L	6	GLN
1	L	7	SER
1	L	9	SER
1	L	12	THR
1	L	18	LYS
1	L	24	THR
1	L	39	LYS
1	L	42	GLN
1	L	43	PRO
1	L	45	LYS
1	L	74	THR
1	L	90	ASN
1	L	98	PHE
1	L	106	LEU
1	L	116	SER
1	L	123	GLU
1	L	126	THR
1	L	136	LEU
1	L	143	ASP
1	L	145	ASN
1	L	154	GLU
1	L	162	SER
1	L	165	ASP
1	L	168	SER
1	L	169	LYS
1	L	172	THR
1	L	175	MET
1	L	185	GLU
1	L	191	SER
1	L	194	CYS
1	L	195	GLU
1	L	197	THR
1	L	203	SER
1	L	207	LYS
1	L	208	SER
1	L	211	ARG
2	H	1	GLU
2	H	13	LYS
2	H	17	SER

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Mol	Chain	Res	Type
2	H	41	PRO
2	H	45	LEU
2	H	50	THR
2	H	51	ILE
2	H	52(A)	ASN
2	H	61	ASP
2	H	62	SER
2	H	71	ARG
2	H	77	THR
2	H	81	GLN
2	H	89	MET
2	H	97	ARG
2	H	99	ASP
2	H	100(A)	ASN
2	H	108	LEU
2	H	115	LYS
2	H	119	PRO
2	H	130	ASP
2	H	133	THR
2	H	153	THR
2	H	154	LEU
2	H	166	LEU
2	H	168	SER
2	H	179	GLN
2	H	198	THR
2	H	203	GLN
2	H	204	SER
2	H	205	ILE
2	H	209	ASN
2	H	218	LYS
2	H	219	VAL
2	H	228	ARG
3	P	100	TYR
3	P	101	ASP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (9) such sidechains are listed below:

Mol	Chain	Res	Type
1	L	6	GLN
1	L	37	GLN
1	L	145	ASN
1	L	210	ASN

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Mol	Chain	Res	Type
2	H	81	GLN
2	H	100(A)	ASN
2	H	105	GLN
2	H	172	HIS
2	H	179	GLN

5.3.3 RNA

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates

There are no 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

EDS was not executed - this section will therefore be empty.

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

EDS was not executed - this section will therefore be empty.

6.3 Carbohydrates

EDS was not executed - this section will therefore be empty.

6.4 Ligands

EDS was not executed - this section will therefore be empty.

6.5 Other polymers

EDS was not executed - this section will therefore be empty.