Full wwPDB X-ray Structure Validation Report (i)

Jan 31, 2016 – 07:30 PM GMT

PDB ID	:	1FVP
Title	:	FLAVOPROTEIN 390
Authors	:	Kita, A.; Miki, K.
Deposited on	:	1995-07-07
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
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:

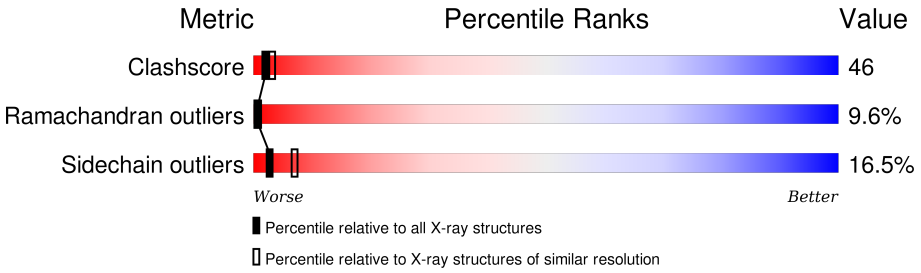
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)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

1 Overall quality at a glance (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	102246	2422 (2.70-2.70)
Ramachandran outliers	100387	2382 (2.70-2.70)
Sidechain outliers	100360	2382 (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.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	231	32% 51% 15% •
1	B	231	28% 50% 20% •

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 3997 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.

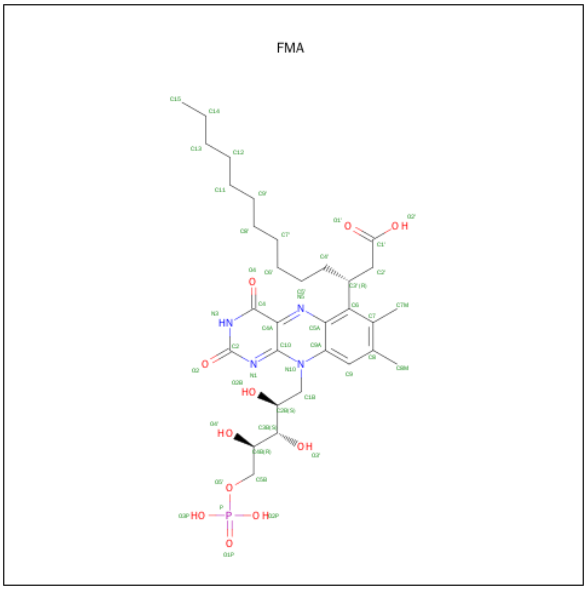
- Molecule 1 is a protein called FLAVOPROTEIN 390.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	231	Total	C	N	O	S	0	0	0
			1874	1193	306	367	8			
1	B	231	Total	C	N	O	S	0	0	0
			1874	1193	306	367	8			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	64	PRO	SER	CONFLICT	UNP P12745
B	64	PRO	SER	CONFLICT	UNP P12745

- Molecule 2 is 6-(3-TETRADECANOIC ACID) FLAVINE MONONUCLEOTIDE (three-letter code: FMA) (formula: $C_{31}H_{47}N_4O_{11}P$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	0	0
			47	31	4	11	1		

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	0	0
			47	31	4	11	1		
2	B	1	Total	C	N	O	P	0	0
			47	31	4	11	1		
2	B	1	Total	C	N	O	P	0	0
			47	31	4	11	1		

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	37	Total	O	0	0
			37	37		
3	B	24	Total	O	0	0
			24	24		

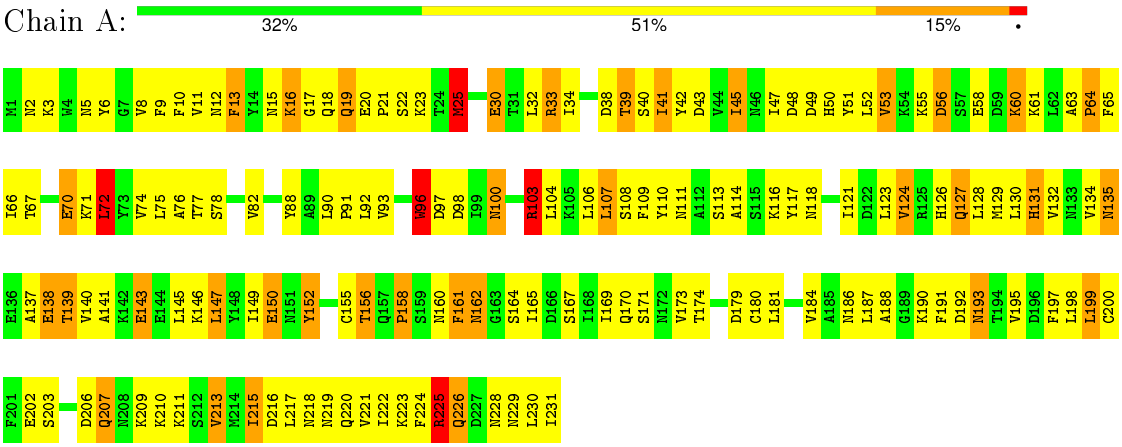
3 Residue-property plots (i)

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.

Note EDS was not executed.

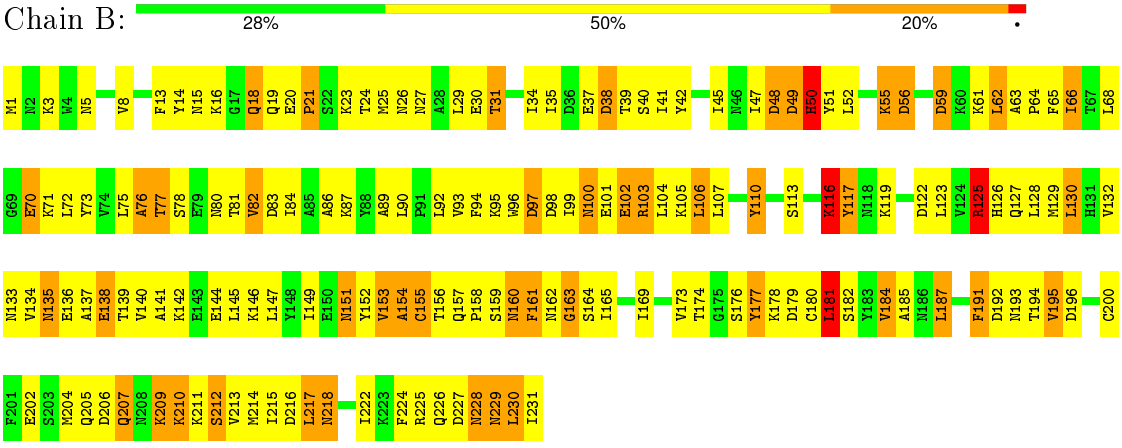
- Molecule 1: FLAVOPROTEIN 390

Chain A:



- Molecule 1: FLAVOPROTEIN 390

Chain B:



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 43 2 2	Depositor
Cell constants a, b, c, α, β, γ	76.80Å 76.80Å 242.00Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	6.00 – 2.70	Depositor
% Data completeness (in resolution range)	(Not available) (6.00-2.70)	Depositor
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	PROLSQ, X-PLOR 3.1	Depositor
R, R_{free}	0.240 , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	3997	wwPDB-VP
Average B, all atoms (Å^2)	35.0	wwPDB-VP

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: FMA

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	0.77	0/1907	1.62	15/2578 (0.6%)
1	B	0.76	0/1907	1.57	14/2578 (0.5%)
All	All	0.76	0/3814	1.59	29/5156 (0.6%)

There are no bond length outliers.

All (29) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	96	TRP	CA-CB-CG	15.08	142.36	113.70
1	B	125	ARG	NE-CZ-NH1	10.21	125.41	120.30
1	A	103	ARG	NE-CZ-NH1	7.92	124.26	120.30
1	A	33	ARG	NE-CZ-NH2	-7.49	116.56	120.30
1	B	98	ASP	CA-CB-CG	6.97	128.74	113.40
1	B	98	ASP	CB-CG-OD1	6.87	124.48	118.30
1	A	179	ASP	CB-CG-OD1	6.83	124.45	118.30
1	B	59	ASP	CB-CG-OD1	6.74	124.36	118.30
1	A	96	TRP	CB-CG-CD2	6.46	135.00	126.60
1	B	50	HIS	CA-CB-CG	6.24	124.20	113.60
1	B	103	ARG	CD-NE-CZ	6.20	132.28	123.60
1	A	72	LEU	CA-CB-CG	6.12	129.39	115.30
1	B	125	ARG	NE-CZ-NH2	-6.00	117.30	120.30
1	A	103	ARG	NE-CZ-NH2	-5.83	117.38	120.30
1	A	111	ASN	CB-CA-C	5.70	121.81	110.40
1	B	187	LEU	CB-CA-C	5.58	120.80	110.20
1	A	143	GLU	CG-CD-OE1	5.56	129.42	118.30
1	A	25	MET	CA-CB-CG	-5.50	103.95	113.30
1	A	202	GLU	CA-CB-CG	5.40	125.28	113.40
1	B	117	TYR	CB-CG-CD1	5.39	124.23	121.00
1	B	152	TYR	C-N-CA	5.37	135.12	121.70
1	B	110	TYR	CA-CB-CG	5.27	123.42	113.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	33	ARG	NE-CZ-NH1	5.21	122.91	120.30
1	A	135	ASN	CB-CA-C	5.21	120.82	110.40
1	A	216	ASP	CB-CG-OD2	-5.18	113.64	118.30
1	B	38	ASP	CB-CG-OD1	5.15	122.94	118.30
1	B	163	GLY	N-CA-C	-5.10	100.34	113.10
1	A	109	PHE	CA-CB-CG	5.09	126.12	113.90
1	B	56	ASP	CB-CG-OD1	5.04	122.83	118.30

There are no chirality outliers.

There are no planarity outliers.

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	1874	0	1851	163	0
1	B	1874	0	1851	189	0
2	A	94	0	88	20	0
2	B	94	0	88	27	0
3	A	37	0	0	3	0
3	B	24	0	0	2	0
All	All	3997	0	3878	359	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 46.

All (359) 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:135:ASN:HD21	1:A:140:VAL:HB	1.21	1.02
1:A:3:LYS:HB2	1:A:230:LEU:HD22	1.41	0.99
1:A:184:VAL:HG21	2:A:233:FMA:H111	1.47	0.95
1:A:25:MET:HG3	2:B:232:FMA:H6'1	1.50	0.94
1:B:1:MET:HE1	2:B:233:FMA:H1'2	1.51	0.93
2:B:232:FMA:N5	2:B:232:FMA:H2'1	1.87	0.88
1:A:145:LEU:HD23	1:A:169:ILE:HG23	1.55	0.88

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:18:GLN:HG2	1:B:147:LEU:HD21	1.56	0.87
1:B:16:LYS:HD2	1:B:19:GLN:HB2	1.59	0.84
2:A:233:FMA:N1	2:A:233:FMA:H2'	1.90	0.84
1:A:75:LEU:HD12	1:A:93:VAL:HG13	1.57	0.84
1:A:181:LEU:HD21	1:A:220:GLN:HE22	1.44	0.83
1:B:3:LYS:HB2	1:B:230:LEU:HD13	1.58	0.83
2:A:233:FMA:N1	2:A:233:FMA:C2B	2.42	0.83
2:A:232:FMA:N5	2:A:232:FMA:H2'1	1.95	0.81
1:B:135:ASN:HD22	1:B:209:LYS:HD2	1.46	0.81
1:A:108:SER:HA	3:A:269:HOH:O	1.82	0.80
1:B:102:GLU:HA	1:B:105:LYS:HG2	1.63	0.80
1:A:98:ASP:HB3	1:A:103:ARG:HB3	1.63	0.79
1:A:61:LYS:HB2	2:A:232:FMA:H4'	1.64	0.79
1:B:93:VAL:HG22	1:B:127:GLN:HB3	1.65	0.79
1:B:66:ILE:HD12	1:B:75:LEU:HB2	1.65	0.79
1:B:133:ASN:HB3	1:B:141:ALA:HB1	1.65	0.78
1:B:41:ILE:HG22	1:B:222:ILE:HG23	1.66	0.76
1:A:225:ARG:HA	1:A:230:LEU:HD12	1.69	0.75
2:A:232:FMA:C2'	2:A:232:FMA:N5	2.49	0.75
1:A:25:MET:HG3	2:B:232:FMA:C6'	2.16	0.75
1:A:135:ASN:ND2	1:A:140:VAL:HB	2.01	0.74
1:B:125:ARG:NH2	1:B:194:THR:HA	2.03	0.74
1:B:20:GLU:HB3	1:B:21:PRO:HD2	1.70	0.73
1:A:126:HIS:HB2	1:A:195:VAL:HG12	1.71	0.73
1:B:137:ALA:O	1:B:140:VAL:HG12	1.88	0.72
1:A:66:ILE:HG13	1:A:93:VAL:HG11	1.71	0.71
1:B:31:THR:HA	1:B:34:ILE:HD12	1.73	0.70
1:B:184:VAL:HG22	2:B:233:FMA:H7'2	1.73	0.69
1:B:77:THR:HG22	1:B:81:THR:HG21	1.74	0.69
1:A:184:VAL:HG21	2:A:233:FMA:C11	2.24	0.68
1:B:133:ASN:ND2	1:B:145:LEU:HB2	2.09	0.68
2:B:233:FMA:N5	2:B:233:FMA:H2'1	2.09	0.67
1:A:61:LYS:CB	2:A:232:FMA:H4'	2.24	0.67
1:B:41:ILE:HD13	1:B:218:ASN:HA	1.77	0.66
1:B:132:VAL:HG22	1:B:173:VAL:HB	1.78	0.66
1:B:50:HIS:O	1:B:52:LEU:N	2.28	0.66
1:B:61:LYS:HB2	3:B:253:HOH:O	1.95	0.66
1:B:153:VAL:HG13	1:B:154:ALA:H	1.61	0.65
1:A:155:CYS:SG	1:A:156:THR:N	2.69	0.65
1:A:3:LYS:NZ	1:A:231:ILE:HD13	2.11	0.65
2:A:233:FMA:O2	2:A:233:FMA:H4'	1.98	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:40:SER:H	1:B:218:ASN:ND2	1.96	0.64
1:A:210:LYS:HA	1:A:213:VAL:HG23	1.78	0.64
1:B:55:LYS:HG3	1:B:59:ASP:HA	1.80	0.64
1:B:99:ILE:HG12	1:B:101:GLU:H	1.63	0.64
1:A:13:PHE:HB3	1:A:16:LYS:NZ	2.13	0.64
1:B:160:ASN:O	1:B:164:SER:N	2.31	0.64
1:A:39:THR:HG21	1:A:42:TYR:HE2	1.63	0.63
1:B:16:LYS:C	1:B:151:ASN:HD21	2.02	0.63
1:A:104:LEU:HD21	1:A:190:LYS:O	1.98	0.63
1:A:131:HIS:HB3	1:A:145:LEU:HD11	1.82	0.62
1:B:107:LEU:HD22	1:B:191:PHE:HD2	1.65	0.62
1:B:207:GLN:HG3	1:B:210:LYS:HD3	1.82	0.62
1:A:181:LEU:HD11	2:A:233:FMA:H5D	1.81	0.61
1:B:16:LYS:NZ	1:B:19:GLN:NE2	2.48	0.61
1:B:133:ASN:HD22	1:B:145:LEU:HB2	1.63	0.61
2:A:232:FMA:H5B	1:B:25:MET:HB2	1.82	0.61
1:A:41:ILE:HD13	1:A:221:VAL:HB	1.82	0.61
1:A:3:LYS:HD2	1:A:231:ILE:HD13	1.82	0.61
1:B:65:PHE:CD2	1:B:72:LEU:HD11	2.36	0.61
1:B:87:LYS:O	1:B:119:LYS:HG3	2.00	0.61
1:A:156:THR:O	1:A:158:PRO:HD3	2.00	0.61
1:A:70:GLU:HA	1:B:45:ILE:HG23	1.82	0.61
1:A:230:LEU:C	1:A:231:ILE:HD12	2.20	0.61
1:A:181:LEU:HD21	1:A:220:GLN:NE2	2.14	0.61
1:B:161:PHE:HB2	1:B:165:ILE:HG23	1.81	0.60
1:B:145:LEU:HD13	1:B:174:THR:HG22	1.83	0.60
1:B:146:LYS:HA	1:B:169:ILE:HD11	1.82	0.60
1:A:128:LEU:HD22	1:A:195:VAL:HG21	1.83	0.60
1:A:8:VAL:O	1:A:45:ILE:HA	2.00	0.60
1:B:160:ASN:ND2	1:B:165:ILE:HA	2.15	0.60
1:A:75:LEU:HD12	1:A:93:VAL:CG1	2.32	0.60
1:B:19:GLN:HA	1:B:23:LYS:HD3	1.83	0.60
1:B:134:VAL:HG13	1:B:177:TYR:H	1.66	0.60
1:B:211:LYS:HE3	1:B:215:ILE:HD12	1.84	0.59
1:B:184:VAL:O	1:B:187:LEU:N	2.34	0.59
1:A:34:ILE:HD13	1:A:211:LYS:HA	1.83	0.59
1:A:93:VAL:HG23	1:A:127:GLN:HB2	1.84	0.59
1:A:103:ARG:HA	1:A:106:LEU:HD12	1.84	0.59
1:A:130:LEU:O	1:A:199:LEU:HA	2.02	0.59
1:A:221:VAL:O	1:A:225:ARG:HG2	2.02	0.59
1:B:133:ASN:HD21	1:B:144:GLU:HG3	1.66	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:103:ARG:HH12	1:B:130:LEU:HD23	1.67	0.59
1:B:230:LEU:O	1:B:231:ILE:HB	2.03	0.58
1:B:68:LEU:HD12	1:B:73:TYR:CD1	2.38	0.58
1:A:40:SER:N	1:A:218:ASN:ND2	2.52	0.58
1:A:34:ILE:HA	1:A:38:ASP:HB2	1.84	0.58
1:B:137:ALA:O	1:B:139:THR:N	2.37	0.58
1:B:41:ILE:HG23	1:B:218:ASN:ND2	2.19	0.57
1:B:40:SER:H	1:B:218:ASN:HD21	1.52	0.57
1:B:40:SER:OG	1:B:222:ILE:HD13	2.05	0.57
1:B:113:SER:O	1:B:116:LYS:HB3	2.03	0.57
1:A:13:PHE:HZ	1:A:155:CYS:HB3	1.70	0.57
1:A:40:SER:H	1:A:218:ASN:ND2	2.02	0.56
2:B:232:FMA:C5'	2:B:232:FMA:HM72	2.34	0.56
1:B:133:ASN:ND2	1:B:144:GLU:HG3	2.21	0.56
1:B:30:GLU:O	1:B:34:ILE:HG13	2.06	0.56
1:A:135:ASN:HB3	1:A:141:ALA:HB2	1.86	0.56
2:B:232:FMA:H122	2:B:232:FMA:H6'2	1.88	0.56
1:B:92:LEU:HB2	1:B:126:HIS:ND1	2.21	0.56
1:B:145:LEU:HD13	1:B:174:THR:CG2	2.36	0.56
1:B:48:ASP:OD1	1:B:50:HIS:ND1	2.37	0.56
1:B:160:ASN:C	1:B:162:ASN:H	2.09	0.56
1:B:161:PHE:HB2	1:B:165:ILE:CG2	2.36	0.56
1:B:61:LYS:CD	2:B:232:FMA:O3P	2.54	0.55
1:A:12:ASN:ND2	1:B:62:LEU:HD23	2.21	0.55
1:A:53:VAL:HB	1:A:55:LYS:HE2	1.88	0.55
1:A:32:LEU:HD11	1:B:72:LEU:HD22	1.87	0.55
1:B:35:ILE:HG23	1:B:42:TYR:HB2	1.89	0.55
1:B:82:VAL:HG21	1:B:106:LEU:HD12	1.88	0.55
1:B:16:LYS:HZ2	1:B:19:GLN:NE2	2.04	0.55
1:B:96:TRP:HA	1:B:129:MET:O	2.07	0.55
1:B:138:GLU:HG2	1:B:176:SER:HB3	1.87	0.55
1:A:9:PHE:CZ	1:A:200:CYS:HB2	2.41	0.55
1:A:58:GLU:HB2	1:A:60:LYS:HG3	1.89	0.55
1:A:207:GLN:HE21	1:A:210:LYS:HE2	1.70	0.55
1:A:39:THR:HG21	1:A:42:TYR:CE2	2.42	0.55
1:A:3:LYS:HZ3	1:A:231:ILE:HD13	1.70	0.54
1:B:61:LYS:HD2	2:B:232:FMA:O3P	2.06	0.54
1:B:66:ILE:CD1	1:B:75:LEU:HD13	2.36	0.54
1:A:222:ILE:HG21	3:A:242:HOH:O	2.06	0.54
1:B:142:LYS:O	1:B:146:LYS:HB2	2.07	0.54
1:A:104:LEU:HD23	1:A:107:LEU:HD22	1.88	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:76:ALA:HB2	1:A:92:LEU:HD22	1.89	0.54
1:A:104:LEU:HD23	1:A:107:LEU:CD2	2.38	0.54
1:A:130:LEU:HD13	1:A:173:VAL:HG21	1.87	0.54
1:B:140:VAL:HG13	1:B:141:ALA:H	1.73	0.54
1:B:128:LEU:HB2	1:B:195:VAL:HG13	1.90	0.54
1:A:30:GLU:O	1:A:34:ILE:HG13	2.07	0.54
1:B:16:LYS:HZ2	1:B:24:THR:HG22	1.73	0.54
1:B:49:ASP:O	1:B:52:LEU:HG	2.08	0.54
1:A:222:ILE:O	1:A:226:GLN:HG3	2.08	0.53
1:B:135:ASN:HA	1:B:209:LYS:NZ	2.24	0.53
1:B:80:ASN:O	1:B:83:ASP:N	2.42	0.53
1:B:135:ASN:O	1:B:137:ALA:N	2.41	0.53
1:A:219:ASN:N	1:A:219:ASN:HD22	2.07	0.53
1:B:128:LEU:N	1:B:196:ASP:O	2.29	0.53
1:A:184:VAL:C	1:A:186:ASN:H	2.11	0.53
1:B:19:GLN:HG2	1:B:23:LYS:NZ	2.24	0.53
1:B:16:LYS:O	1:B:151:ASN:ND2	2.42	0.53
1:A:121:ILE:HG22	1:A:124:VAL:HG11	1.90	0.53
1:A:139:THR:HG22	1:A:143:GLU:OE1	2.09	0.52
1:B:184:VAL:CG2	2:B:233:FMA:H7'2	2.38	0.52
1:B:224:PHE:O	1:B:227:ASP:HB3	2.09	0.52
1:A:116:LYS:C	1:A:118:ASN:H	2.12	0.52
1:A:25:MET:HG3	2:B:232:FMA:C5'	2.40	0.52
1:A:129:MET:HA	1:A:198:LEU:O	2.09	0.52
1:B:87:LYS:HG3	1:B:117:TYR:CE2	2.45	0.52
1:A:25:MET:HG3	2:B:232:FMA:H5B	1.92	0.52
1:B:16:LYS:NZ	1:B:19:GLN:HE22	2.07	0.51
1:A:13:PHE:HB3	1:A:16:LYS:HZ2	1.76	0.51
1:A:135:ASN:HD22	1:A:141:ALA:N	2.09	0.51
1:A:9:PHE:CZ	1:A:96:TRP:HD1	2.28	0.51
1:A:74:VAL:O	1:A:92:LEU:HA	2.10	0.51
1:B:229:ASN:O	1:B:230:LEU:HG	2.11	0.51
2:A:233:FMA:C2	2:A:233:FMA:H4'	2.40	0.51
1:B:173:VAL:HG21	1:B:184:VAL:HG12	1.92	0.51
1:B:40:SER:N	1:B:218:ASN:HD21	2.09	0.51
1:B:159:SER:O	1:B:160:ASN:HB3	2.11	0.51
1:A:13:PHE:O	2:B:232:FMA:H8'1	2.10	0.51
1:A:225:ARG:HB3	1:A:230:LEU:HB2	1.92	0.50
1:A:114:ALA:HB1	1:A:121:ILE:HG12	1.93	0.50
1:B:224:PHE:O	1:B:228:ASN:OD1	2.30	0.50
1:B:76:ALA:O	1:B:78:SER:N	2.45	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:145:LEU:O	1:A:149:ILE:HG12	2.11	0.50
1:A:110:TYR:CE1	1:A:121:ILE:HD13	2.46	0.50
1:B:134:VAL:HG13	1:B:177:TYR:N	2.27	0.50
1:B:35:ILE:HA	1:B:39:THR:OG1	2.12	0.50
1:A:160:ASN:HB3	1:A:164:SER:O	2.11	0.50
1:B:147:LEU:O	1:B:151:ASN:N	2.44	0.49
1:A:65:PHE:CE2	2:A:232:FMA:H132	2.47	0.49
1:B:8:VAL:O	1:B:45:ILE:HA	2.13	0.49
1:B:193:ASN:HD22	2:B:233:FMA:H4'	1.78	0.49
1:B:63:ALA:HB1	1:B:65:PHE:CE1	2.47	0.49
1:A:88:TYR:HE1	1:B:26:ASN:HD21	1.59	0.49
1:A:219:ASN:O	1:A:223:LYS:HE2	2.11	0.49
1:B:133:ASN:HB3	1:B:141:ALA:CB	2.40	0.49
1:B:213:VAL:HG13	2:B:233:FMA:H151	1.95	0.49
1:A:30:GLU:OE2	1:A:33:ARG:NE	2.38	0.49
1:A:56:ASP:OD2	1:A:60:LYS:HB2	2.13	0.49
1:A:110:TYR:CD1	1:A:110:TYR:O	2.65	0.49
1:A:206:ASP:O	1:A:209:LYS:N	2.43	0.49
1:A:184:VAL:HG21	2:A:233:FMA:C9'	2.43	0.49
1:B:41:ILE:CD1	1:B:218:ASN:HA	2.42	0.49
1:A:51:TYR:OH	1:B:62:LEU:HD21	2.13	0.48
1:B:133:ASN:HB2	1:B:145:LEU:HD12	1.94	0.48
1:B:209:LYS:O	1:B:213:VAL:HG23	2.13	0.48
1:B:76:ALA:O	1:B:77:THR:C	2.52	0.48
1:B:138:GLU:HG2	1:B:176:SER:CB	2.43	0.48
1:B:125:ARG:NH1	1:B:196:ASP:OD1	2.42	0.48
1:B:50:HIS:C	1:B:52:LEU:H	2.17	0.48
1:A:146:LYS:HG2	1:A:150:GLU:OE1	2.14	0.48
1:A:96:TRP:HE3	1:A:97:ASP:N	2.10	0.48
1:A:34:ILE:HG23	1:A:38:ASP:HB2	1.96	0.48
1:B:100:ASN:OD1	1:B:187:LEU:HD11	2.12	0.48
1:B:128:LEU:HD22	1:B:195:VAL:HG11	1.96	0.48
1:A:71:LYS:HD2	3:A:268:HOH:O	2.12	0.48
1:A:11:VAL:HG21	1:A:16:LYS:HD2	1.95	0.48
1:B:100:ASN:ND2	1:B:104:LEU:HD22	2.29	0.48
1:B:82:VAL:HG22	1:B:92:LEU:CD2	2.44	0.48
1:A:110:TYR:OH	1:A:124:VAL:HG21	2.14	0.48
1:B:212:SER:O	1:B:216:ASP:HB2	2.13	0.48
1:B:78:SER:O	1:B:106:LEU:HD11	2.14	0.47
1:A:18:GLN:HG2	1:A:147:LEU:HD23	1.95	0.47
1:B:149:ILE:HG22	1:B:165:ILE:HD12	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:20:GLU:OE1	1:B:23:LYS:HD2	2.14	0.47
1:A:11:VAL:CG2	1:A:16:LYS:HD2	2.44	0.47
1:A:40:SER:N	1:A:218:ASN:HD21	2.11	0.47
1:B:169:ILE:CG2	1:B:174:THR:HG21	2.44	0.47
2:A:233:FMA:N1	2:A:233:FMA:C3B	2.78	0.47
2:B:233:FMA:N5	2:B:233:FMA:C2'	2.77	0.47
1:B:3:LYS:NZ	1:B:5:ASN:OD1	2.48	0.47
1:B:102:GLU:O	1:B:106:LEU:HB2	2.14	0.47
1:A:134:VAL:HG22	1:A:180:CYS:SG	2.55	0.47
1:B:16:LYS:CA	1:B:151:ASN:HD21	2.27	0.47
1:A:218:ASN:OD1	1:A:219:ASN:ND2	2.47	0.47
1:A:13:PHE:HB3	1:A:16:LYS:HZ3	1.80	0.47
2:B:232:FMA:N5	2:B:232:FMA:C2'	2.64	0.47
1:A:61:LYS:O	1:B:14:TYR:HE2	1.97	0.47
1:A:206:ASP:O	1:A:207:GLN:C	2.51	0.47
1:A:225:ARG:O	1:A:226:GLN:C	2.53	0.47
1:B:134:VAL:C	1:B:209:LYS:HZ2	2.18	0.47
1:A:78:SER:O	1:A:82:VAL:HB	2.14	0.47
1:A:48:ASP:HA	1:A:50:HIS:CE1	2.50	0.46
1:A:13:PHE:CZ	1:A:155:CYS:HB3	2.49	0.46
1:A:132:VAL:HA	1:A:173:VAL:O	2.15	0.46
1:B:225:ARG:O	1:B:227:ASP:N	2.49	0.46
1:A:67:THR:HG21	1:B:47:ILE:HG13	1.98	0.46
1:B:27:ASN:ND2	1:B:207:GLN:OE1	2.48	0.46
2:B:232:FMA:H5B	2:B:232:FMA:HM72	1.97	0.46
1:B:227:ASP:C	1:B:229:ASN:H	2.19	0.46
1:B:103:ARG:NH1	1:B:130:LEU:HD23	2.31	0.46
1:B:211:LYS:HE3	1:B:215:ILE:CD1	2.45	0.46
1:B:134:VAL:O	1:B:209:LYS:HD3	2.16	0.46
1:A:217:LEU:O	1:A:217:LEU:HD12	2.15	0.46
1:A:219:ASN:HA	1:A:222:ILE:HG22	1.97	0.46
1:A:33:ARG:HH12	1:A:38:ASP:CG	2.19	0.46
1:A:149:ILE:O	1:A:152:TYR:N	2.49	0.46
1:A:121:ILE:O	1:A:121:ILE:HD12	2.16	0.46
1:A:146:LYS:HG2	1:A:146:LYS:O	2.16	0.46
1:B:179:ASP:O	1:B:180:CYS:C	2.53	0.46
1:B:39:THR:HB	1:B:218:ASN:HD22	1.81	0.45
1:A:123:LEU:N	1:A:123:LEU:HD22	2.32	0.45
1:B:137:ALA:C	1:B:139:THR:H	2.19	0.45
1:A:88:TYR:HB3	1:B:29:LEU:HD11	1.99	0.45
1:A:6:TYR:CE1	2:A:233:FMA:H7'1	2.51	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:217:LEU:O	1:B:218:ASN:C	2.54	0.45
1:B:41:ILE:HG22	1:B:222:ILE:CG2	2.41	0.45
1:A:135:ASN:HB2	1:A:209:LYS:NZ	2.31	0.45
1:B:176:SER:O	1:B:177:TYR:C	2.55	0.45
1:B:217:LEU:HD11	2:B:233:FMA:H8'2	1.99	0.45
1:A:130:LEU:HD22	1:A:173:VAL:HG23	1.98	0.45
1:A:191:PHE:O	1:A:193:ASN:N	2.50	0.45
1:A:224:PHE:HE1	1:A:230:LEU:HD11	1.82	0.44
1:A:38:ASP:O	1:A:39:THR:HG23	2.17	0.44
1:B:162:ASN:HD22	1:B:162:ASN:HA	1.55	0.44
1:B:16:LYS:HG3	1:B:151:ASN:ND2	2.32	0.44
1:B:27:ASN:O	1:B:30:GLU:N	2.49	0.44
1:A:16:LYS:O	1:A:19:GLN:HG3	2.17	0.44
1:B:19:GLN:HB3	1:B:24:THR:HG23	1.99	0.44
1:A:63:ALA:HA	1:A:64:PRO:HD2	1.82	0.44
1:A:184:VAL:HG21	2:A:233:FMA:H9'1	1.99	0.44
1:A:67:THR:HG22	1:B:45:ILE:HD11	2.00	0.44
1:B:95:LYS:NZ	3:B:274:HOH:O	2.50	0.44
1:A:100:ASN:OD1	1:A:187:LEU:HD11	2.16	0.44
1:B:76:ALA:HB1	1:B:106:LEU:HD12	1.99	0.44
1:A:113:SER:O	1:A:114:ALA:C	2.56	0.44
1:A:167:SER:O	1:A:171:SER:N	2.48	0.44
1:B:149:ILE:CG2	1:B:165:ILE:HD12	2.48	0.44
1:A:223:LYS:HB2	1:A:223:LYS:HE2	1.76	0.44
1:A:187:LEU:O	1:A:188:ALA:C	2.56	0.44
1:B:184:VAL:HG21	2:B:233:FMA:H9'1	2.00	0.44
1:B:184:VAL:C	1:B:187:LEU:H	2.21	0.44
1:A:167:SER:HA	1:A:170:GLN:HB2	2.00	0.44
1:B:181:LEU:HB3	1:B:182:SER:H	1.64	0.44
1:B:84:ILE:HG21	2:B:232:FMA:C7	2.47	0.43
1:B:75:LEU:HD12	1:B:93:VAL:O	2.18	0.43
1:B:77:THR:CG2	1:B:81:THR:HG21	2.45	0.43
1:B:55:LYS:CG	1:B:59:ASP:HA	2.46	0.43
1:B:89:ALA:HB2	1:B:119:LYS:HB3	1.99	0.43
1:B:158:PRO:O	1:B:160:ASN:N	2.47	0.43
1:A:96:TRP:NE1	1:A:131:HIS:CE1	2.86	0.43
1:A:39:THR:HG22	1:A:218:ASN:HB2	2.01	0.43
1:B:135:ASN:HA	1:B:209:LYS:HZ1	1.83	0.43
1:B:15:ASN:O	1:B:16:LYS:C	2.57	0.43
1:B:116:LYS:HG2	1:B:116:LYS:O	2.18	0.43
1:A:3:LYS:CB	1:A:230:LEU:HD22	2.30	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:145:LEU:HD22	1:A:174:THR:CG2	2.47	0.43
1:A:98:ASP:O	1:A:103:ARG:NH2	2.51	0.43
1:B:64:PRO:HG3	1:B:77:THR:HG21	2.00	0.43
1:A:207:GLN:NE2	1:A:210:LYS:NZ	2.67	0.43
1:A:211:LYS:O	1:A:215:ILE:HG23	2.18	0.43
1:A:13:PHE:CB	1:A:16:LYS:HZ3	2.31	0.43
1:B:165:ILE:O	1:B:169:ILE:HG13	2.19	0.43
1:A:34:ILE:O	1:A:39:THR:OG1	2.35	0.43
1:A:12:ASN:HB2	1:A:47:ILE:CG2	2.48	0.43
1:B:125:ARG:NH1	1:B:195:VAL:H	2.16	0.43
1:B:31:THR:O	1:B:34:ILE:N	2.52	0.43
1:B:95:LYS:HE2	1:B:97:ASP:OD1	2.18	0.43
1:A:191:PHE:C	1:A:193:ASN:N	2.71	0.43
1:A:199:LEU:HD12	1:A:199:LEU:H	1.84	0.42
1:A:221:VAL:O	1:A:223:LYS:N	2.52	0.42
1:B:204:MET:CE	1:B:213:VAL:HG21	2.49	0.42
1:B:94:PHE:HZ	1:B:107:LEU:HD13	1.83	0.42
1:A:90:LEU:HA	1:A:91:PRO:HD3	1.86	0.42
1:B:146:LYS:NZ	1:B:146:LYS:HB2	2.34	0.42
2:B:233:FMA:C2B	2:B:233:FMA:N1	2.81	0.42
1:B:200:CYS:SG	1:B:202:GLU:HB2	2.60	0.42
1:A:230:LEU:O	1:A:231:ILE:HD12	2.19	0.42
1:A:67:THR:CG2	1:B:47:ILE:HG13	2.50	0.42
1:B:70:GLU:CD	1:B:70:GLU:H	2.21	0.42
1:A:19:GLN:H	1:A:19:GLN:HG2	1.68	0.42
1:B:205:GLN:O	1:B:207:GLN:N	2.52	0.42
1:B:83:ASP:O	1:B:86:ALA:HB3	2.20	0.42
2:B:232:FMA:H5D	2:B:232:FMA:HM72	2.02	0.42
1:B:13:PHE:HZ	1:B:16:LYS:HE2	1.84	0.42
1:B:82:VAL:HG22	1:B:92:LEU:HD22	2.02	0.42
1:A:10:PHE:CB	2:B:232:FMA:H141	2.50	0.42
1:B:145:LEU:HD23	1:B:145:LEU:O	2.20	0.42
1:B:218:ASN:OD1	1:B:222:ILE:HD11	2.20	0.42
1:B:16:LYS:HZ3	1:B:19:GLN:HE22	1.68	0.42
1:B:125:ARG:HH12	1:B:195:VAL:H	1.68	0.42
1:A:219:ASN:H	1:A:219:ASN:HD22	1.68	0.42
1:B:50:HIS:NE2	1:B:97:ASP:OD1	2.53	0.41
1:A:55:LYS:HA	1:A:60:LYS:O	2.20	0.41
1:B:82:VAL:HG21	1:B:106:LEU:CD1	2.49	0.41
1:B:125:ARG:NH1	1:B:195:VAL:O	2.53	0.41
1:A:184:VAL:O	1:A:187:LEU:N	2.52	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:132:VAL:HA	1:B:173:VAL:O	2.20	0.41
1:A:5:ASN:OD1	1:A:43:ASP:OD1	2.38	0.41
1:B:169:ILE:HG23	1:B:174:THR:HG21	2.03	0.41
2:A:232:FMA:H141	1:B:47:ILE:HD13	2.02	0.41
1:A:132:VAL:HG22	1:A:173:VAL:CG1	2.50	0.41
1:A:161:PHE:O	1:A:162:ASN:OD1	2.38	0.41
1:B:19:GLN:HG2	1:B:23:LYS:HZ3	1.84	0.41
1:A:114:ALA:CB	1:A:121:ILE:HG12	2.49	0.41
1:A:137:ALA:O	1:A:138:GLU:C	2.57	0.41
1:A:72:LEU:HG	2:A:232:FMA:C15	2.51	0.41
1:B:31:THR:HG22	1:B:214:MET:CE	2.50	0.41
1:B:95:LYS:HA	1:B:129:MET:SD	2.60	0.41
1:A:20:GLU:O	1:A:23:LYS:N	2.54	0.41
1:A:40:SER:H	1:A:218:ASN:HD22	1.65	0.41
1:A:16:LYS:O	1:A:17:GLY:C	2.59	0.41
1:A:96:TRP:CZ3	1:A:97:ASP:HB3	2.56	0.41
1:A:107:LEU:O	1:A:107:LEU:HG	2.19	0.41
2:B:232:FMA:H122	2:B:232:FMA:C6'	2.51	0.41
1:B:64:PRO:HG3	1:B:81:THR:HG21	2.03	0.41
1:A:184:VAL:CG2	2:A:233:FMA:H111	2.34	0.40
1:B:160:ASN:O	1:B:162:ASN:N	2.54	0.40
1:B:225:ARG:C	1:B:227:ASP:N	2.75	0.40
1:B:75:LEU:C	1:B:77:THR:H	2.25	0.40
1:B:185:ALA:CB	2:B:233:FMA:HM82	2.51	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	229/231 (99%)	170 (74%)	44 (19%)	15 (7%)	1 2

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	B	229/231 (99%)	147 (64%)	53 (23%)	29 (13%)	0 0
All	All	458/462 (99%)	317 (69%)	97 (21%)	44 (10%)	1 1

All (44) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	51	TYR
1	B	136	GLU
1	B	138	GLU
1	B	153	VAL
1	B	177	TYR
1	B	218	ASN
1	B	229	ASN
1	A	41	ILE
1	A	56	ASP
1	A	229	ASN
1	B	116	LYS
1	B	122	ASP
1	B	160	ASN
1	B	181	LEU
1	B	230	LEU
1	A	19	GLN
1	A	21	PRO
1	A	100	ASN
1	A	225	ARG
1	B	77	THR
1	B	135	ASN
1	B	156	THR
1	B	178	LYS
1	B	192	ASP
1	B	210	LYS
1	B	226	GLN
1	A	15	ASN
1	A	138	GLU
1	A	192	ASP
1	A	226	GLN
1	B	49	ASP
1	B	76	ALA
1	B	154	ALA
1	B	161	PHE
1	A	64	PRO
1	A	117	TYR

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Mol	Chain	Res	Type
1	A	162	ASN
1	B	21	PRO
1	B	110	TYR
1	B	217	LEU
1	A	158	PRO
1	B	155	CYS
1	B	206	ASP
1	B	163	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	212/212 (100%)	175 (82%)	37 (18%)	2 6
1	B	212/212 (100%)	179 (84%)	33 (16%)	3 8
All	All	424/424 (100%)	354 (84%)	70 (16%)	3 7

All (70) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	2	ASN
1	A	13	PHE
1	A	16	LYS
1	A	22	SER
1	A	25	MET
1	A	30	GLU
1	A	39	THR
1	A	45	ILE
1	A	49	ASP
1	A	52	LEU
1	A	53	VAL
1	A	60	LYS
1	A	70	GLU
1	A	72	LEU
1	A	77	THR

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Mol	Chain	Res	Type
1	A	96	TRP
1	A	103	ARG
1	A	107	LEU
1	A	124	VAL
1	A	127	GLN
1	A	131	HIS
1	A	139	THR
1	A	147	LEU
1	A	150	GLU
1	A	152	TYR
1	A	156	THR
1	A	161	PHE
1	A	165	ILE
1	A	193	ASN
1	A	197	PHE
1	A	199	LEU
1	A	203	SER
1	A	207	GLN
1	A	213	VAL
1	A	215	ILE
1	A	225	ARG
1	A	228	ASN
1	B	18	GLN
1	B	31	THR
1	B	37	GLU
1	B	38	ASP
1	B	48	ASP
1	B	50	HIS
1	B	55	LYS
1	B	56	ASP
1	B	62	LEU
1	B	66	ILE
1	B	70	GLU
1	B	71	LYS
1	B	82	VAL
1	B	90	LEU
1	B	97	ASP
1	B	100	ASN
1	B	102	GLU
1	B	106	LEU
1	B	116	LYS
1	B	123	LEU

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Mol	Chain	Res	Type
1	B	125	ARG
1	B	130	LEU
1	B	151	ASN
1	B	155	CYS
1	B	157	GLN
1	B	181	LEU
1	B	184	VAL
1	B	191	PHE
1	B	195	VAL
1	B	207	GLN
1	B	209	LYS
1	B	212	SER
1	B	228	ASN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (18) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	5	ASN
1	A	12	ASN
1	A	27	ASN
1	A	127	GLN
1	A	135	ASN
1	A	162	ASN
1	A	170	GLN
1	A	207	GLN
1	A	218	ASN
1	A	219	ASN
1	A	220	GLN
1	B	2	ASN
1	B	19	GLN
1	B	26	ASN
1	B	120	ASN
1	B	151	ASN
1	B	162	ASN
1	B	218	ASN

5.3.3 RNA

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)

4 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the chemical component dictionary. The Link column lists molecule types, if any, to which the group is linked. 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 $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
2	FMA	A	232	-	43,49,49	4.29	16 (37%)	40,69,69	2.87	16 (40%)
2	FMA	A	233	-	43,49,49	4.24	18 (41%)	40,69,69	2.89	15 (37%)
2	FMA	B	232	-	43,49,49	4.30	20 (46%)	40,69,69	2.95	16 (40%)
2	FMA	B	233	-	43,49,49	4.23	18 (41%)	40,69,69	2.90	18 (45%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the chemical component dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	FMA	A	232	-	-	0/35/37/37	0/3/3/3
2	FMA	A	233	-	-	0/35/37/37	0/3/3/3
2	FMA	B	232	-	-	0/35/37/37	0/3/3/3
2	FMA	B	233	-	-	0/35/37/37	0/3/3/3

All (72) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	232	FMA	C6-C5A	-17.53	1.39	1.54
2	B	232	FMA	C6-C5A	-17.32	1.39	1.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	233	FMA	C6-C5A	-16.94	1.39	1.54
2	B	233	FMA	C6-C5A	-16.93	1.39	1.54
2	A	232	FMA	C5A-N5	-9.37	1.34	1.47
2	A	232	FMA	C7-C6	-9.30	1.37	1.55
2	A	233	FMA	C7-C6	-9.09	1.37	1.55
2	B	233	FMA	C5A-N5	-9.01	1.34	1.47
2	A	233	FMA	C5A-N5	-8.87	1.34	1.47
2	B	232	FMA	C5A-N5	-8.86	1.34	1.47
2	B	232	FMA	C7-C6	-8.83	1.38	1.55
2	B	233	FMA	C7-C6	-8.72	1.38	1.55
2	B	233	FMA	C9-C9A	-7.20	1.36	1.53
2	B	232	FMA	C9-C9A	-7.17	1.36	1.53
2	A	233	FMA	C9-C9A	-7.14	1.36	1.53
2	A	232	FMA	C9-C9A	-6.95	1.37	1.53
2	B	233	FMA	C9-C8	-6.69	1.38	1.53
2	A	232	FMA	C9-C8	-6.68	1.38	1.53
2	B	232	FMA	C9-C8	-6.68	1.38	1.53
2	A	233	FMA	C9-C8	-6.59	1.38	1.53
2	A	232	FMA	C5A-C9A	-5.88	1.46	1.52
2	A	232	FMA	C4A-C4	-5.87	1.42	1.53
2	B	232	FMA	C5A-C9A	-5.78	1.46	1.52
2	B	233	FMA	C5A-C9A	-5.50	1.47	1.52
2	A	233	FMA	C4A-C4	-5.40	1.43	1.53
2	A	233	FMA	C5A-C9A	-5.36	1.47	1.52
2	B	233	FMA	C4A-C4	-5.25	1.43	1.53
2	B	232	FMA	C4A-C4	-5.23	1.43	1.53
2	B	232	FMA	C8-C7	-5.12	1.44	1.54
2	A	232	FMA	C8-C7	-4.94	1.44	1.54
2	A	233	FMA	C8-C7	-4.87	1.44	1.54
2	B	232	FMA	P-O3P	-4.86	1.37	1.54
2	B	233	FMA	C8-C7	-4.82	1.45	1.54
2	B	233	FMA	P-O3P	-4.69	1.37	1.54
2	B	232	FMA	C9A-N10	-4.63	1.38	1.48
2	A	232	FMA	P-O3P	-4.57	1.38	1.54
2	A	233	FMA	P-O3P	-4.48	1.38	1.54
2	B	233	FMA	C9A-N10	-4.45	1.39	1.48
2	A	233	FMA	C9A-N10	-4.39	1.39	1.48
2	A	232	FMA	C9A-N10	-3.69	1.40	1.48
2	A	232	FMA	C4A-N5	-3.19	1.30	1.45
2	A	233	FMA	C4A-N5	-3.06	1.31	1.45
2	B	233	FMA	C4A-N5	-3.01	1.31	1.45
2	B	232	FMA	C4A-N5	-2.92	1.32	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	233	FMA	O2-C2	-2.91	1.17	1.23
2	A	233	FMA	O2-C2	-2.73	1.17	1.23
2	B	232	FMA	O2-C2	-2.70	1.17	1.23
2	B	233	FMA	P-O2P	-2.65	1.45	1.54
2	B	232	FMA	P-O2P	-2.61	1.45	1.54
2	A	232	FMA	P-O2P	-2.59	1.45	1.54
2	A	233	FMA	P-O2P	-2.59	1.45	1.54
2	B	232	FMA	C3'-C6	-2.57	1.46	1.53
2	A	232	FMA	O2-C2	-2.56	1.18	1.23
2	B	232	FMA	O3'-C3B	-2.36	1.37	1.43
2	A	233	FMA	C3'-C6	-2.29	1.47	1.53
2	B	233	FMA	C3'-C6	-2.18	1.48	1.53
2	A	232	FMA	O3'-C3B	-2.02	1.38	1.43
2	B	232	FMA	O4'-C4B	2.22	1.48	1.43
2	B	232	FMA	C5B-C4B	2.32	1.55	1.51
2	B	232	FMA	O5'-C5B	2.33	1.54	1.44
2	B	233	FMA	O5'-C5B	2.43	1.54	1.44
2	A	232	FMA	O5'-C5B	2.45	1.54	1.44
2	B	233	FMA	O4'-C4B	2.55	1.49	1.43
2	A	233	FMA	O5'-C5B	2.58	1.55	1.44
2	A	233	FMA	C5B-C4B	2.74	1.55	1.51
2	A	233	FMA	C1B-C2B	4.40	1.59	1.52
2	B	232	FMA	C1B-C2B	4.44	1.59	1.52
2	B	233	FMA	C1B-C2B	4.51	1.59	1.52
2	B	232	FMA	C2-N3	5.00	1.45	1.37
2	B	233	FMA	C2-N3	5.06	1.45	1.37
2	A	233	FMA	C2-N3	5.24	1.46	1.37
2	A	232	FMA	C2-N3	5.42	1.46	1.37

All (65) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	232	FMA	O2-C2-N3	-5.99	109.88	121.82
2	B	232	FMA	O2-C2-N3	-4.92	112.00	121.82
2	A	233	FMA	O2-C2-N3	-4.81	112.23	121.82
2	B	233	FMA	O2-C2-N3	-4.74	112.38	121.82
2	A	233	FMA	O2B-C2B-C1B	-3.91	101.21	110.45
2	A	232	FMA	O2B-C2B-C1B	-3.21	102.87	110.45
2	A	232	FMA	O5'-P-O1P	-3.02	99.45	107.14
2	B	233	FMA	O5'-P-O1P	-2.92	99.70	107.14
2	B	233	FMA	O2B-C2B-C1B	-2.82	103.79	110.45
2	A	233	FMA	O5'-P-O1P	-2.81	99.99	107.14

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	233	FMA	C4'-C3'-C2'	-2.78	106.13	111.61
2	B	232	FMA	O5'-P-O1P	-2.70	100.28	107.14
2	B	232	FMA	O4-C4-N3	-2.47	116.29	120.93
2	A	232	FMA	C9A-C5A-N5	2.07	116.48	111.02
2	A	232	FMA	C8-C9-C9A	2.25	122.11	112.53
2	B	232	FMA	C7M-C7-C8	2.26	115.09	111.10
2	B	233	FMA	C8-C9-C9A	2.30	122.30	112.53
2	A	233	FMA	C7M-C7-C8	2.37	115.29	111.10
2	B	233	FMA	O4-C4-C4A	2.37	123.30	119.47
2	A	233	FMA	C8-C9-C9A	2.39	122.69	112.53
2	B	232	FMA	C8-C9-C9A	2.46	122.98	112.53
2	B	233	FMA	C7M-C7-C8	2.46	115.45	111.10
2	B	233	FMA	O2-C2-N1	2.47	128.60	122.86
2	A	233	FMA	O2-C2-N1	2.54	128.75	122.86
2	A	233	FMA	O3P-P-O1P	2.57	118.86	110.58
2	A	232	FMA	O3P-P-O1P	2.59	118.92	110.58
2	B	233	FMA	O3P-P-O1P	2.62	119.03	110.58
2	A	232	FMA	N3-C2-N1	2.63	119.02	116.14
2	A	233	FMA	N3-C2-N1	2.63	119.02	116.14
2	B	233	FMA	N3-C2-N1	2.63	119.02	116.14
2	A	232	FMA	C7M-C7-C8	2.80	116.06	111.10
2	B	233	FMA	O2B-C2B-C3B	2.81	116.08	109.02
2	B	232	FMA	O4-C4-C4A	2.82	124.03	119.47
2	B	232	FMA	C4'-C3'-C6	3.08	120.59	112.57
2	B	232	FMA	O2-C2-N1	3.27	130.45	122.86
2	B	233	FMA	C8M-C8-C9	3.40	117.32	111.19
2	A	232	FMA	O2-C2-N1	3.55	131.10	122.86
2	B	233	FMA	C7-C6-C5A	3.58	117.77	109.22
2	B	232	FMA	O3P-P-O1P	3.69	122.47	110.58
2	A	233	FMA	C8M-C8-C9	3.77	117.98	111.19
2	A	233	FMA	C7-C6-C5A	3.78	118.25	109.22
2	A	233	FMA	C9-C9A-C5A	3.80	117.52	110.19
2	B	232	FMA	C7-C6-C5A	3.90	118.55	109.22
2	B	232	FMA	C9-C9A-C5A	3.95	117.82	110.19
2	A	232	FMA	C9-C9A-C5A	4.02	117.94	110.19
2	B	233	FMA	C9-C9A-C5A	4.05	118.01	110.19
2	A	232	FMA	C7-C6-C5A	4.11	119.04	109.22
2	A	232	FMA	C8M-C8-C9	4.18	118.71	111.19
2	B	232	FMA	C8M-C8-C9	4.24	118.83	111.19
2	B	232	FMA	C9-C8-C7	5.52	118.03	109.33
2	B	233	FMA	C7M-C7-C6	5.53	122.78	113.51
2	A	232	FMA	C7M-C7-C6	5.55	122.81	113.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	233	FMA	C7M-C7-C6	5.68	123.03	113.51
2	B	233	FMA	C9-C9A-N10	5.75	124.77	113.03
2	B	232	FMA	C7M-C7-C6	5.75	123.16	113.51
2	A	233	FMA	C9-C8-C7	5.80	118.47	109.33
2	A	232	FMA	C9-C9A-N10	5.91	125.12	113.03
2	B	233	FMA	C9-C8-C7	5.93	118.68	109.33
2	A	232	FMA	C9-C8-C7	6.05	118.86	109.33
2	A	233	FMA	C9-C9A-N10	6.05	125.40	113.03
2	B	232	FMA	C9-C9A-N10	6.38	126.08	113.03
2	A	232	FMA	C8M-C8-C7	8.20	122.43	112.37
2	B	232	FMA	C8M-C8-C7	8.78	123.14	112.37
2	A	233	FMA	C8M-C8-C7	9.11	123.55	112.37
2	B	233	FMA	C8M-C8-C7	9.48	124.00	112.37

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

4 monomers are involved in 47 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	232	FMA	8	0
2	A	233	FMA	12	0
2	B	232	FMA	16	0
2	B	233	FMA	11	0

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

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.