Full wwPDB X-ray Structure Validation Report (i)

May 29, 2024 – 10:55 AM EDT

PDB ID	:	1HIL
Title	:	STRUCTURAL EVIDENCE FOR INDUCED FIT AS A MECHANISM FOR ANTIGEN-ANTIBODY RECOGNITION
Authors	:	Rini, J.M.; Wilson, I.A.
Deposited on	:	1992-07-08
Resolution	:	2.00 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
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

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

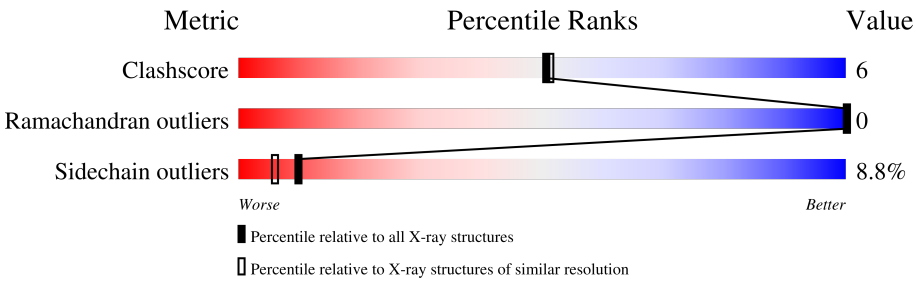
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36.2

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 2.00 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	141614	9178 (2.00-2.00)
Ramachandran outliers	138981	9054 (2.00-2.00)
Sidechain outliers	138945	9053 (2.00-2.00)

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 of the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. 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%

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	217	78% 18% • •
1	C	217	74% 21% •
2	B	220	84% 11% • •
2	D	220	75% 19% • • •

2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 6765 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
			Total	C	N	O	S			
1	A	217	1680	1047	279	347	7	0	0	0
1	C	217	1680	1047	279	347	7	0	0	0

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	B	214	1628	1028	270	323	7	0	0	0
2	D	214	1617	1022	267	321	7	0	0	1

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	227	PRO	-	insertion	GB 533229
D	227	PRO	-	insertion	GB 533229

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
3	A	38	38	38	0	0
3	B	42	42	42	0	0
3	C	39	39	39	0	0
3	D	41	41	41	0	0

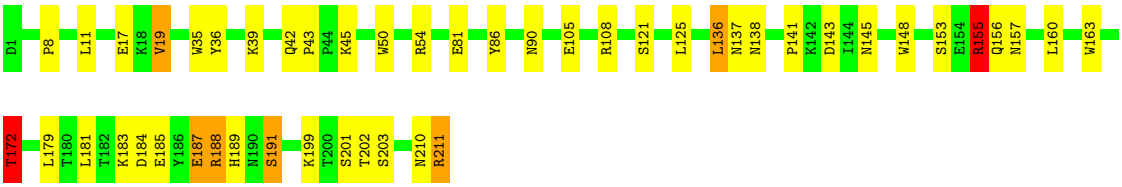
3 Residue-property plots (i)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. 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. 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.

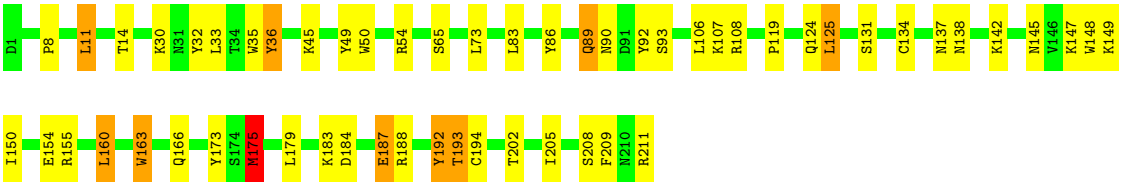
• Molecule 1: IGG2A-KAPPA 17/9 FAB (LIGHT CHAIN)

Chain A:



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

Chain C:

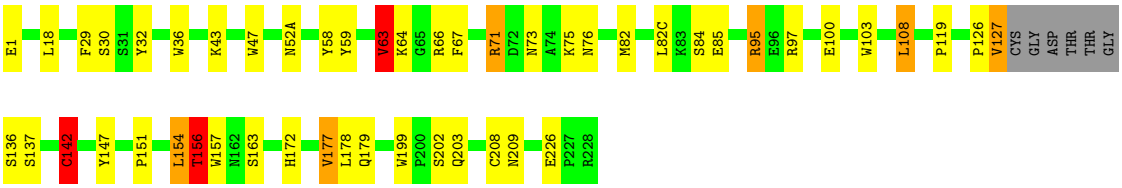


• Molecule 2: IGG2A-KAPPA 17/9 FAB (HEAVY CHAIN)

Chain B:

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

Chain D:



4 Data and refinement statistics (i)

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

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	90.04Å 82.80Å 73.40Å 90.00° 122.60° 90.00°	Depositor
Resolution (Å)	6.00 – 2.00	Depositor
% Data completeness (in resolution range)	(Not available) (6.00-2.00)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	X-PLOR	Depositor
R, R_{free}	0.195 , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	6765	wwPDB-VP
Average B, all atoms ($Å^2$)	23.0	wwPDB-VP

5 Model quality (i)

5.1 Standard geometry (i)

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	0.82	1/1718 (0.1%)	1.45	26/2334 (1.1%)
1	C	0.84	0/1718	1.48	24/2334 (1.0%)
2	B	0.85	0/1668	1.51	25/2270 (1.1%)
2	D	0.88	0/1657	1.53	27/2258 (1.2%)
All	All	0.85	1/6761 (0.0%)	1.49	102/9196 (1.1%)

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	D	0	2

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	19	VAL	CA-CB	5.29	1.65	1.54

All (102) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	D	95	ARG	NE-CZ-NH2	-9.90	115.35	120.30
1	C	148	TRP	CD1-CG-CD2	9.50	113.90	106.30
2	B	47	TRP	CD1-CG-CD2	9.39	113.81	106.30
1	A	148	TRP	CD1-CG-CD2	9.22	113.68	106.30
1	C	163	TRP	CD1-CG-CD2	9.18	113.64	106.30
2	D	47	TRP	CD1-CG-CD2	8.90	113.42	106.30
1	C	163	TRP	CE2-CD2-CG	-8.22	100.72	107.30
2	D	199	TRP	CD1-CG-CD2	8.18	112.84	106.30
2	B	97	ARG	NE-CZ-NH2	-8.13	116.23	120.30
1	A	50	TRP	CD1-CG-CD2	8.00	112.70	106.30
1	C	148	TRP	CE2-CD2-CG	-7.93	100.96	107.30

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	36	TRP	CD1-CG-CD2	7.89	112.61	106.30
2	B	38	ARG	NE-CZ-NH1	7.79	124.19	120.30
1	A	86	TYR	CB-CG-CD2	-7.71	116.37	121.00
1	A	211	ARG	NE-CZ-NH2	-7.68	116.46	120.30
1	C	160	LEU	CA-CB-CG	7.67	132.94	115.30
2	B	157	TRP	CD1-CG-CD2	7.61	112.39	106.30
2	D	156	THR	N-CA-CB	-7.60	95.86	110.30
2	D	142	CYS	CA-CB-SG	-7.53	100.44	114.00
2	B	199	TRP	CD1-CG-CD2	7.39	112.21	106.30
1	A	54	ARG	NE-CZ-NH1	7.35	123.98	120.30
1	A	148	TRP	CE2-CD2-CG	-7.35	101.42	107.30
1	A	163	TRP	CD1-CG-CD2	7.29	112.14	106.30
1	A	35	TRP	CD1-CG-CD2	7.26	112.11	106.30
1	C	30	LYS	CB-CG-CD	-7.24	92.77	111.60
2	B	47	TRP	CE2-CD2-CG	-7.21	101.53	107.30
2	D	157	TRP	CD1-CG-CD2	7.15	112.02	106.30
2	D	199	TRP	CE2-CD2-CG	-7.04	101.67	107.30
1	C	50	TRP	CD1-CG-CD2	7.03	111.92	106.30
2	D	47	TRP	CE2-CD2-CG	-7.01	101.69	107.30
2	B	199	TRP	CE2-CD2-CG	-6.95	101.74	107.30
1	A	163	TRP	CE2-CD2-CG	-6.94	101.75	107.30
2	B	157	TRP	CE2-CD2-CG	-6.93	101.75	107.30
1	A	136	LEU	CA-CB-CG	6.91	131.18	115.30
1	C	148	TRP	CG-CD1-NE1	-6.89	103.21	110.10
1	A	54	ARG	NE-CZ-NH2	-6.86	116.87	120.30
2	B	47	TRP	CG-CD1-NE1	-6.83	103.27	110.10
1	C	35	TRP	CD1-CG-CD2	6.80	111.74	106.30
2	D	177	VAL	CG1-CB-CG2	-6.78	100.06	110.90
1	C	163	TRP	CG-CD2-CE3	6.77	139.99	133.90
2	B	36	TRP	CE2-CD2-CG	-6.74	101.91	107.30
1	C	86	TYR	CB-CG-CD2	-6.73	116.96	121.00
1	C	163	TRP	CB-CG-CD1	-6.73	118.25	127.00
1	A	148	TRP	CG-CD1-NE1	-6.72	103.38	110.10
1	A	188	ARG	NE-CZ-NH2	-6.68	116.96	120.30
2	D	47	TRP	CG-CD1-NE1	-6.54	103.56	110.10
2	D	157	TRP	CE2-CD2-CG	-6.54	102.07	107.30
2	D	71	ARG	NE-CZ-NH2	-6.48	117.06	120.30
1	C	54	ARG	NE-CZ-NH1	6.47	123.53	120.30
2	D	103	TRP	CD1-CG-CD2	6.39	111.41	106.30
2	D	59	TYR	CB-CG-CD2	-6.39	117.17	121.00
1	C	54	ARG	NE-CZ-NH2	-6.35	117.13	120.30
2	D	36	TRP	CD1-CG-CD2	6.29	111.33	106.30

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	177	VAL	CG1-CB-CG2	-6.26	100.88	110.90
2	D	154	LEU	CA-CB-CG	6.26	129.70	115.30
2	B	103	TRP	CE2-CD2-CG	-6.24	102.31	107.30
1	C	163	TRP	CG-CD1-NE1	-6.21	103.89	110.10
2	D	103	TRP	CE2-CD2-CG	-6.17	102.36	107.30
2	D	36	TRP	CE2-CD2-CG	-6.10	102.42	107.30
2	B	63	VAL	N-CA-CB	-6.06	98.17	111.50
1	A	50	TRP	CE2-CD2-CG	-6.00	102.50	107.30
1	A	187	GLU	CA-CB-CG	-5.99	100.22	113.40
2	D	127	VAL	N-CA-C	-5.96	94.89	111.00
1	A	35	TRP	CE2-CD2-CG	-5.94	102.55	107.30
1	C	187	GLU	CA-CB-CG	-5.93	100.36	113.40
2	B	103	TRP	CD1-CG-CD2	5.91	111.02	106.30
1	A	35	TRP	CG-CD1-NE1	-5.90	104.20	110.10
1	C	50	TRP	CG-CD1-NE1	-5.90	104.20	110.10
1	A	50	TRP	CG-CD1-NE1	-5.86	104.24	110.10
1	C	36	TYR	CB-CG-CD2	-5.86	117.49	121.00
2	B	142	CYS	CA-CB-SG	-5.83	103.50	114.00
2	D	178	LEU	CA-CB-CG	5.81	128.67	115.30
2	D	58	TYR	CB-CG-CD1	-5.80	117.52	121.00
1	C	35	TRP	CE2-CD2-CG	-5.80	102.66	107.30
2	D	108	LEU	CA-CB-CG	5.76	128.54	115.30
1	C	108	ARG	NE-CZ-NH2	-5.71	117.44	120.30
1	A	211	ARG	NE-CZ-NH1	5.71	123.15	120.30
1	A	155	ARG	NE-CZ-NH1	5.69	123.14	120.30
1	C	175	MET	CG-SD-CE	-5.68	91.11	100.20
1	A	108	ARG	NE-CZ-NH1	5.67	123.14	120.30
1	A	17	GLU	CA-CB-CG	5.65	125.84	113.40
2	D	63	VAL	N-CA-CB	-5.64	99.08	111.50
2	D	63	VAL	CA-CB-CG2	-5.56	102.56	110.90
2	B	157	TRP	CG-CD1-NE1	-5.56	104.54	110.10
1	A	153	SER	N-CA-CB	-5.55	102.17	110.50
2	B	203	GLN	CA-CB-CG	5.55	125.61	113.40
2	B	97	ARG	NE-CZ-NH1	5.50	123.05	120.30
2	B	32	TYR	CB-CG-CD1	-5.46	117.73	121.00
2	D	199	TRP	CG-CD1-NE1	-5.38	104.72	110.10
1	A	36	TYR	CB-CG-CD2	-5.35	117.79	121.00
2	B	10	ASP	CB-CG-OD1	5.32	123.09	118.30
1	A	172	THR	N-CA-CB	-5.31	100.22	110.30
2	B	228	ARG	NE-CZ-NH1	5.30	122.95	120.30
1	C	50	TRP	CE2-CD2-CG	-5.28	103.08	107.30
2	B	157	TRP	CB-CG-CD1	-5.28	120.14	127.00

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	D	71	ARG	NE-CZ-NH1	5.24	122.92	120.30
1	A	148	TRP	CB-CG-CD1	-5.20	120.24	127.00
1	C	192	TYR	CB-CG-CD1	-5.20	117.88	121.00
2	B	1	GLU	N-CA-C	-5.14	97.13	111.00
1	C	33	LEU	CA-CB-CG	5.12	127.07	115.30
2	D	75	LYS	CA-CB-CG	-5.05	102.29	113.40
2	B	89	MET	CG-SD-CE	-5.01	92.18	100.20

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	D	126	PRO	Mainchain,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	1680	0	1614	17	0
1	C	1680	0	1616	25	0
2	B	1628	0	1590	5	0
2	D	1617	0	1577	24	0
3	A	38	0	0	1	0
3	B	42	0	0	0	0
3	C	39	0	0	2	0
3	D	41	0	0	0	0
All	All	6765	0	6397	67	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 6.

All (67) 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:D:142:CYS:HG	2:D:208:CYS:HG	0.89	0.84

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:163:SER:H	2:D:209:ASN:HD21	1.33	0.77
2:D:142:CYS:HG	2:D:208:CYS:CB	1.99	0.75
2:D:142:CYS:SG	2:D:208:CYS:CB	2.79	0.70
1:C:106:LEU:H	1:C:166:GLN:HE22	1.40	0.69
2:D:163:SER:H	2:D:209:ASN:ND2	1.91	0.68
1:C:8:PRO:HG3	1:C:11:LEU:HG	1.76	0.68
1:A:138:ASN:HA	1:A:172:THR:HG23	1.77	0.66
1:C:125:LEU:HD12	1:C:183:LYS:HG3	1.78	0.65
2:D:32:TYR:CE2	2:D:97:ARG:HG3	2.32	0.64
2:D:30:SER:O	2:D:52(A):ASN:HB2	1.99	0.62
2:D:119:PRO:HB3	2:D:147:TYR:HB3	1.82	0.62
2:B:119:PRO:HB3	2:B:147:TYR:HB3	1.81	0.62
1:A:43:PRO:HD2	1:A:45:LYS:NZ	2.15	0.61
1:A:42:GLN:HG3	3:A:216:HOH:O	2.02	0.60
2:D:82:MET:HE2	2:D:82(C):LEU:HD21	1.85	0.59
1:A:43:PRO:HD2	1:A:45:LYS:HZ1	1.69	0.58
1:A:125:LEU:HD12	1:A:183:LYS:HG3	1.86	0.58
2:D:142:CYS:CB	2:D:208:CYS:HG	2.16	0.56
1:A:138:ASN:HA	1:A:172:THR:CG2	2.33	0.56
1:C:150:ILE:HD11	1:C:179:LEU:HD21	1.86	0.56
1:C:187:GLU:HA	1:C:211:ARG:NH2	2.21	0.55
1:C:184:ASP:HB3	1:C:188:ARG:NH2	2.22	0.55
3:C:237:HOH:O	2:D:43:LYS:HD2	2.06	0.54
1:C:32:TYR:HB2	1:C:92:TYR:HB2	1.90	0.54
2:D:156:THR:HG22	2:D:209:ASN:HB2	1.88	0.54
1:C:163:TRP:CD1	1:C:175:MET:HG3	2.42	0.53
2:D:71:ARG:HE	2:D:73:ASN:HD21	1.55	0.53
1:C:8:PRO:CG	1:C:11:LEU:HG	2.39	0.53
1:C:184:ASP:HB3	1:C:188:ARG:HH22	1.73	0.52
1:A:137:ASN:HB3	1:A:138:ASN:HD22	1.76	0.51
1:C:124:GLN:NE2	3:C:219:HOH:O	2.41	0.51
2:D:63:VAL:HG13	2:D:67:PHE:HB2	1.93	0.51
1:C:149:LYS:HB2	1:C:193:THR:HG23	1.93	0.49
2:D:71:ARG:NE	2:D:73:ASN:HD21	2.12	0.48
2:D:156:THR:HG22	2:D:209:ASN:HD22	1.77	0.48
1:A:141:PRO:HG2	1:A:199:LYS:HD3	1.95	0.48
1:C:137:ASN:HB3	1:C:138:ASN:HD22	1.79	0.48
2:B:63:VAL:HG13	2:B:67:PHE:HB2	1.96	0.47
2:D:71:ARG:HE	2:D:73:ASN:ND2	2.12	0.47
2:D:142:CYS:CB	2:D:208:CYS:SG	3.02	0.47
2:B:194:THR:HG22	2:B:196:SER:H	1.80	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:8:PRO:HG3	1:A:11:LEU:HD13	1.97	0.46
1:A:191:SER:OG	1:A:210:ASN:ND2	2.49	0.46
1:C:124:GLN:NE2	1:C:131:SER:H	2.15	0.45
1:C:49:TYR:CD2	2:D:100:GLU:HG3	2.52	0.45
1:C:149:LYS:HA	1:C:154:GLU:HA	1.98	0.45
1:C:150:ILE:HD12	1:C:155:ARG:HD2	1.98	0.45
1:C:142:LYS:HD3	1:C:173:TYR:CE2	2.51	0.45
2:D:66:ARG:HH11	2:D:66:ARG:HD2	1.66	0.44
1:A:155:ARG:HH11	1:A:155:ARG:HB2	1.82	0.44
1:C:138:ASN:HD21	2:D:172:HIS:HE1	1.67	0.43
1:A:39:LYS:HE2	1:A:81:GLU:O	2.18	0.43
1:A:155:ARG:HB2	1:A:155:ARG:NH1	2.34	0.42
1:A:185:GLU:O	1:A:189:HIS:HD2	2.03	0.42
1:A:211:ARG:HG2	1:A:211:ARG:HH11	1.84	0.42
1:A:160:LEU:HD11	2:B:177:VAL:HG23	2.01	0.42
2:D:29:PHE:CD2	2:D:76:ASN:HA	2.55	0.42
1:C:124:GLN:HE22	1:C:131:SER:H	1.69	0.41
1:C:134:CYS:SG	1:C:194:CYS:CB	3.09	0.41
2:B:32:TYR:CE2	2:B:97:ARG:HG3	2.56	0.41
1:C:160:LEU:HD22	2:D:177:VAL:HG23	2.03	0.41
1:C:192:TYR:HB2	1:C:209:PHE:CE1	2.56	0.41
2:D:142:CYS:SG	2:D:208:CYS:HB2	2.59	0.41
1:C:36:TYR:OH	1:C:89:GLN:NE2	2.54	0.40
1:C:119:PRO:HB3	1:C:209:PHE:CE2	2.57	0.40
1:A:188:ARG:HE	1:A:188:ARG:HB3	1.73	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	215/217 (99%)	211 (98%)	4 (2%)	0	100 100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	C	215/217 (99%)	212 (99%)	3 (1%)	0	100	100
2	B	210/220 (96%)	204 (97%)	6 (3%)	0	100	100
2	D	210/220 (96%)	204 (97%)	6 (3%)	0	100	100
All	All	850/874 (97%)	831 (98%)	19 (2%)	0	100	100

There are no Ramachandran outliers to report.

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	194/194 (100%)	175 (90%)	19 (10%)	8	4
1	C	194/194 (100%)	176 (91%)	18 (9%)	9	5
2	B	183/187 (98%)	173 (94%)	10 (6%)	21	17
2	D	182/187 (97%)	163 (90%)	19 (10%)	7	4
All	All	753/762 (99%)	687 (91%)	66 (9%)	10	6

All (66) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	19	VAL
1	A	90	ASN
1	A	105	GLU
1	A	121	SER
1	A	136	LEU
1	A	143	ASP
1	A	145	ASN
1	A	155	ARG
1	A	156	GLN
1	A	157	ASN
1	A	172	THR
1	A	179	LEU
1	A	181	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	184	ASP
1	A	187	GLU
1	A	191	SER
1	A	201	SER
1	A	202	THR
1	A	203	SER
2	B	95	ARG
2	B	127	VAL
2	B	136	SER
2	B	151	PRO
2	B	166	LEU
2	B	167	SER
2	B	179	GLN
2	B	195	SER
2	B	202	SER
2	B	228	ARG
1	C	11	LEU
1	C	14	THR
1	C	45	LYS
1	C	65	SER
1	C	73	LEU
1	C	83	LEU
1	C	89	GLN
1	C	90	ASN
1	C	93	SER
1	C	107	LYS
1	C	125	LEU
1	C	145	ASN
1	C	147	LYS
1	C	175	MET
1	C	193	THR
1	C	202	THR
1	C	205	ILE
1	C	208	SER
2	D	1	GLU
2	D	18	LEU
2	D	63	VAL
2	D	64	LYS
2	D	84	SER
2	D	85	GLU
2	D	95	ARG
2	D	108	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	D	127	VAL
2	D	136	SER
2	D	137	SER
2	D	142	CYS
2	D	151	PRO
2	D	154	LEU
2	D	156	THR
2	D	179	GLN
2	D	202	SER
2	D	203	GLN
2	D	226	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (10) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	138	ASN
1	A	210	ASN
2	B	203	GLN
1	C	37	GLN
1	C	89	GLN
1	C	124	GLN
1	C	138	ASN
1	C	166	GLN
2	D	73	ASN
2	D	209	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)

There are no monosaccharides in this entry.

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)

EDS was not executed - this section is therefore empty.

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

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates (i)

EDS was not executed - this section is therefore empty.

6.4 Ligands (i)

EDS was not executed - this section is therefore empty.

6.5 Other polymers (i)

EDS was not executed - this section is therefore empty.