Full wwPDB X-ray Structure Validation Report (i)

Jun 13, 2024 – 07:57 AM EDT

PDB ID	:	1MCS
Title	:	PRINCIPLES AND PITFALLS IN DESIGNING SITE DIRECTED PEPTIDE LIGANDS
Authors	:	Edmundson, A.B.; Harris, D.L.; Fan, Z.-C.; Guddat, L.W.
Deposited on	:	1993-02-25
Resolution	:	2.70 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:

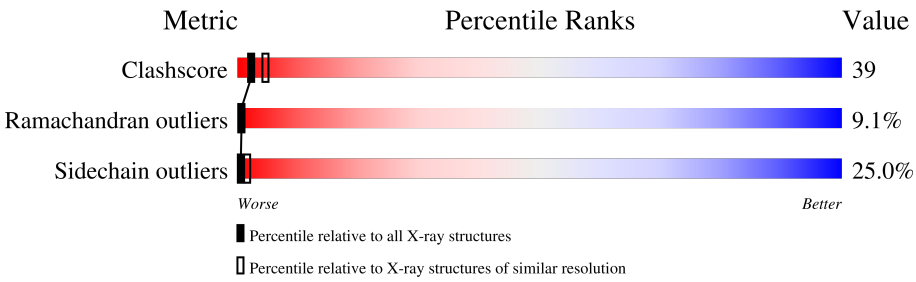
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (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 2.70 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	3122 (2.70-2.70)
Ramachandran outliers	138981	3069 (2.70-2.70)
Sidechain outliers	138945	3069 (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 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	216	31% 47% 19% •
1	B	216	33% 48% 17% •
2	P	5	80% 20%

2 Entry composition (i)

There are 2 unique types of molecules in this entry. The entry contains 3251 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 IMMUNOGLOBULIN LAMBDA DIMER MCG (LIGHT CHAIN).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	216	1605	1000	266	334	5	0	0	0
1	B	216	1605	1000	266	334	5	0	0	0

There are 44 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	20	ILE	PHE	CONFLICT	PIR S14675
A	23	THR	SER	CONFLICT	PIR S14675
A	29	VAL	ILE	CONFLICT	PIR S14675
A	31	GLY	ASN	CONFLICT	PIR S14675
A	39	GLN	ARG	CONFLICT	PIR S14675
A	42	ALA	PRO	CONFLICT	PIR S14675
A	48	VAL	LEU	CONFLICT	PIR S14675
A	49	ILE	MET	CONFLICT	PIR S14675
A	54	ASN	THR	CONFLICT	PIR S14675
A	62	ASP	ASN	CONFLICT	PIR S14675
A	94	GLU	ALA	CONFLICT	PIR S14675
A	97	ASP	ASN	CONFLICT	PIR S14675
A	98	ASN	SER	CONFLICT	PIR S14675
A	99	PHE	LEU	CONFLICT	PIR S14675
A	100	VAL	ILE	CONFLICT	PIR S14675
A	103	THR	GLY	CONFLICT	PIR S14675
A	106	LYS	ARG	CONFLICT	PIR S14675
A	107	VAL	LEU	CONFLICT	PIR S14675
A	116	ASN	ALA	CONFLICT	PIR S14675
A	118	THR	SER	CONFLICT	PIR S14675
A	156	GLY	SER	CONFLICT	PIR S14675
A	167	LYS	THR	CONFLICT	PIR S14675
B	20	ILE	PHE	CONFLICT	PIR S14675
B	23	THR	SER	CONFLICT	PIR S14675

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
B	29	VAL	ILE	CONFLICT	PIR S14675
B	31	GLY	ASN	CONFLICT	PIR S14675
B	39	GLN	ARG	CONFLICT	PIR S14675
B	42	ALA	PRO	CONFLICT	PIR S14675
B	48	VAL	LEU	CONFLICT	PIR S14675
B	49	ILE	MET	CONFLICT	PIR S14675
B	54	ASN	THR	CONFLICT	PIR S14675
B	62	ASP	ASN	CONFLICT	PIR S14675
B	94	GLU	ALA	CONFLICT	PIR S14675
B	97	ASP	ASN	CONFLICT	PIR S14675
B	98	ASN	SER	CONFLICT	PIR S14675
B	99	PHE	LEU	CONFLICT	PIR S14675
B	100	VAL	ILE	CONFLICT	PIR S14675
B	103	THR	GLY	CONFLICT	PIR S14675
B	106	LYS	ARG	CONFLICT	PIR S14675
B	107	VAL	LEU	CONFLICT	PIR S14675
B	116	ASN	ALA	CONFLICT	PIR S14675
B	118	THR	SER	CONFLICT	PIR S14675
B	156	GLY	SER	CONFLICT	PIR S14675
B	167	LYS	THR	CONFLICT	PIR S14675

- Molecule 2 is a protein called PEPTIDE N-ACETYL-L-GLN-D-PHE-L-HIS-D-PRO-OH.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
2	P	5	41	27	7	7	0	0	0

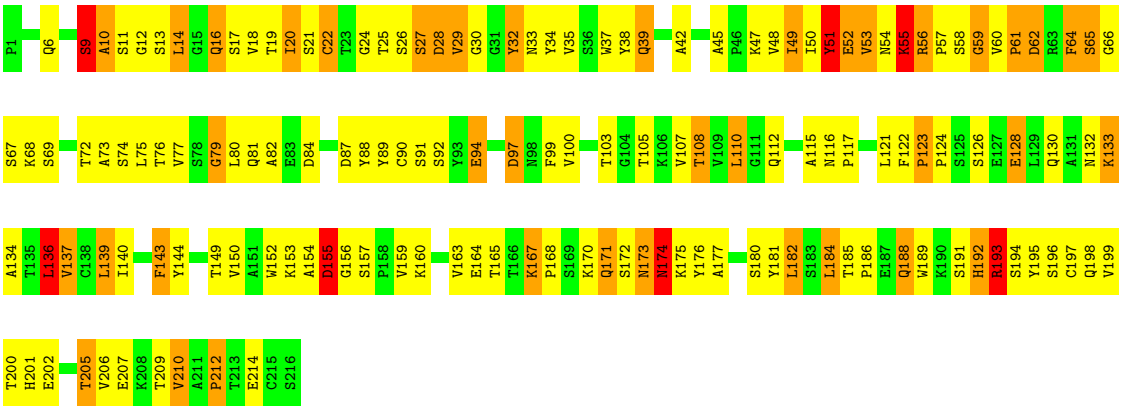
3 Residue-property plots (i)

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.

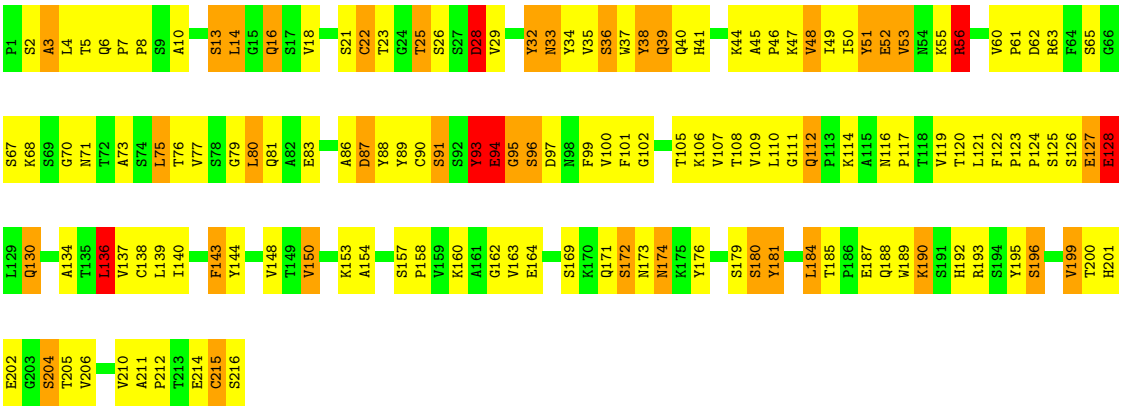
• Molecule 1: IMMUNOGLOBULIN LAMBDA DIMER MCG (LIGHT CHAIN)

Chain A: 31% 47% 19% •



• Molecule 1: IMMUNOGLOBULIN LAMBDA DIMER MCG (LIGHT CHAIN)

Chain B: 33% 48% 17% •



• Molecule 2: PEPTIDE N-ACETYL-L-GLN-D-PHE-L-HIS-D-PRO-OH

Chain P: 80% 20%

ACE0
Q1
F2
H3
P4

4 Data and refinement statistics (i)

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

Property	Value	Source
Space group	P 31 2 1	Depositor
Cell constants a, b, c, α, β, γ	72.30Å 72.30Å 185.90Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	6.00 – 2.70	Depositor
% Data completeness (in resolution range)	(Not available) (6.00-2.70)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	PROLSQ, X-PLOR	Depositor
R, R_{free}	0.183 , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	3251	wwPDB-VP
Average B, all atoms ($Å^2$)	0.0	wwPDB-VP

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: ACE, DPR, DPN

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	0.86	0/1644	1.45	11/2241 (0.5%)
1	B	0.87	0/1644	1.40	11/2241 (0.5%)
2	P	0.72	0/19	1.65	0/23
All	All	0.86	0/3307	1.43	22/4505 (0.5%)

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	A	0	1
2	P	0	1
All	All	0	2

There are no bond length outliers.

All (22) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	136	LEU	CA-CB-CG	9.87	138.00	115.30
1	A	51	TYR	CA-CB-CG	8.23	129.04	113.40
1	A	136	LEU	CA-CB-CG	7.14	131.73	115.30
1	A	193	ARG	NE-CZ-NH1	6.74	123.67	120.30
1	A	51	TYR	CB-CG-CD1	6.68	125.01	121.00
1	B	128	GLU	CA-CB-CG	6.42	127.51	113.40
1	B	51	TYR	CA-CB-CG	6.41	125.58	113.40
1	B	56	ARG	NE-CZ-NH1	6.40	123.50	120.30
1	B	22	CYS	CB-CA-C	6.40	123.19	110.40
1	A	22	CYS	CA-CB-SG	6.19	125.14	114.00
1	A	87	ASP	CB-CG-OD1	6.11	123.80	118.30

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	174	ASN	N-CA-CB	5.93	121.27	110.60
1	B	181	TYR	CA-CB-CG	5.74	124.31	113.40
1	B	193	ARG	NE-CZ-NH1	5.66	123.13	120.30
1	A	90	CYS	CA-CB-SG	5.60	124.08	114.00
1	A	97	ASP	CB-CG-OD1	5.53	123.27	118.30
1	B	22	CYS	CA-CB-SG	5.49	123.88	114.00
1	A	51	TYR	CB-CG-CD2	-5.32	117.81	121.00
1	B	87	ASP	CA-CB-CG	5.26	124.97	113.40
1	B	193	ARG	NE-CZ-NH2	-5.23	117.69	120.30
1	A	79	GLY	N-CA-C	-5.13	100.28	113.10
1	B	93	TYR	CB-CG-CD1	5.04	124.02	121.00

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	167	LYS	Peptide
2	P	3	HIS	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	1605	0	1540	137	0
1	B	1605	0	1540	130	0
2	P	41	0	34	10	0
All	All	3251	0	3114	248	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 39.

All (248) 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:A:167:LYS:HB3	1:A:168:PRO:CD	1.85	1.05

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:167:LYS:HB3	1:A:168:PRO:HD3	1.06	1.04
1:A:167:LYS:CB	1:A:168:PRO:HD3	1.86	1.03
1:B:105:THR:HG22	1:B:106:LYS:H	1.40	0.84
1:B:86:ALA:HB3	1:B:88:TYR:HE1	1.44	0.83
1:B:40:GLN:O	1:B:86:ALA:HB1	1.79	0.82
1:A:65:SER:HB2	1:A:76:THR:HB	1.62	0.82
1:B:13:SER:H	1:B:16:GLN:HB2	1.44	0.81
1:A:200:THR:HB	1:A:205:THR:HG23	1.63	0.81
1:A:171:GLN:HG3	1:A:175:LYS:O	1.83	0.79
1:A:53:VAL:HG21	1:A:68:LYS:HB2	1.63	0.78
1:A:153:LYS:HB2	1:A:196:SER:HB2	1.66	0.78
1:B:51:TYR:HB2	2:P:2:DPN:HZ	1.65	0.77
1:B:77:VAL:HG11	1:B:80:LEU:HD22	1.68	0.76
1:B:49:ILE:O	1:B:60:VAL:HG11	1.86	0.75
1:B:80:LEU:HD21	1:B:107:VAL:HG11	1.68	0.74
1:B:16:GLN:O	1:B:80:LEU:HB2	1.87	0.74
1:A:168:PRO:HB2	1:A:176:TYR:HD2	1.53	0.74
1:A:20:ILE:HG12	1:A:75:LEU:HB3	1.68	0.73
1:B:48:VAL:HG11	2:P:0:ACE:H3	1.70	0.73
1:A:10:ALA:HB3	1:A:107:VAL:HG22	1.70	0.72
1:A:16:GLN:O	1:A:80:LEU:HB2	1.89	0.72
1:A:50:ILE:HD13	1:A:56:ARG:HG3	1.72	0.71
1:A:171:GLN:HB2	1:B:164:GLU:OE1	1.90	0.71
1:A:168:PRO:HB2	1:A:176:TYR:CD2	2.26	0.70
1:A:139:LEU:HD11	1:B:181:TYR:CD2	2.26	0.70
1:B:6:GLN:NE2	1:B:88:TYR:O	2.25	0.70
1:B:134:ALA:O	1:B:184:LEU:HD12	1.91	0.70
1:B:125:SER:HB3	1:B:128:GLU:HB3	1.75	0.69
1:A:121:LEU:HD12	1:A:122:PHE:H	1.57	0.69
1:A:150:VAL:HG22	1:A:199:VAL:HG22	1.74	0.69
1:B:29:VAL:HG22	1:B:68:LYS:HE3	1.73	0.68
1:A:165:THR:HA	1:A:180:SER:HA	1.76	0.68
1:B:51:TYR:CB	2:P:2:DPN:HZ	2.23	0.68
1:B:96:SER:HA	1:B:99:PHE:HE1	1.59	0.67
1:A:124:PRO:HD3	1:A:136:LEU:HD22	1.76	0.67
1:A:51:TYR:HE2	1:B:97:ASP:HA	1.58	0.67
1:A:171:GLN:O	1:A:173:ASN:N	2.27	0.67
1:B:44:LYS:HD3	1:B:45:ALA:O	1.94	0.67
1:A:34:TYR:O	1:A:92:SER:HA	1.94	0.66
1:B:163:VAL:HA	1:B:181:TYR:O	1.96	0.66
1:B:26:SER:HB3	1:B:28:ASP:HB3	1.77	0.66

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:198:GLN:HB3	1:A:207:GLU:HG3	1.78	0.66
1:B:56:ARG:HB3	1:B:60:VAL:HB	1.78	0.65
1:A:164:GLU:CD	1:B:171:GLN:HB3	2.17	0.65
1:B:124:PRO:HD3	1:B:136:LEU:HD13	1.79	0.65
1:A:139:LEU:HD13	1:B:137:VAL:CG2	2.27	0.64
1:A:171:GLN:HG2	1:A:177:ALA:HB2	1.78	0.64
1:B:36:SER:HB3	2:P:2:DPN:HE2	1.79	0.64
1:A:139:LEU:HD13	1:B:137:VAL:HG21	1.80	0.63
1:A:45:ALA:HA	1:B:89:TYR:CE2	2.33	0.63
1:A:61:PRO:HB2	1:A:64:PHE:HD2	1.64	0.63
1:A:61:PRO:HB2	1:A:64:PHE:CD2	2.34	0.63
1:A:99:PHE:CE2	2:P:1:GLN:HB2	2.33	0.63
1:B:32:TYR:OH	1:B:93:TYR:HB3	1.99	0.63
1:A:11:SER:HB3	1:A:110:LEU:HD21	1.81	0.62
1:B:3:ALA:O	1:B:25:THR:HB	1.99	0.62
1:B:14:LEU:H	1:B:14:LEU:HD22	1.65	0.62
1:B:86:ALA:HB3	1:B:88:TYR:CE1	2.32	0.61
1:B:192:HIS:O	1:B:212:PRO:HG2	1.99	0.61
1:A:128:GLU:HG2	1:A:133:LYS:HE3	1.82	0.61
1:B:13:SER:N	1:B:16:GLN:HB2	2.15	0.61
1:A:155:ASP:OD2	1:A:192:HIS:HB2	2.01	0.61
1:A:165:THR:HG23	1:A:180:SER:HB2	1.81	0.61
1:A:49:ILE:O	1:A:57:PRO:HD2	2.01	0.60
1:A:12:GLY:HA3	1:A:80:LEU:HD21	1.84	0.60
1:B:75:LEU:HD12	1:B:76:THR:N	2.17	0.60
1:B:14:LEU:HD13	1:B:109:VAL:HG11	1.83	0.59
1:A:124:PRO:HG3	1:A:134:ALA:HB1	1.83	0.59
1:B:10:ALA:O	1:B:107:VAL:HA	2.02	0.59
1:B:35:VAL:HG11	1:B:73:ALA:HB1	1.83	0.59
1:B:96:SER:O	1:B:97:ASP:HB2	2.02	0.59
1:B:123:PRO:HA	1:B:136:LEU:HD13	1.85	0.59
1:A:37:TRP:HB2	1:A:50:ILE:HB	1.84	0.59
1:A:51:TYR:HE2	1:B:97:ASP:CA	2.16	0.59
1:A:132:ASN:O	1:A:132:ASN:ND2	2.36	0.59
1:B:169:SER:O	1:B:176:TYR:HA	2.03	0.59
1:A:58:SER:H	1:B:97:ASP:HB3	1.68	0.58
1:A:56:ARG:HD2	1:A:64:PHE:O	2.04	0.57
1:A:88:TYR:HB2	1:A:105:THR:CG2	2.35	0.57
1:B:49:ILE:O	1:B:50:ILE:HG13	2.04	0.57
1:B:117:PRO:HB3	1:B:140:ILE:HG23	1.87	0.57
1:A:19:THR:HA	1:A:75:LEU:O	2.04	0.57

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:28:ASP:HB3	1:A:94:GLU:HB3	1.87	0.57
1:A:35:VAL:HA	1:A:91:SER:O	2.05	0.56
1:A:121:LEU:HD12	1:A:122:PHE:N	2.20	0.56
1:B:33:ASN:O	1:B:53:VAL:HG23	2.05	0.56
1:B:179:SER:O	1:B:180:SER:HB2	2.04	0.56
1:B:188:GLN:H	1:B:188:GLN:NE2	2.04	0.56
1:B:119:VAL:HG21	1:B:206:VAL:HG23	1.88	0.56
1:B:154:ALA:HB2	1:B:195:TYR:CE1	2.41	0.56
1:A:20:ILE:CG1	1:A:75:LEU:HB3	2.36	0.55
1:A:184:LEU:HD11	1:A:195:TYR:CE2	2.41	0.55
1:A:39:GLN:HG2	1:A:88:TYR:CE2	2.42	0.55
1:B:37:TRP:HB2	1:B:50:ILE:HB	1.89	0.55
1:B:153:LYS:HZ3	1:B:196:SER:HB2	1.72	0.55
1:B:41:HIS:HB2	1:B:44:LYS:HD2	1.89	0.55
1:B:56:ARG:HG2	1:B:60:VAL:HG12	1.89	0.55
1:A:123:PRO:HG3	1:A:210:VAL:HG11	1.89	0.54
1:A:159:VAL:HG11	1:A:182:LEU:HD11	1.89	0.54
1:A:184:LEU:HD11	1:A:195:TYR:OH	2.07	0.54
1:B:143:PHE:HD1	1:B:143:PHE:H	1.55	0.54
1:A:13:SER:N	1:A:16:GLN:HE21	2.05	0.54
1:B:29:VAL:HG11	1:B:71:ASN:HD22	1.72	0.54
1:A:140:ILE:HG23	1:A:199:VAL:HG11	1.90	0.54
1:B:93:TYR:O	1:B:95:GLY:N	2.41	0.54
1:A:139:LEU:HD11	1:B:181:TYR:HD2	1.73	0.54
1:B:110:LEU:HD11	1:B:114:LYS:HE3	1.90	0.53
1:B:200:THR:HG23	1:B:205:THR:OG1	2.08	0.53
1:B:140:ILE:HG12	1:B:199:VAL:HG21	1.91	0.53
1:A:84:ASP:HB2	1:A:88:TYR:OH	2.08	0.53
1:B:190:LYS:HD2	1:B:190:LYS:C	2.29	0.53
1:A:13:SER:N	1:A:80:LEU:HD23	2.23	0.53
1:A:132:ASN:OD1	1:A:186:PRO:HG2	2.08	0.52
1:A:12:GLY:O	1:A:110:LEU:HD22	2.10	0.52
1:A:134:ALA:O	1:A:184:LEU:HB2	2.09	0.52
1:B:111:GLY:O	1:B:112:GLN:HB2	2.09	0.52
1:B:150:VAL:HG21	1:B:180:SER:OG	2.08	0.52
1:B:32:TYR:CZ	1:B:93:TYR:HB3	2.44	0.52
1:A:27:SER:O	1:A:32:TYR:HE1	1.92	0.52
1:A:51:TYR:HE2	1:B:97:ASP:N	2.07	0.52
1:B:96:SER:HA	1:B:99:PHE:CE1	2.43	0.52
1:B:121:LEU:HD12	1:B:122:PHE:H	1.75	0.52
1:A:21:SER:HA	1:A:73:ALA:O	2.11	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:50:ILE:HD12	1:A:54:ASN:HA	1.92	0.51
1:A:48:VAL:O	1:A:57:PRO:HG2	2.09	0.51
1:A:193:ARG:O	1:A:212:PRO:HD2	2.11	0.51
1:B:14:LEU:CD1	1:B:109:VAL:HG11	2.40	0.51
1:A:9:SER:O	1:A:105:THR:OG1	2.29	0.51
1:B:143:PHE:HE2	1:B:148:VAL:HB	1.76	0.51
1:B:189:TRP:CZ3	1:B:212:PRO:HG3	2.47	0.50
1:A:19:THR:OG1	1:A:76:THR:HA	2.12	0.50
1:A:186:PRO:HA	1:A:189:TRP:HB3	1.94	0.50
1:B:127:GLU:HA	1:B:130:GLN:HB2	1.94	0.50
1:B:7:PRO:O	1:B:105:THR:HG23	2.12	0.50
1:A:121:LEU:HD22	1:A:197:CYS:HB3	1.93	0.50
1:A:163:VAL:HA	1:A:181:TYR:O	2.12	0.49
1:B:93:TYR:CE1	2:P:2:DPN:HA	2.46	0.49
1:A:20:ILE:O	1:A:74:SER:HA	2.12	0.49
1:A:37:TRP:HA	1:A:89:TYR:O	2.11	0.49
1:B:6:GLN:OE1	1:B:102:GLY:HA3	2.13	0.49
1:B:49:ILE:HA	1:B:60:VAL:HG21	1.95	0.49
1:A:45:ALA:HA	1:B:89:TYR:HE2	1.78	0.49
1:A:184:LEU:HD11	1:A:195:TYR:CZ	2.47	0.49
1:A:198:GLN:HA	1:A:206:VAL:O	2.13	0.49
1:B:143:PHE:CE2	1:B:148:VAL:HB	2.48	0.49
1:A:16:GLN:HG2	1:A:17:SER:N	2.27	0.49
1:B:75:LEU:HD21	1:B:88:TYR:HD2	1.77	0.49
1:A:156:GLY:O	1:A:157:SER:C	2.52	0.48
1:B:187:GLU:HB3	1:B:188:GLN:NE2	2.29	0.48
1:A:153:LYS:HD2	1:A:156:GLY:O	2.13	0.48
1:B:44:LYS:HG2	1:B:45:ALA:H	1.78	0.48
1:B:93:TYR:HE1	1:B:99:PHE:CZ	2.33	0.47
1:A:57:PRO:HA	1:B:97:ASP:HA	1.96	0.47
1:B:94:GLU:OE1	1:B:100:VAL:HG22	2.14	0.47
1:A:64:PHE:CD1	1:A:77:VAL:HG22	2.50	0.47
1:A:185:THR:N	1:A:188:GLN:OE1	2.48	0.47
1:A:115:ALA:HB3	1:A:144:TYR:N	2.29	0.47
1:B:7:PRO:HA	1:B:8:PRO:HD3	1.82	0.47
1:B:171:GLN:C	1:B:173:ASN:H	2.18	0.47
1:A:13:SER:O	1:A:16:GLN:HB3	2.15	0.47
1:A:124:PRO:CD	1:A:136:LEU:HD22	2.42	0.47
1:A:150:VAL:HG11	1:A:180:SER:HB3	1.95	0.47
1:A:91:SER:HA	1:A:100:VAL:O	2.15	0.47
1:A:38:TYR:O	1:A:88:TYR:HA	2.15	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:24:GLY:HA3	1:A:29:VAL:HB	1.96	0.46
1:A:34:TYR:CE2	2:P:4:DPR:HD3	2.51	0.46
1:B:117:PRO:HB3	1:B:140:ILE:CG2	2.44	0.46
1:A:167:LYS:CB	1:A:168:PRO:CD	2.65	0.46
1:A:48:VAL:HG21	1:B:99:PHE:HB2	1.98	0.46
1:A:150:VAL:HG11	1:A:180:SER:CB	2.45	0.46
1:A:159:VAL:HG22	1:A:159:VAL:O	2.15	0.46
1:B:80:LEU:HD21	1:B:107:VAL:CG1	2.41	0.46
1:A:11:SER:HA	1:A:108:THR:O	2.17	0.45
1:A:137:VAL:CG2	1:B:139:LEU:HD22	2.46	0.45
1:B:2:SER:C	1:B:4:LEU:H	2.19	0.45
1:A:51:TYR:CE2	1:B:97:ASP:N	2.84	0.45
1:A:168:PRO:CB	1:A:176:TYR:HD2	2.26	0.45
1:B:179:SER:O	1:B:180:SER:CB	2.65	0.45
1:B:171:GLN:O	1:B:173:ASN:N	2.49	0.45
1:A:51:TYR:HE2	1:B:97:ASP:H	1.64	0.45
1:B:32:TYR:HE2	1:B:94:GLU:HA	1.82	0.45
1:A:53:VAL:CG2	1:A:68:LYS:HB2	2.40	0.45
1:A:126:SER:O	1:A:130:GLN:HG2	2.17	0.45
1:B:29:VAL:CG1	1:B:71:ASN:HD22	2.30	0.45
1:A:47:LYS:HA	1:A:47:LYS:HD3	1.71	0.44
1:A:54:ASN:HB2	1:A:66:GLY:O	2.17	0.44
1:A:124:PRO:HD3	1:A:136:LEU:CD2	2.46	0.44
1:A:159:VAL:CG1	1:A:182:LEU:HD11	2.47	0.44
1:B:39:GLN:HG2	1:B:47:LYS:HD3	1.99	0.44
1:B:35:VAL:HG11	1:B:73:ALA:CB	2.47	0.44
1:B:35:VAL:HA	1:B:91:SER:O	2.18	0.44
1:A:50:ILE:HD12	1:A:55:LYS:H	1.82	0.44
1:B:7:PRO:HD3	1:B:21:SER:O	2.17	0.44
1:B:13:SER:O	1:B:80:LEU:HB3	2.17	0.44
1:A:54:ASN:O	1:A:55:LYS:HB2	2.17	0.44
1:A:59:GLY:O	1:A:60:VAL:HG23	2.18	0.44
1:B:56:ARG:HG2	1:B:60:VAL:CG1	2.48	0.43
1:B:157:SER:HA	1:B:158:PRO:HD2	1.75	0.43
1:A:50:ILE:CD1	1:A:55:LYS:H	2.31	0.43
1:A:52:GLU:O	1:A:54:ASN:N	2.47	0.43
1:B:61:PRO:C	1:B:63:ARG:H	2.22	0.43
1:B:143:PHE:HE2	1:B:148:VAL:CB	2.30	0.43
1:B:119:VAL:HG12	1:B:138:CYS:SG	2.58	0.43
1:B:18:VAL:CG2	1:B:80:LEU:HD23	2.49	0.43
1:B:153:LYS:NZ	1:B:196:SER:HB2	2.33	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:88:TYR:HB2	1:A:105:THR:HG23	2.01	0.43
1:A:186:PRO:O	1:A:189:TRP:HB3	2.19	0.43
1:B:38:TYR:CE1	1:B:91:SER:HB2	2.54	0.43
1:B:144:TYR:O	1:B:201:HIS:CE1	2.72	0.42
1:A:6:GLN:HE22	1:A:89:TYR:HA	1.84	0.42
1:A:99:PHE:HD2	2:P:1:GLN:NE2	2.17	0.42
1:A:191:SER:OG	1:A:192:HIS:CD2	2.72	0.42
1:A:16:GLN:CG	1:A:17:SER:N	2.83	0.42
1:B:116:ASN:OD1	1:B:204:SER:OG	2.34	0.42
1:B:61:PRO:O	1:B:63:ARG:N	2.52	0.42
1:A:140:ILE:HG12	1:A:199:VAL:CG2	2.50	0.42
1:A:154:ALA:CA	1:A:159:VAL:HB	2.50	0.42
1:B:90:CYS:O	1:B:101:PHE:HA	2.20	0.42
1:B:163:VAL:HG23	1:B:181:TYR:O	2.19	0.42
1:A:65:SER:O	1:A:75:LEU:HD12	2.19	0.42
1:B:40:GLN:OE1	1:B:46:PRO:HG3	2.20	0.42
1:B:184:LEU:HB2	1:B:185:THR:H	1.68	0.42
1:A:143:PHE:HD2	1:A:201:HIS:CE1	2.38	0.41
1:B:75:LEU:HD21	1:B:88:TYR:CD2	2.56	0.41
1:A:152:TRP:HB3	1:A:159:VAL:CG1	2.51	0.41
1:A:57:PRO:HB3	1:B:97:ASP:O	2.20	0.41
1:B:48:VAL:CG1	2:P:0:ACE:H3	2.46	0.41
1:B:51:TYR:CE1	1:B:55:LYS:HB2	2.56	0.41
1:A:82:ALA:HB1	1:A:112:GLN:OE1	2.21	0.41
1:B:4:LEU:HA	1:B:23:THR:O	2.20	0.41
1:A:50:ILE:HG21	1:A:53:VAL:O	2.20	0.41
1:B:211:ALA:HA	1:B:212:PRO:HD3	1.79	0.41
1:B:36:SER:CB	2:P:2:DPN:HE2	2.49	0.41
1:B:120:THR:HG22	1:B:122:PHE:CE1	2.56	0.41
1:B:171:GLN:O	1:B:174:ASN:N	2.51	0.41
1:A:60:VAL:HA	1:A:61:PRO:HD2	1.73	0.40
1:A:170:LYS:HD3	1:A:174:ASN:OD1	2.21	0.40
1:A:51:TYR:CE2	1:B:97:ASP:HA	2.46	0.40
1:A:14:LEU:HD23	1:A:110:LEU:O	2.22	0.40
1:A:84:ASP:HB2	1:A:88:TYR:HH	1.85	0.40
1:A:116:ASN:HA	1:A:117:PRO:HD3	1.82	0.40
1:B:90:CYS:O	1:B:90:CYS:SG	2.79	0.40
1:A:49:ILE:HD12	1:A:60:VAL:HG13	2.03	0.40
1:A:117:PRO:HD3	1:A:201:HIS:CD2	2.56	0.40
1:A:152:TRP:H	1:A:160:LYS:HD3	1.87	0.40
1:A:154:ALA:HB3	1:A:157:SER:O	2.22	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:40:GLN:O	1:B:86:ALA:CB	2.60	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	214/216 (99%)	155 (72%)	38 (18%)	21 (10%)	0	0
1	B	214/216 (99%)	164 (77%)	33 (15%)	17 (8%)	1	1
2	P	2/5 (40%)	1 (50%)	0	1 (50%)	0	0
All	All	430/437 (98%)	320 (74%)	71 (16%)	39 (9%)	1	0

All (39) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	10	ALA
1	A	14	LEU
1	A	55	LYS
1	A	172	SER
1	A	173	ASN
1	A	174	ASN
1	A	192	HIS
1	A	212	PRO
1	B	48	VAL
1	B	62	ASP
1	B	94	GLU
1	B	112	GLN
1	B	180	SER
1	B	202	GLU
1	A	61	PRO
1	A	79	GLY

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	193	ARG
1	B	34	TYR
1	B	52	GLU
1	B	172	SER
1	A	29	VAL
1	A	42	ALA
1	A	62	ASP
1	A	155	ASP
1	B	3	ALA
1	B	28	ASP
1	A	16	GLN
1	B	70	GLY
1	B	215	CYS
1	A	59	GLY
1	B	79	GLY
2	P	1	GLN
1	A	9	SER
1	A	49	ILE
1	A	123	PRO
1	B	53	VAL
1	B	95	GLY
1	A	30	GLY
1	B	162	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	181/181 (100%)	135 (75%)	46 (25%)	0 1
1	B	181/181 (100%)	136 (75%)	45 (25%)	0 1
2	P	2/2 (100%)	2 (100%)	0	100 100
All	All	364/364 (100%)	273 (75%)	91 (25%)	0 1

All (91) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	9	SER
1	A	18	VAL
1	A	20	ILE
1	A	22	CYS
1	A	25	THR
1	A	26	SER
1	A	27	SER
1	A	28	ASP
1	A	32	TYR
1	A	33	ASN
1	A	39	GLN
1	A	51	TYR
1	A	52	GLU
1	A	53	VAL
1	A	55	LYS
1	A	56	ARG
1	A	62	ASP
1	A	64	PHE
1	A	65	SER
1	A	67	SER
1	A	69	SER
1	A	72	THR
1	A	81	GLN
1	A	94	GLU
1	A	97	ASP
1	A	103	THR
1	A	108	THR
1	A	110	LEU
1	A	128	GLU
1	A	133	LYS
1	A	136	LEU
1	A	137	VAL
1	A	139	LEU
1	A	143	PHE
1	A	149	THR
1	A	155	ASP
1	A	171	GLN
1	A	182	LEU
1	A	184	LEU
1	A	188	GLN
1	A	194	SER
1	A	202	GLU
1	A	205	THR

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	209	THR
1	A	210	VAL
1	A	214	GLU
1	B	5	THR
1	B	13	SER
1	B	14	LEU
1	B	16	GLN
1	B	22	CYS
1	B	25	THR
1	B	28	ASP
1	B	32	TYR
1	B	33	ASN
1	B	36	SER
1	B	38	TYR
1	B	39	GLN
1	B	52	GLU
1	B	56	ARG
1	B	65	SER
1	B	67	SER
1	B	75	LEU
1	B	80	LEU
1	B	81	GLN
1	B	83	GLU
1	B	87	ASP
1	B	91	SER
1	B	93	TYR
1	B	94	GLU
1	B	96	SER
1	B	108	THR
1	B	126	SER
1	B	127	GLU
1	B	128	GLU
1	B	130	GLN
1	B	136	LEU
1	B	143	PHE
1	B	150	VAL
1	B	160	LYS
1	B	172	SER
1	B	174	ASN
1	B	184	LEU
1	B	190	LYS
1	B	196	SER

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	199	VAL
1	B	204	SER
1	B	210	VAL
1	B	214	GLU
1	B	215	CYS
1	B	216	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (15) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	16	GLN
1	A	71	ASN
1	A	81	GLN
1	A	130	GLN
1	A	171	GLN
1	A	173	ASN
1	A	192	HIS
1	A	198	GLN
1	A	201	HIS
1	B	54	ASN
1	B	71	ASN
1	B	81	GLN
1	B	130	GLN
1	B	188	GLN
2	P	1	GLN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

2 non-standard protein/DNA/RNA residues are modelled in this entry.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

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.