Full wwPDB X-ray Structure Validation Report ⓘ

May 17, 2020 – 12:47 am BST

PDB ID	:	4AM0
Title	:	Structure of Dengue virus strain 4 DIII in complex with Fab 2H12
Authors	:	Midgley, C.M.; Flanagan, A.; Mongkolsapaya, J.; Grimes, J.M.; Screaton, G.R.
Deposited on	:	2012-03-06
Resolution	:	3.02 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 ⓘ symbol.

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

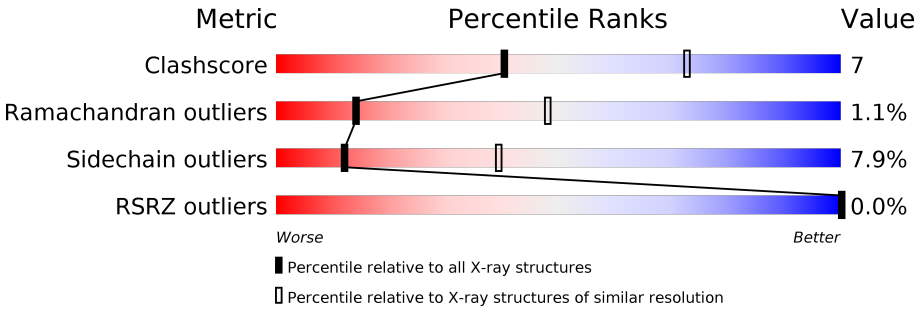
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.11
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.11

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 3.02 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	2734 (3.04-3.00)
Ramachandran outliers	138981	2640 (3.04-3.00)
Sidechain outliers	138945	2643 (3.04-3.00)
RSRZ outliers	127900	2287 (3.04-3.00)

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 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% 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.

Mol	Chain	Length	Quality of chain
1	A	217	73% 23%
1	C	217	75% 19%
1	E	217	72% 20% 5%
1	H	217	74% 21%
2	B	212	82% 15%
2	D	212	84% 14%
2	F	212	81% 16%

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Mol	Chain	Length	Quality of chain
2	L	212	83% 14% •
3	Q	101	61% 27% • 10%
3	R	101	68% 22% 5% 5%
3	S	101	63% 26% • 9%
3	T	101	71% 18% 5% 6%

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 15830 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 2H12, HEAVY CHAIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	211	Total	C	N	O	S	0	0	0
			1580	996	255	321	8			
1	C	211	Total	C	N	O	S	0	0	0
			1580	996	255	321	8			
1	E	212	Total	C	N	O	S	0	0	0
			1584	998	256	322	8			
1	H	214	Total	C	N	O	S	0	0	0
			1596	1005	258	325	8			

- Molecule 2 is a protein called FAB 2H12, LIGHT CHAIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	212	Total	C	N	O	S	0	0	0
			1655	1031	283	334	7			
2	D	212	Total	C	N	O	S	0	0	0
			1655	1031	283	334	7			
2	F	212	Total	C	N	O	S	0	0	0
			1655	1031	283	334	7			
2	L	212	Total	C	N	O	S	0	0	0
			1655	1031	283	334	7			

- Molecule 3 is a protein called ENVELOPE PROTEIN,.

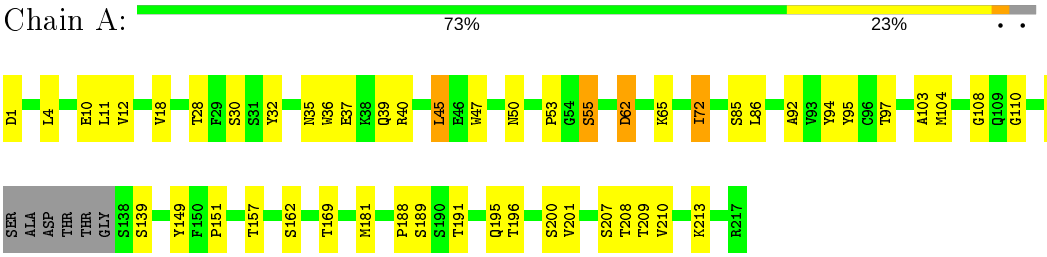
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	Q	91	Total	C	N	O	S	0	0	0
			696	443	114	135	4			
3	R	96	Total	C	N	O	S	0	0	0
			736	468	122	142	4			
3	S	92	Total	C	N	O	S	0	0	0
			706	451	116	135	4			
3	T	95	Total	C	N	O	S	0	0	0
			732	466	121	141	4			

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 the various outlier classes 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.

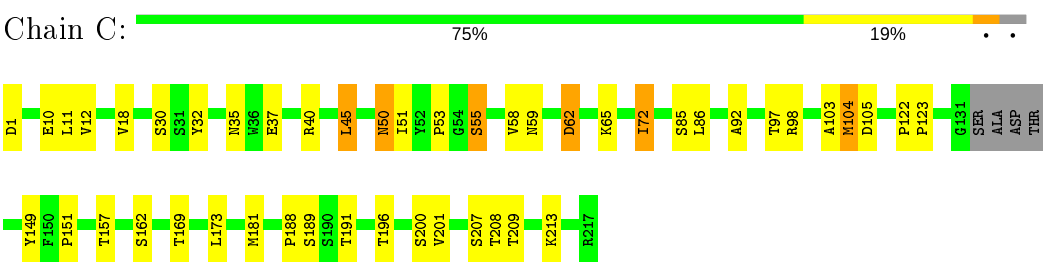
- Molecule 1: FAB 2H12, HEAVY CHAIN

Chain A:



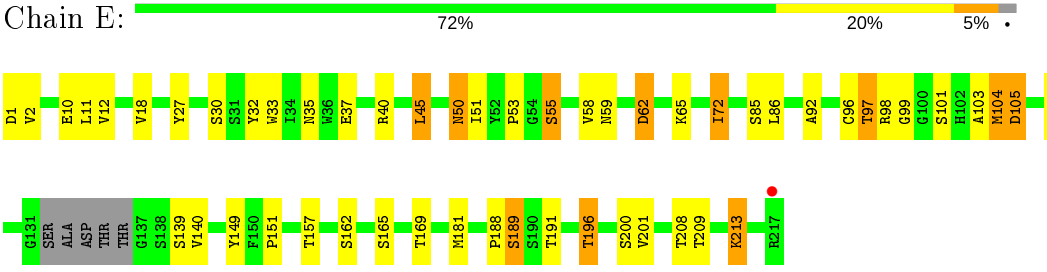
- Molecule 1: FAB 2H12, HEAVY CHAIN

Chain C:



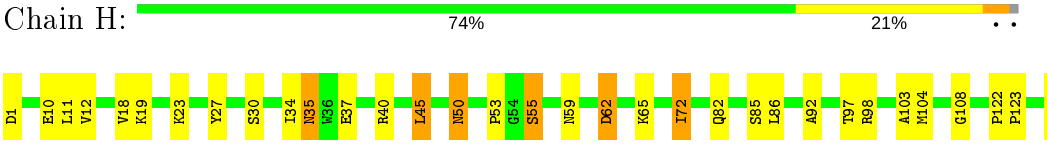
- Molecule 1: FAB 2H12, HEAVY CHAIN

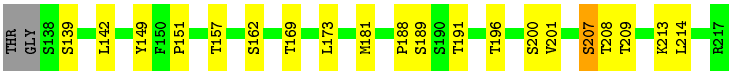
Chain E:



- Molecule 1: FAB 2H12, HEAVY CHAIN

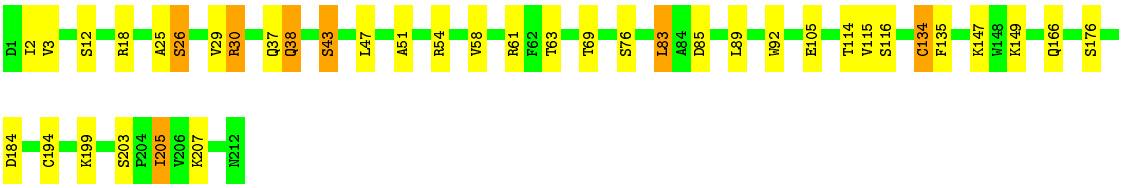
Chain H:





• Molecule 2: FAB 2H12, LIGHT CHAIN

Chain B:

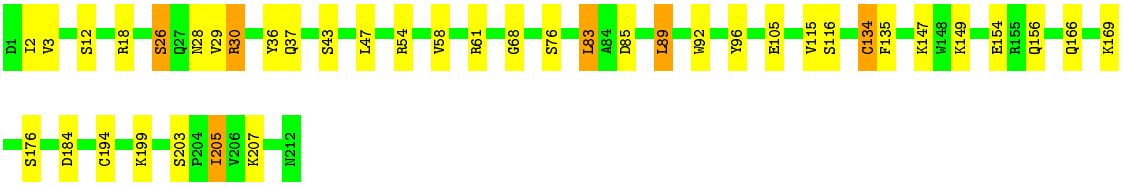


• Molecule 2: FAB 2H12, LIGHT CHAIN

Chain D:

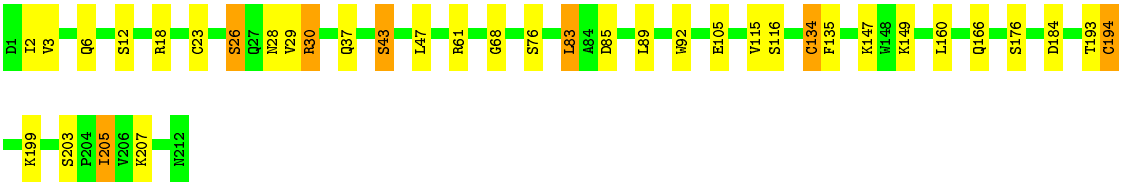
• Molecule 2: FAB 2H12, LIGHT CHAIN

Chain F:



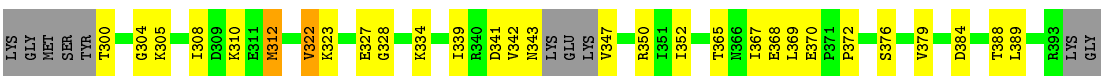
• Molecule 2: FAB 2H12, LIGHT CHAIN

Chain L:



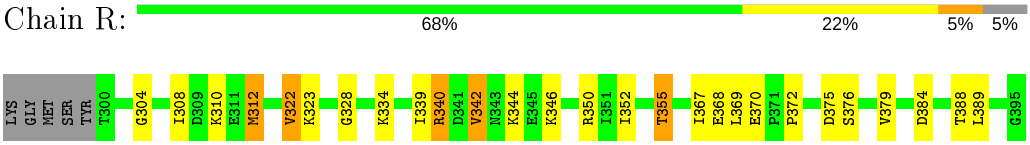
• Molecule 3: ENVELOPE PROTEIN,

Chain Q:



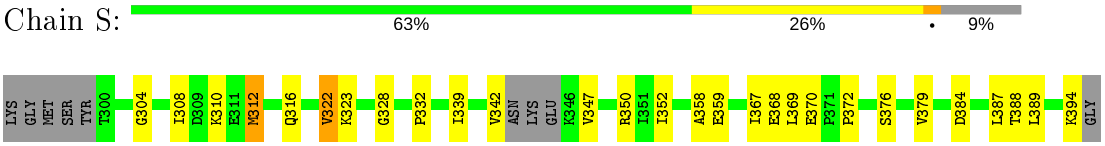
• Molecule 3: ENVELOPE PROTEIN,

Chain R:



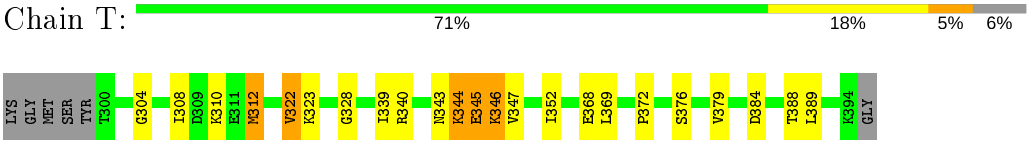
• Molecule 3: ENVELOPE PROTEIN,

Chain S:



• Molecule 3: ENVELOPE PROTEIN,

Chain T:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α, β, γ	69.93Å 92.80Å 96.59Å 118.55° 90.33° 104.05°	Depositor
Resolution (Å)	41.99 – 3.02 41.99 – 3.02	Depositor EDS
% Data completeness (in resolution range)	95.7 (41.99-3.02) 96.1 (41.99-3.02)	Depositor EDS
R_{merge}	0.11	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.85 (at 3.01Å)	Xtriage
Refinement program	BUSTER 2.11.2	Depositor
R, R_{free}	0.196 , 0.252 0.206 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å^2)	38.7	Xtriage
Anisotropy	0.866	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.33 , 19.9	EDS
L-test for twinning[2]	$< \|L\| > = 0.46$, $< L^2 > = 0.28$	Xtriage
Estimated twinning fraction	0.097 for -h,-k-l,l	Xtriage
F_o,F_c correlation	0.90	EDS
Total number of atoms	15830	wwPDB-VP
Average B, all atoms (Å^2)	44.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.23% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

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	A	0.55	0/1622	0.78	0/2217
1	C	0.57	0/1622	0.79	0/2217
1	E	0.55	0/1626	0.79	0/2222
1	H	0.55	0/1638	0.79	0/2239
2	B	0.51	0/1693	0.72	0/2299
2	D	0.47	0/1693	0.69	0/2299
2	F	0.48	0/1693	0.70	0/2299
2	L	0.48	0/1693	0.69	0/2299
3	Q	0.57	0/710	0.82	0/963
3	R	0.56	0/751	0.81	0/1016
3	S	0.56	0/720	0.76	0/974
3	T	0.56	0/747	0.85	1/1011 (0.1%)
All	All	0.53	0/16208	0.76	1/22055 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	T	345	GLU	C-N-CA	6.18	137.15	121.70

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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	1580	0	1526	27	0
1	C	1580	0	1526	27	0
1	E	1584	0	1529	35	0
1	H	1596	0	1538	30	0
2	B	1655	0	1588	15	0
2	D	1655	0	1588	13	0
2	F	1655	0	1588	17	0
2	L	1655	0	1588	16	0
3	Q	696	0	685	15	0
3	R	736	0	734	14	0
3	S	706	0	705	15	0
3	T	732	0	731	12	0
All	All	15830	0	15326	221	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 7.

All (221) 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:208:THR:HG22	1:H:208:THR:HG22	1.20	1.18
1:C:208:THR:HG22	1:E:208:THR:HG22	1.38	1.06
1:E:97:THR:HG21	1:E:104:MET:HG3	1.37	1.06
1:E:97:THR:HG21	1:E:104:MET:CG	1.95	0.95
2:F:134:CYS:HG	2:F:194:CYS:HG	0.91	0.87
3:R:340:ARG:HH21	3:R:379:VAL:HG21	1.40	0.87
1:C:97:THR:HG21	1:C:104:MET:HG2	1.56	0.86
1:E:50:ASN:ND2	1:E:59:ASN:HB2	1.97	0.79
2:D:134:CYS:HG	2:D:194:CYS:HG	1.32	0.77
1:A:208:THR:CG2	1:H:208:THR:HG22	2.12	0.74
3:Q:305:LYS:HE3	3:Q:327:GLU:OE1	1.87	0.73
1:H:97:THR:HG21	1:H:104:MET:HB3	1.71	0.72
1:E:62:ASP:HA	1:E:65:LYS:HG3	1.74	0.69
2:D:37:GLN:HB2	2:D:47:LEU:HD11	1.75	0.68
1:E:11:LEU:HD22	1:E:151:PRO:HG3	1.75	0.68
1:A:62:ASP:HA	1:A:65:LYS:HG3	1.75	0.68
1:H:62:ASP:HA	1:H:65:LYS:HG3	1.76	0.68
1:H:97:THR:HG21	1:H:104:MET:CB	2.24	0.68
1:E:12:VAL:HG11	1:E:18:VAL:HB	1.77	0.67
3:R:312:MET:HG2	3:R:322:VAL:HG13	1.76	0.67
2:L:37:GLN:HB2	2:L:47:LEU:HD11	1.77	0.67
1:A:12:VAL:HG11	1:A:18:VAL:HB	1.76	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:62:ASP:HA	1:C:65:LYS:HG3	1.74	0.67
1:A:30:SER:HA	1:A:53:PRO:HB2	1.76	0.67
2:B:134:CYS:HG	2:B:194:CYS:HG	1.39	0.67
3:Q:312:MET:HG2	3:Q:322:VAL:HG13	1.77	0.67
1:C:11:LEU:HD22	1:C:151:PRO:HG3	1.77	0.66
3:S:312:MET:HG2	3:S:322:VAL:HG13	1.77	0.66
3:R:334:LYS:HD3	3:R:355:THR:HG22	1.78	0.66
1:E:30:SER:HA	1:E:53:PRO:HB2	1.77	0.65
3:T:312:MET:HG2	3:T:322:VAL:HG13	1.77	0.65
2:L:134:CYS:HG	2:L:194:CYS:CB	2.08	0.65
2:B:37:GLN:HB2	2:B:47:LEU:HD11	1.79	0.65
1:E:53:PRO:HA	1:E:72:ILE:HD13	1.79	0.65
1:H:30:SER:HA	1:H:53:PRO:HB2	1.79	0.65
1:H:12:VAL:HG11	1:H:18:VAL:HB	1.80	0.64
1:A:11:LEU:HD22	1:A:151:PRO:HG3	1.78	0.64
1:H:11:LEU:HD22	1:H:151:PRO:HG3	1.78	0.64
2:F:37:GLN:HB2	2:F:47:LEU:HD11	1.77	0.64
1:C:12:VAL:HG11	1:C:18:VAL:HB	1.80	0.64
1:C:30:SER:HA	1:C:53:PRO:HB2	1.79	0.63
1:H:53:PRO:HA	1:H:72:ILE:HD13	1.78	0.63
1:A:35:ASN:ND2	1:A:47:TRP:HE1	1.97	0.63
1:C:32:TYR:O	1:C:53:PRO:HD2	1.99	0.63
3:R:339:ILE:HD11	3:R:369:LEU:HD22	1.82	0.62
1:A:53:PRO:HA	1:A:72:ILE:HD13	1.81	0.61
1:C:53:PRO:HA	1:C:72:ILE:HD13	1.83	0.61
1:A:97:THR:HG21	1:A:104:MET:HB3	1.82	0.60
1:C:50:ASN:ND2	1:C:59:ASN:HB2	2.17	0.60
1:E:123:PRO:HB3	1:E:149:TYR:HB3	1.85	0.59
3:S:350:ARG:HH11	3:S:370:GLU:HG2	1.68	0.59
1:C:97:THR:CG2	1:C:104:MET:HG2	2.29	0.59
2:L:3:VAL:H	2:L:26:SER:HB3	1.68	0.59
1:E:50:ASN:HD21	1:E:59:ASN:HB2	1.67	0.58
1:E:32:TYR:O	1:E:53:PRO:HD2	2.03	0.58
1:H:37:GLU:HB3	1:H:45:LEU:HD23	1.86	0.58
1:A:37:GLU:HB3	1:A:45:LEU:HD23	1.86	0.58
1:C:123:PRO:HB3	1:C:149:TYR:HB3	1.86	0.58
3:R:308:ILE:HD11	3:R:389:LEU:HD21	1.86	0.57
1:A:123:PRO:HB3	1:A:149:TYR:HB3	1.86	0.57
2:F:205:ILE:HD11	2:F:207:LYS:HE2	1.87	0.57
2:F:3:VAL:H	2:F:26:SER:HB3	1.69	0.57
1:H:123:PRO:HB3	1:H:149:TYR:HB3	1.86	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:3:VAL:H	2:D:26:SER:HB3	1.70	0.56
3:S:308:ILE:HD11	3:S:389:LEU:HD21	1.87	0.56
1:A:108:GLY:O	2:B:43:SER:OG	2.19	0.56
3:Q:300:THR:N	3:Q:334:LYS:HZ3	2.03	0.56
1:E:37:GLU:HB3	1:E:45:LEU:HD23	1.87	0.56
1:E:51:ILE:HD12	1:E:58:VAL:HG22	1.87	0.56
1:H:34:ILE:HA	1:H:97:THR:O	2.05	0.56
1:A:12:VAL:HG21	1:A:86:LEU:HD13	1.87	0.56
2:B:3:VAL:H	2:B:26:SER:HB3	1.71	0.56
2:B:147:LYS:HE3	2:B:149:LYS:HE3	1.87	0.55
3:T:339:ILE:HG22	3:T:347:VAL:HB	1.88	0.55
1:E:12:VAL:HG21	1:E:86:LEU:HD13	1.88	0.55
2:L:147:LYS:HE3	2:L:149:LYS:HE3	1.88	0.55
3:Q:350:ARG:HD2	3:Q:370:GLU:O	2.07	0.55
2:B:205:ILE:HD11	2:B:207:LYS:HE2	1.89	0.55
2:F:147:LYS:HE3	2:F:149:LYS:HE3	1.89	0.54
2:F:154:GLU:OE2	2:F:156:GLN:NE2	2.38	0.54
3:S:350:ARG:HD2	3:S:370:GLU:O	2.08	0.54
2:L:205:ILE:HD11	2:L:207:LYS:HE2	1.91	0.53
1:C:12:VAL:HG21	1:C:86:LEU:HD13	1.91	0.53
1:H:97:THR:HG22	1:H:98:ARG:N	2.23	0.53
2:D:147:LYS:HE3	2:D:149:LYS:HE3	1.90	0.53
1:C:37:GLU:HB3	1:C:45:LEU:HD23	1.89	0.53
1:H:97:THR:HG22	1:H:98:ARG:O	2.09	0.52
1:H:173:LEU:HD13	2:L:160:LEU:HD22	1.91	0.52
3:R:372:PRO:HG2	3:R:376:SER:HB3	1.91	0.52
3:Q:308:ILE:HD11	3:Q:389:LEU:HD21	1.92	0.52
1:H:50:ASN:ND2	1:H:59:ASN:HB2	2.25	0.51
1:E:108:GLY:O	2:F:43:SER:OG	2.24	0.51
3:T:339:ILE:HD11	3:T:369:LEU:HD22	1.92	0.51
1:H:12:VAL:HG21	1:H:86:LEU:HD13	1.91	0.51
1:A:35:ASN:HD22	1:A:47:TRP:HE1	1.57	0.51
3:T:308:ILE:HD11	3:T:389:LEU:HD21	1.93	0.51
3:T:347:VAL:HG21	3:T:372:PRO:HG3	1.93	0.51
2:F:61:ARG:HB3	2:F:76:SER:O	2.10	0.51
2:D:30:ARG:HD2	2:D:92:TRP:CH2	2.46	0.50
1:E:97:THR:HG21	1:E:104:MET:HG2	1.87	0.50
3:Q:379:VAL:HG22	3:Q:388:THR:HG22	1.92	0.50
2:L:61:ARG:HB3	2:L:76:SER:O	2.12	0.50
3:T:379:VAL:HG22	3:T:388:THR:HG22	1.93	0.50
2:D:205:ILE:HD11	2:D:207:LYS:HE2	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:R:340:ARG:NH2	3:R:379:VAL:HG21	2.19	0.49
2:B:61:ARG:HB3	2:B:76:SER:O	2.12	0.49
1:E:97:THR:CG2	1:E:104:MET:HG3	2.27	0.49
2:D:61:ARG:HB3	2:D:76:SER:O	2.12	0.49
3:Q:339:ILE:HD11	3:Q:369:LEU:HD22	1.93	0.49
3:S:379:VAL:HG22	3:S:388:THR:HG22	1.95	0.49
1:E:104:MET:HB2	2:F:36:TYR:OH	2.13	0.49
3:S:332:PRO:HA	3:S:358:ALA:O	2.12	0.49
2:L:30:ARG:HD2	2:L:92:TRP:CH2	2.48	0.49
3:T:372:PRO:HG2	3:T:376:SER:HB3	1.93	0.49
2:F:30:ARG:HD2	2:F:92:TRP:CH2	2.48	0.48
1:A:36:TRP:HA	1:A:95:TYR:O	2.13	0.48
1:A:210:VAL:HG22	1:H:207:SER:HB2	1.95	0.48
3:T:352:ILE:HB	3:T:368:GLU:HB3	1.95	0.48
1:H:157:THR:HB	1:H:200:SER:HB2	1.96	0.48
3:R:352:ILE:HB	3:R:368:GLU:HB3	1.96	0.48
1:A:122:PRO:HG3	1:H:122:PRO:HG3	1.95	0.47
2:B:18:ARG:HG3	2:B:76:SER:HA	1.96	0.47
3:Q:350:ARG:HH11	3:Q:370:GLU:HG2	1.78	0.47
2:D:134:CYS:HG	2:D:194:CYS:CB	2.26	0.47
2:L:18:ARG:HG3	2:L:76:SER:HA	1.95	0.47
3:Q:352:ILE:HB	3:Q:368:GLU:HB3	1.96	0.47
1:A:50:ASN:ND2	3:S:316:GLN:OE1	2.47	0.47
1:E:97:THR:HG23	1:E:104:MET:HA	1.97	0.47
2:D:18:ARG:HG3	2:D:76:SER:HA	1.95	0.47
1:C:40:ARG:HG3	1:C:92:ALA:HB2	1.97	0.47
1:E:188:PRO:O	1:E:191:THR:HG22	2.15	0.47
2:B:30:ARG:HD2	2:B:92:TRP:CH2	2.49	0.46
1:C:188:PRO:O	1:C:191:THR:HG22	2.16	0.46
1:H:40:ARG:HG3	1:H:92:ALA:HB2	1.97	0.46
3:S:310:LYS:HB3	3:S:323:LYS:HB2	1.97	0.46
1:C:157:THR:HB	1:C:200:SER:HB2	1.97	0.46
2:F:18:ARG:HG3	2:F:76:SER:HA	1.98	0.46
3:S:352:ILE:HB	3:S:368:GLU:HB3	1.98	0.45
1:A:157:THR:HB	1:A:200:SER:HB2	1.97	0.45
1:E:157:THR:HB	1:E:200:SER:HB2	1.98	0.45
3:Q:341:ASP:C	3:Q:343:ASN:H	2.18	0.45
2:B:83:LEU:HD21	2:B:166:GLN:HB3	1.97	0.45
1:H:108:GLY:O	2:L:43:SER:OG	2.33	0.45
1:C:35:ASN:HB2	1:C:97:THR:CG2	2.47	0.45
2:B:2:ILE:HD13	2:B:29:VAL:HG12	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:Q:304:GLY:HA3	3:Q:328:GLY:HA3	1.99	0.45
1:H:188:PRO:O	1:H:191:THR:HG22	2.17	0.45
3:S:339:ILE:HD11	3:S:369:LEU:HD22	1.99	0.45
3:T:340:ARG:NH1	3:T:345:GLU:OE1	2.49	0.45
1:A:188:PRO:O	1:A:191:THR:HG22	2.16	0.45
1:C:51:ILE:HD11	1:C:72:ILE:HG12	1.99	0.45
3:R:379:VAL:HG22	3:R:388:THR:HG22	1.99	0.45
1:H:27:TYR:CE2	1:H:98:ARG:HD2	2.52	0.45
1:H:35:ASN:HD22	1:H:97:THR:HB	1.82	0.45
1:C:51:ILE:HD12	1:C:58:VAL:HG22	1.98	0.45
3:Q:305:LYS:HB3	3:Q:327:GLU:HB2	1.98	0.45
1:H:19:LYS:HG3	1:H:82:GLN:HG3	1.99	0.44
1:E:40:ARG:HG3	1:E:92:ALA:HB2	2.00	0.44
3:R:350:ARG:HB3	3:R:370:GLU:O	2.18	0.44
2:D:2:ILE:HD13	2:D:29:VAL:HG12	1.99	0.44
1:E:35:ASN:ND2	1:E:97:THR:HG22	2.32	0.44
3:S:304:GLY:HA3	3:S:328:GLY:HA3	2.00	0.44
1:C:201:VAL:O	1:C:209:THR:HA	2.18	0.44
3:R:310:LYS:HB3	3:R:323:LYS:HB2	1.99	0.44
1:A:40:ARG:HG3	1:A:92:ALA:HB2	1.99	0.43
3:T:344:LYS:HA	3:T:345:GLU:HA	1.74	0.43
1:A:201:VAL:O	1:A:209:THR:HA	2.17	0.43
1:E:201:VAL:O	1:E:209:THR:HA	2.18	0.43
1:A:169:THR:HG23	1:A:181:MET:HE1	2.00	0.43
2:B:115:VAL:HA	2:B:135:PHE:O	2.19	0.43
2:F:83:LEU:HD21	2:F:166:GLN:HB3	1.99	0.43
1:E:98:ARG:HB3	1:E:105:ASP:OD1	2.18	0.43
2:L:6:GLN:HG3	2:L:23:CYS:HB2	2.01	0.43
1:C:173:LEU:HD13	2:D:160:LEU:HD22	2.01	0.43
2:F:115:VAL:HA	2:F:135:PHE:O	2.19	0.43
2:F:2:ILE:HD13	2:F:29:VAL:HG12	2.00	0.43
1:H:97:THR:CG2	1:H:98:ARG:N	2.81	0.43
3:T:304:GLY:HA3	3:T:328:GLY:HA3	2.00	0.43
3:Q:310:LYS:HB3	3:Q:323:LYS:HB2	2.00	0.43
1:E:35:ASN:O	1:E:96:CYS:HA	2.18	0.42
1:H:142:LEU:HD22	1:H:214:LEU:HD12	2.00	0.42
1:C:169:THR:HG23	1:C:181:MET:HE1	2.00	0.42
3:R:322:VAL:HG23	3:R:367:ILE:HB	2.01	0.42
2:D:28:ASN:OD1	2:D:68:GLY:HA2	2.19	0.42
1:A:28:THR:O	1:A:32:TYR:HD1	2.02	0.42
2:D:115:VAL:HA	2:D:135:PHE:O	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:122:PRO:HG3	1:E:122:PRO:HG3	2.02	0.42
1:A:191:THR:O	1:A:195:GLN:HB2	2.19	0.42
3:S:347:VAL:HG21	3:S:372:PRO:HG3	2.02	0.42
1:C:98:ARG:O	1:C:104:MET:HA	2.19	0.42
2:L:83:LEU:HD21	2:L:166:GLN:HB3	2.01	0.42
3:S:322:VAL:HG23	3:S:367:ILE:HB	2.02	0.42
3:Q:372:PRO:HG2	3:Q:376:SER:HB3	2.02	0.42
1:A:94:TYR:O	1:A:110:GLY:HA2	2.20	0.42
1:E:196:THR:HG23	1:E:213:LYS:NZ	2.35	0.42
1:H:201:VAL:O	1:H:209:THR:HA	2.19	0.42
2:L:2:ILE:HD13	2:L:29:VAL:HG12	2.02	0.42
3:S:372:PRO:HG2	3:S:376:SER:HB3	2.02	0.42
1:C:35:ASN:HB2	1:C:97:THR:HG23	2.02	0.41
3:R:304:GLY:HA3	3:R:328:GLY:HA3	2.02	0.41
2:F:54:ARG:HD3	2:F:58:VAL:O	2.20	0.41
1:E:33:TRP:O	1:E:99:GLY:N	2.50	0.41
3:Q:322:VAL:HG23	3:Q:367:ILE:HB	2.03	0.41
1:E:97:THR:CG2	1:E:104:MET:HA	2.51	0.41
1:C:208:THR:CG2	1:E:208:THR:HG22	2.28	0.41
2:L:28:ASN:OD1	2:L:68:GLY:HA2	2.20	0.41
2:B:54:ARG:HD3	2:B:58:VAL:O	2.20	0.41
1:E:169:THR:HG23	1:E:181:MET:HE1	2.02	0.41
2:L:149:LYS:HB2	2:L:193:THR:HB	2.02	0.41
3:R:342:VAL:HG13	3:R:375:ASP:HB2	2.03	0.41
3:S:350:ARG:NH2	3:S:372:PRO:HA	2.36	0.41
1:C:105:ASP:N	1:C:105:ASP:OD1	2.53	0.41
2:F:28:ASN:OD1	2:F:68:GLY:HA2	2.20	0.41
2:B:25:ALA:HB3	2:B:69:THR:HA	2.03	0.41
3:T:310:LYS:HB3	3:T:323:LYS:HB2	2.02	0.41
1:A:39:GLN:HE22	2:B:38:GLN:HE22	1.69	0.40
1:E:2:VAL:HG13	1:E:27:TYR:CD1	2.56	0.40
1:H:169:THR:HG23	1:H:181:MET:HE1	2.03	0.40
2:L:115:VAL:HA	2:L:135:PHE:O	2.20	0.40
1:E:140:VAL:HG12	1:E:189:SER:HA	2.03	0.40
2:F:89:LEU:HD11	2:F:96:TYR:HB3	2.03	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	207/217 (95%)	193 (93%)	11 (5%)	3 (1%)	11	41
1	C	207/217 (95%)	194 (94%)	10 (5%)	3 (1%)	11	41
1	E	208/217 (96%)	193 (93%)	11 (5%)	4 (2%)	8	34
1	H	210/217 (97%)	195 (93%)	11 (5%)	4 (2%)	8	34
2	B	210/212 (99%)	195 (93%)	13 (6%)	2 (1%)	15	50
2	D	210/212 (99%)	196 (93%)	12 (6%)	2 (1%)	15	50
2	F	210/212 (99%)	197 (94%)	12 (6%)	1 (0%)	29	66
2	L	210/212 (99%)	197 (94%)	12 (6%)	1 (0%)	29	66
3	Q	87/101 (86%)	83 (95%)	3 (3%)	1 (1%)	14	48
3	R	94/101 (93%)	87 (93%)	7 (7%)	0	100	100
3	S	88/101 (87%)	82 (93%)	5 (6%)	1 (1%)	14	48
3	T	93/101 (92%)	88 (95%)	4 (4%)	1 (1%)	14	48
All	All	2034/2120 (96%)	1900 (93%)	111 (6%)	23 (1%)	14	48

All (23) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	103	ALA
2	D	83	LEU
1	H	103	ALA
3	T	346	LYS
1	A	189	SER
2	B	83	LEU
1	C	189	SER
1	E	103	ALA
1	E	189	SER
2	F	83	LEU
1	H	189	SER
2	L	83	LEU

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Mol	Chain	Res	Type
1	A	55	SER
1	H	55	SER
1	H	132	SER
3	Q	342	VAL
1	A	103	ALA
2	B	51	ALA
1	C	55	SER
2	D	51	ALA
1	E	55	SER
1	E	105	ASP
3	S	359	GLU

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	182/186 (98%)	169 (93%)	13 (7%)	14	44
1	C	182/186 (98%)	168 (92%)	14 (8%)	13	41
1	E	182/186 (98%)	166 (91%)	16 (9%)	10	34
1	H	183/186 (98%)	168 (92%)	15 (8%)	11	38
2	B	189/189 (100%)	172 (91%)	17 (9%)	9	33
2	D	189/189 (100%)	175 (93%)	14 (7%)	13	42
2	F	189/189 (100%)	175 (93%)	14 (7%)	13	42
2	L	189/189 (100%)	174 (92%)	15 (8%)	12	39
3	Q	78/86 (91%)	73 (94%)	5 (6%)	17	49
3	R	82/86 (95%)	74 (90%)	8 (10%)	8	29
3	S	79/86 (92%)	73 (92%)	6 (8%)	13	41
3	T	82/86 (95%)	76 (93%)	6 (7%)	14	43
All	All	1806/1844 (98%)	1663 (92%)	143 (8%)	12	39

All (143) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1	ASP
1	A	4	LEU
1	A	10	GLU
1	A	45	LEU
1	A	55	SER
1	A	62	ASP
1	A	72	ILE
1	A	85	SER
1	A	139	SER
1	A	162	SER
1	A	196	THR
1	A	207	SER
1	A	213	LYS
2	B	12	SER
2	B	26	SER
2	B	30	ARG
2	B	38	GLN
2	B	43	SER
2	B	63	THR
2	B	85	ASP
2	B	89	LEU
2	B	105	GLU
2	B	114	THR
2	B	116	SER
2	B	134	CYS
2	B	176	SER
2	B	184	ASP
2	B	199	LYS
2	B	203	SER
2	B	205	ILE
1	C	1	ASP
1	C	10	GLU
1	C	45	LEU
1	C	50	ASN
1	C	55	SER
1	C	62	ASP
1	C	72	ILE
1	C	85	SER
1	C	104	MET
1	C	139	SER
1	C	162	SER
1	C	196	THR
1	C	207	SER

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Mol	Chain	Res	Type
1	C	213	LYS
2	D	12	SER
2	D	26	SER
2	D	30	ARG
2	D	43	SER
2	D	85	ASP
2	D	89	LEU
2	D	105	GLU
2	D	116	SER
2	D	134	CYS
2	D	176	SER
2	D	184	ASP
2	D	199	LYS
2	D	203	SER
2	D	205	ILE
1	E	1	ASP
1	E	10	GLU
1	E	45	LEU
1	E	50	ASN
1	E	55	SER
1	E	62	ASP
1	E	72	ILE
1	E	85	SER
1	E	97	THR
1	E	101	SER
1	E	104	MET
1	E	139	SER
1	E	162	SER
1	E	165	SER
1	E	196	THR
1	E	213	LYS
2	F	12	SER
2	F	26	SER
2	F	30	ARG
2	F	85	ASP
2	F	89	LEU
2	F	105	GLU
2	F	116	SER
2	F	134	CYS
2	F	169	LYS
2	F	176	SER
2	F	184	ASP

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Mol	Chain	Res	Type
2	F	199	LYS
2	F	203	SER
2	F	205	ILE
1	H	1	ASP
1	H	10	GLU
1	H	23	LYS
1	H	35	ASN
1	H	45	LEU
1	H	50	ASN
1	H	55	SER
1	H	62	ASP
1	H	72	ILE
1	H	85	SER
1	H	139	SER
1	H	162	SER
1	H	196	THR
1	H	207	SER
1	H	213	LYS
2	L	12	SER
2	L	26	SER
2	L	30	ARG
2	L	43	SER
2	L	85	ASP
2	L	89	LEU
2	L	105	GLU
2	L	116	SER
2	L	134	CYS
2	L	176	SER
2	L	184	ASP
2	L	194	CYS
2	L	199	LYS
2	L	203	SER
2	L	205	ILE
3	Q	312	MET
3	Q	322	VAL
3	Q	347	VAL
3	Q	365	THR
3	Q	384	ASP
3	R	312	MET
3	R	322	VAL
3	R	340	ARG
3	R	342	VAL

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Mol	Chain	Res	Type
3	R	344	LYS
3	R	346	LYS
3	R	355	THR
3	R	384	ASP
3	S	312	MET
3	S	322	VAL
3	S	342	VAL
3	S	384	ASP
3	S	387	LEU
3	S	394	LYS
3	T	312	MET
3	T	322	VAL
3	T	343	ASN
3	T	344	LYS
3	T	346	LYS
3	T	384	ASP

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

Mol	Chain	Res	Type
1	A	35	ASN
1	A	39	GLN
1	A	50	ASN
2	B	38	GLN
1	C	50	ASN
1	C	59	ASN
1	C	102	HIS
1	E	50	ASN
1	H	50	ASN
2	L	190	ASN
2	L	212	ASN
3	Q	316	GLN
3	R	316	GLN
3	S	316	GLN
3	T	316	GLN

5.3.3 RNA

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates

There are no carbohydrates in this entry.

5.6 Ligand geometry

There are no ligands in this entry.

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95^{th} percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled 'Q< 0.9' lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
1	A	211/217 (97%)	-0.68	0 100 100	14, 39, 71, 106	0
1	C	211/217 (97%)	-0.69	0 100 100	12, 39, 68, 103	0
1	E	212/217 (97%)	-0.65	1 (0%) 91 75	12, 38, 75, 125	0
1	H	214/217 (98%)	-0.64	0 100 100	16, 38, 76, 113	0
2	B	212/212 (100%)	-0.66	0 100 100	19, 46, 73, 109	0
2	D	212/212 (100%)	-0.65	0 100 100	20, 53, 71, 91	0
2	F	212/212 (100%)	-0.59	0 100 100	25, 51, 72, 102	0
2	L	212/212 (100%)	-0.59	0 100 100	19, 48, 78, 90	0
3	Q	91/101 (90%)	-0.75	0 100 100	24, 36, 56, 60	0
3	R	96/101 (95%)	-0.75	0 100 100	19, 39, 53, 58	0
3	S	92/101 (91%)	-0.76	0 100 100	20, 37, 53, 68	0
3	T	95/101 (94%)	-0.73	0 100 100	24, 36, 56, 66	0
All	All	2070/2120 (97%)	-0.66	1 (0%) 100 100	12, 43, 73, 125	0

All (1) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	E	217	ARG	2.1

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

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

6.3 Carbohydrates

There are no carbohydrates in this entry.

6.4 Ligands

There are no ligands in this entry.

6.5 Other polymers

There are no such residues in this entry.