Full wwPDB X-ray Structure Validation Report (i)

Jan 31, 2016 – 07:27 PM GMT

PDB ID	:	1FPT
Title	:	THREE-DIMENSIONAL STRUCTURE OF THE COMPLEX BETWEEN THE FAB FRAGMENT OF AN NEUTRALIZING ANTIBODY FOR TYPE 1 POLIOVIRUS AND ITS VIRAL EPITOPE
Authors	:	Wien, M.W.; Hogle, J.M.
Deposited on	:	1995-01-26
Resolution	:	3.00 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
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 (i)) were used in the production of this report:

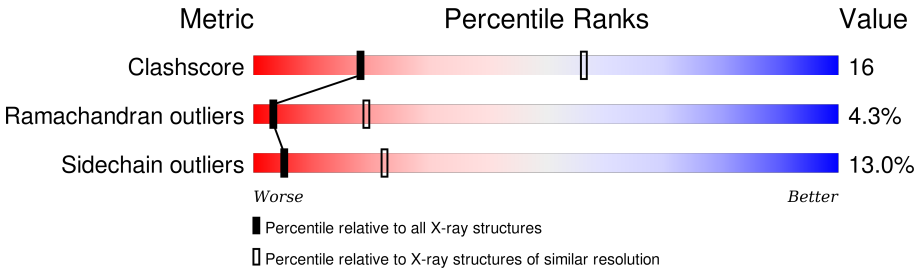
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	trunk26865

1 Overall quality at a glance

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 3.00 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	102246	1912 (3.00-3.00)
Ramachandran outliers	100387	1853 (3.00-3.00)
Sidechain outliers	100360	1856 (3.00-3.00)

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 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	P	18	22% 22% 6% 11% 39%
2	L	219	50% 39% 8% ·
3	H	220	54% 32% 10% ·

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 3465 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 FAB FRAGMENT OF AN NEUTRALIZING ANTIBODY FOR TYPE 1 POLIOVIRUS.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
1	P	11	83	47	15	21	0	0	0

- Molecule 2 is a protein called IGG2A-KAPPA C3 FAB (LIGHT CHAIN).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	L	219	1691	1061	283	341	6	0	0	0

- Molecule 3 is a protein called IGG2A-KAPPA C3 FAB (HEAVY CHAIN).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
3	H	220	1652	1045	269	332	6	0	0	0

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
4	H	20	20	20	0	0
4	L	17	Total	O	0	0
			17	17		
4	P	2	Total	O	0	0
			2	2		

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.

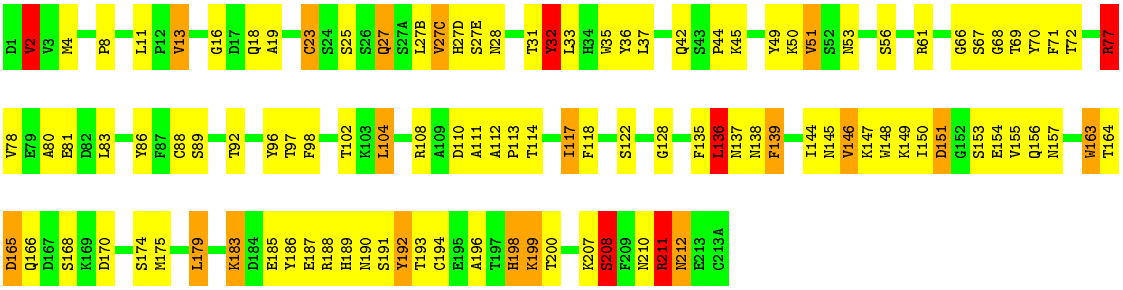
Note EDS was not executed.

• Molecule 1: FAB FRAGMENT OF AN NEUTRALIZING ANTIBODY FOR TYPE 1 POLIOVIRUS

Chain P:

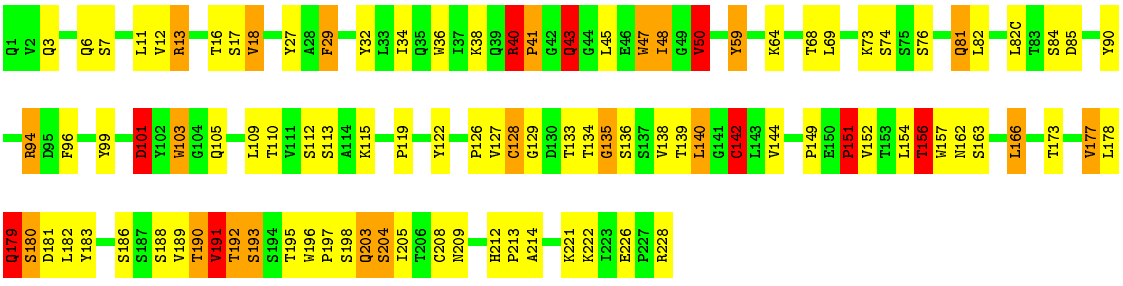
• Molecule 2: IGG2A-KAPPA C3 FAB (LIGHT CHAIN)

Chain L:



• Molecule 3: IGG2A-KAPPA C3 FAB (HEAVY CHAIN)

Chain H:



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 63 2 2	Depositor
Cell constants a, b, c, α, β, γ	129.78Å 129.78Å 143.83Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	10.00 – 3.00	Depositor
% Data completeness (in resolution range)	(Not available) (10.00-3.00)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	X-PLOR	Depositor
R, R_{free}	0.230 , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	3465	wwPDB-VP
Average B, all atoms (Å^2)	19.0	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	P	1.15	0/83	2.61	9/110 (8.2%)
2	L	1.11	1/1731 (0.1%)	1.96	48/2351 (2.0%)
3	H	1.10	2/1693 (0.1%)	2.07	56/2314 (2.4%)
All	All	1.11	3/3507 (0.1%)	2.03	113/4775 (2.4%)

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	P	0	1
2	L	0	1
3	H	0	2
All	All	0	4

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	H	186	SER	CA-CB	-5.72	1.44	1.52
2	L	35	TRP	CG-CD2	-5.70	1.33	1.43
3	H	196	TRP	CG-CD2	-5.02	1.35	1.43

All (113) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	H	142	CYS	CA-CB-SG	-11.87	92.64	114.00
3	H	99	TYR	CB-CG-CD1	-11.30	114.22	121.00
2	L	211	ARG	NE-CZ-NH1	10.43	125.51	120.30
3	H	47	TRP	CD1-CG-CD2	10.11	114.38	106.30
3	H	36	TRP	CD1-CG-CD2	9.13	113.61	106.30
2	L	148	TRP	CD1-CG-CD2	8.76	113.31	106.30
2	L	61	ARG	NE-CZ-NH1	8.71	124.65	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	L	49	TYR	CA-C-N	8.69	136.31	117.20
2	L	148	TRP	CE2-CD2-CG	-8.59	100.43	107.30
3	H	157	TRP	CD1-CG-CD2	8.49	113.09	106.30
2	L	51	VAL	CG1-CB-CG2	-8.27	97.67	110.90
3	H	157	TRP	CE2-CD2-CG	-8.21	100.73	107.30
3	H	47	TRP	CE2-CD2-CG	-8.12	100.80	107.30
2	L	163	TRP	CD1-CG-CD2	8.10	112.78	106.30
3	H	196	TRP	CD1-CG-CD2	7.90	112.62	106.30
2	L	163	TRP	CE2-CD2-CG	-7.81	101.05	107.30
2	L	61	ARG	NE-CZ-NH2	-7.76	116.42	120.30
3	H	99	TYR	CB-CG-CD2	7.72	125.63	121.00
2	L	211	ARG	NE-CZ-NH2	-7.70	116.45	120.30
3	H	36	TRP	CE2-CD2-CG	-7.69	101.15	107.30
2	L	148	TRP	CG-CD2-CE3	7.65	140.79	133.90
3	H	103	TRP	CD1-CG-CD2	7.55	112.34	106.30
3	H	156	THR	CA-CB-CG2	7.52	122.92	112.40
2	L	136	LEU	CA-CB-CG	7.46	132.47	115.30
3	H	50	VAL	CB-CA-C	-7.44	97.26	111.40
2	L	35	TRP	CD1-CG-CD2	7.36	112.18	106.30
3	H	196	TRP	CE2-CD2-CG	-7.13	101.60	107.30
3	H	151	PRO	N-CA-C	7.11	130.58	112.10
3	H	103	TRP	CE2-CD2-CG	-7.07	101.64	107.30
2	L	148	TRP	CB-CG-CD1	-7.01	117.88	127.00
3	H	18	VAL	CG1-CB-CG2	-7.01	99.68	110.90
1	P	94	ASN	O-C-N	-7.00	107.80	121.10
2	L	192	TYR	CB-CG-CD1	-6.97	116.82	121.00
3	H	144	VAL	CG1-CB-CG2	-6.94	99.80	110.90
2	L	163	TRP	CG-CD2-CE3	6.81	140.03	133.90
3	H	122	TYR	CB-CG-CD2	-6.81	116.92	121.00
2	L	35	TRP	CE2-CD2-CG	-6.77	101.88	107.30
3	H	186	SER	CA-CB-OG	-6.58	93.45	111.20
2	L	27	GLN	CA-CB-CG	-6.57	98.94	113.40
3	H	81	GLN	CA-CB-CG	-6.54	99.02	113.40
2	L	33	LEU	CA-CB-CG	6.49	130.22	115.30
3	H	228	ARG	NE-CZ-NH1	6.45	123.53	120.30
1	P	103	LYS	CB-CG-CD	-6.43	94.89	111.60
3	H	3	GLN	CA-CB-CG	6.43	127.54	113.40
3	H	43	GLN	N-CA-CB	-6.40	99.07	110.60
3	H	179	GLN	CA-C-N	6.39	131.26	117.20
3	H	47	TRP	CG-CD1-NE1	-6.31	103.79	110.10
1	P	95	PRO	N-CD-CG	6.26	112.59	103.20
2	L	49	TYR	CB-CG-CD2	-6.24	117.26	121.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	P	98	THR	CA-CB-CG2	6.19	121.06	112.40
2	L	188	ARG	NE-CZ-NH2	6.12	123.36	120.30
2	L	114	THR	CA-C-N	-6.05	103.90	117.20
3	H	135	GLY	CA-C-N	-6.04	103.91	117.20
3	H	48	ILE	CA-C-N	6.03	128.26	116.20
1	P	98	THR	CA-CB-OG1	-6.01	96.39	109.00
3	H	157	TRP	CB-CG-CD1	-6.00	119.19	127.00
2	L	146	VAL	CG1-CB-CG2	-6.00	101.30	110.90
2	L	49	TYR	CA-C-O	-5.99	107.51	120.10
2	L	183	LYS	CG-CD-CE	-5.97	93.99	111.90
3	H	183	TYR	CB-CG-CD2	-5.95	117.43	121.00
3	H	189	VAL	CG1-CB-CG2	-5.93	101.42	110.90
3	H	94	ARG	NE-CZ-NH2	-5.91	117.35	120.30
2	L	50	LYS	CA-C-N	5.86	130.09	117.20
3	H	204	SER	CB-CA-C	-5.82	99.04	110.10
3	H	179	GLN	O-C-N	-5.81	113.40	122.70
3	H	112	SER	CA-C-N	-5.78	104.49	117.20
2	L	2	VAL	CG1-CB-CG2	-5.74	101.72	110.90
2	L	70	TYR	CB-CG-CD2	-5.73	117.56	121.00
2	L	199	LYS	CD-CE-NZ	-5.73	98.51	111.70
2	L	139	PHE	CB-CG-CD2	-5.72	116.80	120.80
2	L	97	THR	CA-CB-OG1	-5.71	97.01	109.00
1	P	95	PRO	N-CA-C	5.70	126.92	112.10
2	L	77	ARG	CA-C-N	-5.70	104.67	117.20
1	P	99	THR	CA-CB-CG2	5.67	120.34	112.40
2	L	163	TRP	CB-CG-CD1	-5.62	119.70	127.00
2	L	104	LEU	CA-CB-CG	5.60	128.19	115.30
2	L	96	TYR	CB-CG-CD2	-5.57	117.66	121.00
3	H	203	GLN	CA-C-N	5.53	129.35	117.20
2	L	77	ARG	NE-CZ-NH2	5.50	123.05	120.30
3	H	157	TRP	CG-CD2-CE3	5.48	138.83	133.90
3	H	59	TYR	CB-CG-CD1	-5.45	117.73	121.00
3	H	173	THR	CA-CB-CG2	-5.43	104.80	112.40
2	L	13	VAL	CA-C-N	5.42	129.13	117.20
3	H	40	ARG	NE-CZ-NH2	-5.41	117.60	120.30
3	H	43	GLN	CA-CB-CG	5.41	125.29	113.40
3	H	135	GLY	O-C-N	5.38	131.32	122.70
3	H	128	CYS	CA-CB-SG	-5.37	104.34	114.00
3	H	6	GLN	N-CA-C	5.35	125.44	111.00
1	P	101	LYS	CA-C-N	-5.34	105.45	117.20
2	L	179	LEU	CB-CG-CD1	-5.34	101.93	111.00
2	L	32	TYR	CB-CG-CD1	-5.33	117.80	121.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	H	228	ARG	N-CA-C	5.33	125.38	111.00
3	H	196	TRP	CG-CD1-NE1	-5.32	104.78	110.10
3	H	228	ARG	NE-CZ-NH2	-5.32	117.64	120.30
3	H	178	LEU	CA-C-N	5.31	128.88	117.20
3	H	197	PRO	CA-C-N	-5.25	105.64	117.20
2	L	155	VAL	CA-CB-CG2	-5.24	103.03	110.90
2	L	110	ASP	N-CA-C	5.18	124.97	111.00
2	L	137	ASN	N-CA-C	5.16	124.94	111.00
2	L	13	VAL	O-C-N	-5.16	114.44	122.70
2	L	23	CYS	CA-CB-SG	5.14	123.25	114.00
2	L	27(C)	VAL	O-C-N	-5.12	114.50	122.70
2	L	42	GLN	O-C-N	-5.10	114.55	122.70
3	H	177	VAL	CA-CB-CG1	-5.08	103.28	110.90
2	L	212	ASN	CA-C-N	-5.08	106.04	117.20
3	H	36	TRP	CG-CD1-NE1	-5.07	105.03	110.10
3	H	45	LEU	O-C-N	-5.07	114.59	122.70
3	H	156	THR	CA-CB-OG1	-5.04	98.41	109.00
2	L	208	SER	CA-CB-OG	5.04	124.81	111.20
3	H	69	LEU	CB-CG-CD1	-5.04	102.44	111.00
3	H	73	LYS	CA-CB-CG	-5.02	102.35	113.40
1	P	95	PRO	CA-CB-CG	5.02	114.33	104.80
3	H	191	VAL	O-C-N	-5.00	114.70	122.70

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
3	H	40	ARG	Peptide
3	H	59	TYR	Sidechain
2	L	32	TYR	Sidechain
1	P	94	ASN	Mainchain

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	P	83	0	76	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	L	1691	0	1636	57	0
3	H	1652	0	1609	49	0
4	H	20	0	0	0	0
4	L	17	0	0	0	0
4	P	2	0	0	0	0
All	All	3465	0	3321	101	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 16.

All (101) 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:L:27(D):HIS:HB2	2:L:92:THR:HG23	1.38	1.04
2:L:147:LYS:HE3	2:L:154:GLU:HG2	1.51	0.93
2:L:113:PRO:HG3	2:L:144:ILE:HD11	1.61	0.80
2:L:118:PHE:CZ	3:H:140:LEU:HA	2.22	0.73
2:L:112:ALA:HB2	2:L:200:THR:HG21	1.70	0.73
2:L:83:LEU:HD11	2:L:166:GLN:HG2	1.71	0.73
2:L:37:LEU:HD23	2:L:45:LYS:HE2	1.74	0.70
2:L:118:PHE:HZ	3:H:140:LEU:HA	1.56	0.68
2:L:27(B):LEU:HD12	2:L:71:PHE:CE1	2.31	0.66
3:H:156:THR:HG22	3:H:209:ASN:OD1	1.96	0.66
3:H:142:CYS:HG	3:H:208:CYS:CB	2.09	0.65
3:H:119:PRO:HD3	3:H:212:HIS:CD2	2.31	0.65
2:L:13:VAL:HG11	2:L:78:VAL:HG21	1.78	0.64
2:L:151:ASP:HA	2:L:191:SER:HB2	1.79	0.64
2:L:183:LYS:O	2:L:186:TYR:HB3	1.99	0.63
2:L:136:LEU:HD12	2:L:144:ILE:HD13	1.80	0.62
2:L:11:LEU:HD23	2:L:104:LEU:HD23	1.81	0.61
2:L:145:ASN:O	2:L:196:ALA:HA	2.01	0.60
2:L:4:MET:HE1	2:L:27(B):LEU:HD11	1.83	0.60
2:L:32:TYR:HD1	2:L:92:THR:HG1	1.49	0.59
3:H:27:TYR:CE1	3:H:29:PHE:HA	2.37	0.59
3:H:138:VAL:HG23	3:H:193:SER:HA	1.83	0.59
3:H:204:SER:O	3:H:205:ILE:HG13	2.03	0.59
3:H:142:CYS:HB3	3:H:154:LEU:HD11	1.86	0.58
2:L:36:TYR:HE2	2:L:89:SER:HG	1.52	0.58
2:L:144:ILE:HG13	2:L:198:HIS:HD2	1.68	0.57
3:H:32:TYR:CD2	3:H:96:PHE:HA	2.40	0.57
3:H:47:TRP:HZ2	3:H:50:VAL:HG22	1.70	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:H:38:LYS:HB2	3:H:48:ILE:HD11	1.88	0.55
3:H:12:VAL:HG21	3:H:109:LEU:HD21	1.89	0.55
3:H:162:ASN:HD21	3:H:205:ILE:HG13	1.73	0.53
2:L:31:THR:HG21	2:L:71:PHE:CE2	2.44	0.53
2:L:4:MET:HE2	2:L:25:SER:HB3	1.91	0.52
3:H:40:ARG:HG2	3:H:41:PRO:HD3	1.92	0.51
2:L:44:PRO:HG2	3:H:103:TRP:CZ3	2.46	0.51
2:L:136:LEU:HD21	2:L:146:VAL:HG21	1.92	0.51
3:H:40:ARG:HH21	3:H:85:ASP:HA	1.76	0.51
2:L:23:CYS:SG	2:L:88:CYS:CB	3.00	0.50
3:H:27:TYR:OH	3:H:34:ILE:HD11	2.11	0.50
3:H:136:SER:O	3:H:193:SER:HB3	2.11	0.50
3:H:138:VAL:CG2	3:H:193:SER:HA	2.41	0.50
2:L:187:GLU:HA	2:L:211:ARG:HD2	1.93	0.50
1:P:93:ASP:O	1:P:95:PRO:HD3	2.12	0.50
2:L:117:ILE:HD11	2:L:207:LYS:HB3	1.92	0.50
3:H:138:VAL:HB	3:H:191:VAL:HG12	1.94	0.49
2:L:193:THR:OG1	2:L:208:SER:HB3	2.13	0.49
3:H:151:PRO:O	3:H:213:PRO:HD2	2.13	0.49
3:H:181:ASP:O	3:H:182:LEU:HD23	2.14	0.48
3:H:13:ARG:HG3	3:H:16:THR:OG1	2.13	0.48
2:L:135:PHE:CD2	3:H:188:SER:HB3	2.49	0.48
3:H:11:LEU:HD12	3:H:149:PRO:HG3	1.96	0.47
3:H:18:VAL:O	3:H:81:GLN:HA	2.14	0.47
2:L:163:TRP:NE1	2:L:175:MET:SD	2.87	0.47
2:L:156:GLN:HA	2:L:156:GLN:NE2	2.29	0.47
2:L:149:LYS:HG2	2:L:154:GLU:HA	1.97	0.46
3:H:40:ARG:O	3:H:43:GLN:HB3	2.15	0.46
3:H:16:THR:HG22	3:H:17:SER:N	2.29	0.46
2:L:13:VAL:HG12	2:L:78:VAL:HG11	1.97	0.46
2:L:150:ILE:HG12	2:L:192:TYR:CD1	2.50	0.46
2:L:149:LYS:HA	2:L:153:SER:O	2.16	0.46
3:H:203:GLN:O	3:H:204:SER:HB2	2.16	0.46
2:L:27(C):VAL:HG22	2:L:31:THR:OG1	2.17	0.45
2:L:147:LYS:HE3	2:L:154:GLU:CG	2.33	0.45
3:H:180:SER:O	3:H:181:ASP:HB2	2.17	0.45
2:L:16:GLY:O	2:L:77:ARG:HB3	2.17	0.45
2:L:112:ALA:HB2	2:L:200:THR:CG2	2.45	0.44
2:L:67:SER:O	2:L:69:THR:N	2.50	0.44
2:L:86:TYR:CD1	2:L:86:TYR:N	2.84	0.44
2:L:18:GLN:HG2	2:L:19:ALA:N	2.32	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:L:139:PHE:CE1	2:L:174:SER:HA	2.53	0.44
2:L:199:LYS:HG2	2:L:199:LYS:O	2.16	0.44
2:L:198:HIS:ND1	2:L:200:THR:OG1	2.45	0.44
3:H:142:CYS:CB	3:H:154:LEU:HD11	2.47	0.44
3:H:128:CYS:SG	3:H:129:GLY:N	2.90	0.44
3:H:162:ASN:HB2	3:H:166:LEU:HB2	1.99	0.43
2:L:27(D):HIS:O	2:L:28:ASN:N	2.51	0.43
3:H:103:TRP:N	3:H:103:TRP:CD1	2.85	0.43
2:L:80:ALA:HB1	2:L:168:SER:O	2.18	0.43
3:H:192:THR:O	3:H:195:THR:HG22	2.19	0.43
2:L:118:PHE:CE2	3:H:140:LEU:HA	2.54	0.43
3:H:222:LYS:HE3	3:H:226:GLU:HG2	2.01	0.43
2:L:108:ARG:NH2	2:L:111:ALA:HB2	2.34	0.43
2:L:2:VAL:HG22	2:L:27:GLN:HB2	2.01	0.43
3:H:162:ASN:OD1	3:H:205:ILE:HA	2.19	0.42
2:L:164:THR:HG22	2:L:165:ASP:N	2.34	0.42
3:H:191:VAL:HG21	3:H:205:ILE:CD1	2.49	0.42
3:H:191:VAL:HG21	3:H:205:ILE:HD11	2.01	0.42
3:H:47:TRP:CZ2	3:H:50:VAL:HG22	2.53	0.42
2:L:185:GLU:HG2	2:L:189:HIS:HE1	1.84	0.42
2:L:89:SER:HB3	2:L:98:PHE:CD2	2.55	0.42
3:H:94:ARG:HE	3:H:101:ASP:HB3	1.84	0.41
2:L:210:ASN:O	2:L:212:ASN:N	2.53	0.41
2:L:117:ILE:CD1	2:L:207:LYS:HB3	2.50	0.41
3:H:138:VAL:O	3:H:190:THR:HA	2.20	0.41
2:L:66:GLY:HA3	2:L:71:PHE:HA	2.02	0.41
2:L:8:PRO:HG2	2:L:102:THR:HG23	2.02	0.41
3:H:126:PRO:HD3	3:H:140:LEU:HB3	2.04	0.40
3:H:40:ARG:NH2	3:H:85:ASP:HA	2.36	0.40
2:L:135:PHE:CE2	3:H:188:SER:HB3	2.57	0.40
3:H:38:LYS:HD2	3:H:90:TYR:CE2	2.57	0.40
3:H:16:THR:O	3:H:82(C):LEU:HB2	2.22	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

of similar resolution.

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	P	9/18 (50%)	6 (67%)	1 (11%)	2 (22%)	0 0
2	L	217/219 (99%)	189 (87%)	20 (9%)	8 (4%)	4 23
3	H	218/220 (99%)	189 (87%)	20 (9%)	9 (4%)	3 20
All	All	444/457 (97%)	384 (86%)	41 (9%)	19 (4%)	3 19

All (19) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	L	27(E)	SER
2	L	68	GLY
2	L	211	ARG
3	H	135	GLY
3	H	193	SER
2	L	2	VAL
2	L	51	VAL
3	H	76	SER
3	H	84	SER
3	H	101	ASP
1	P	95	PRO
3	H	134	THR
3	H	179	GLN
2	L	138	ASN
2	L	198	HIS
3	H	29	PHE
1	P	94	ASN
3	H	214	ALA
2	L	128	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	P	10/17 (59%)	8 (80%)	2 (20%)	1 8
2	L	196/197 (100%)	179 (91%)	17 (9%)	13 43
3	H	187/187 (100%)	155 (83%)	32 (17%)	2 12
All	All	393/401 (98%)	342 (87%)	51 (13%)	5 22

All (51) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	P	94	ASN
1	P	98	THR
2	L	53	ASN
2	L	56	SER
2	L	72	THR
2	L	77	ARG
2	L	81	GLU
2	L	117	ILE
2	L	122	SER
2	L	136	LEU
2	L	151	ASP
2	L	157	ASN
2	L	165	ASP
2	L	170	ASP
2	L	179	LEU
2	L	190	ASN
2	L	194	CYS
2	L	208	SER
2	L	211	ARG
3	H	7	SER
3	H	13	ARG
3	H	41	PRO
3	H	43	GLN
3	H	50	VAL
3	H	64	LYS
3	H	68	THR
3	H	74	SER
3	H	82	LEU
3	H	101	ASP
3	H	105	GLN
3	H	110	THR
3	H	113	SER
3	H	115	LYS
3	H	127	VAL

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Mol	Chain	Res	Type
3	H	133	THR
3	H	139	THR
3	H	140	LEU
3	H	142	CYS
3	H	151	PRO
3	H	152	VAL
3	H	156	THR
3	H	163	SER
3	H	166	LEU
3	H	177	VAL
3	H	179	GLN
3	H	180	SER
3	H	190	THR
3	H	191	VAL
3	H	192	THR
3	H	198	SER
3	H	221	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
2	L	210	ASN
3	H	212	HIS

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 carbohydrates in this entry.

5.6 Ligand geometry (i)

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.