Full wwPDB X-ray Structure Validation Report ⓘ

Jan 31, 2016 – 08:06 PM GMT

PDB ID	:	1IRJ
Title	:	Crystal Structure of the MRP14 complexed with CHAPS
Authors	:	Itou, H.; Yao, M.; Watanabe, N.; Nishihira, J.; Tanaka, I.
Deposited on	:	2001-10-09
Resolution	:	2.10 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 ⓘ symbol.

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

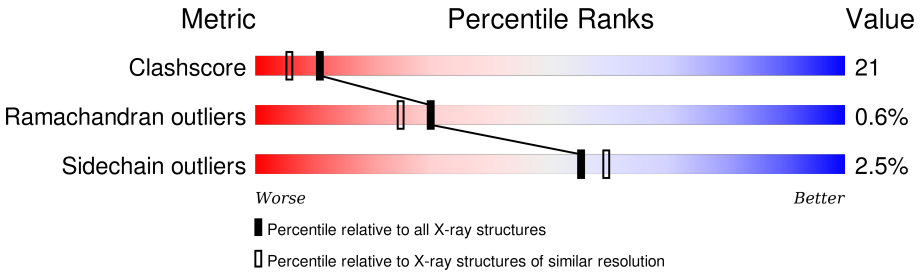
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
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 2.10 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	4460 (2.10-2.10)
Ramachandran outliers	100387	4413 (2.10-2.10)
Sidechain outliers	100360	4414 (2.10-2.10)

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	113	58% 17% • 25%
1	B	113	58% 13% • 26%
1	C	113	46% 25% • • 27%
1	D	113	50% 22% • 27%
1	E	113	48% 25% • 27%
1	F	113	34% 36% • 26%
1	G	113	61% 12% • 26%

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Mol	Chain	Length	Quality of chain
1	H	113	

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 5871 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 Migration Inhibitory Factor-Related Protein 14.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	85	Total	C	N	O	S	0	0	0
			707	445	121	136	5			
1	B	84	Total	C	N	O	S	0	0	0
			700	441	120	134	5			
1	C	83	Total	C	N	O	S	0	0	0
			694	438	119	133	4			
1	D	82	Total	C	N	O	S	0	0	0
			685	432	117	132	4			
1	E	83	Total	C	N	O	S	0	0	0
			694	438	119	133	4			
1	F	84	Total	C	N	O	S	0	0	0
			700	441	120	134	5			
1	G	84	Total	C	N	O	S	0	0	0
			700	441	120	134	5			
1	H	85	Total	C	N	O	S	0	0	0
			707	445	121	136	5			

- Molecule 2 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	G	2	Total	Ca	0	0
			2	2		
2	D	2	Total	Ca	0	0
			2	2		
2	E	2	Total	Ca	0	0
			2	2		
2	H	2	Total	Ca	0	0
			2	2		
2	B	2	Total	Ca	0	0
			2	2		
2	C	2	Total	Ca	0	0
			2	2		

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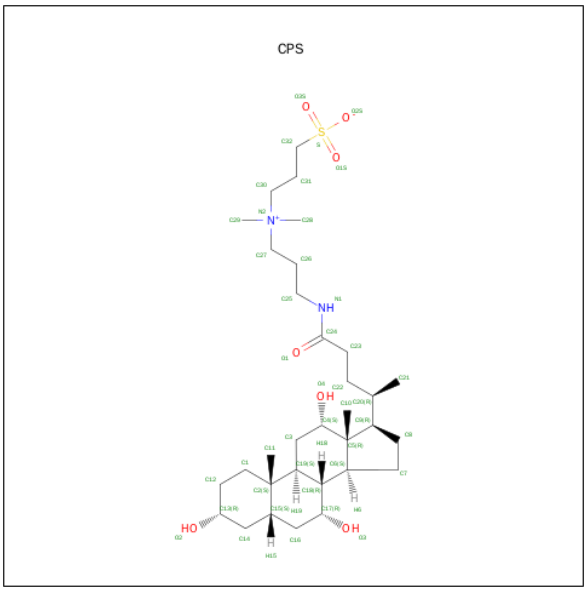
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	2	Total Ca 2 2	0	0
2	F	2	Total Ca 2 2	0	0

- Molecule 3 is 3-[(3-CHOLAMIDOPROPYL)DIMETHYLAMMONIO]-1-PROPANESULFONATE (three-letter code: CPS) (formula: $C_{32}H_{58}N_2O_7S$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	B	1	Total C N O 32 27 1 4	0	0
3	D	1	Total C N O 32 27 1 4	0	0
3	D	1	Total C N O 32 27 1 4	0	0
3	G	1	Total C N O 32 27 1 4	0	0

- Molecule 4 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	19	Total O 19 19	0	0
4	B	28	Total O 28 28	0	0
4	C	6	Total O 6 6	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	D	20	Total O 20 20	0	0
4	E	9	Total O 9 9	0	0
4	F	2	Total O 2 2	0	0
4	G	30	Total O 30 30	0	0
4	H	26	Total O 26 26	0	0

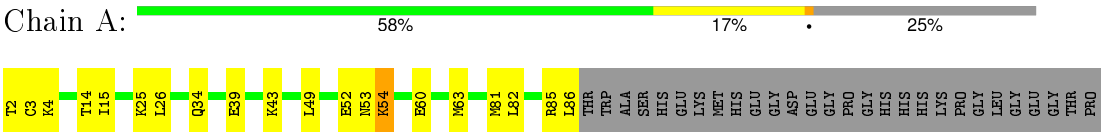
3 Residue-property plots (i)

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.

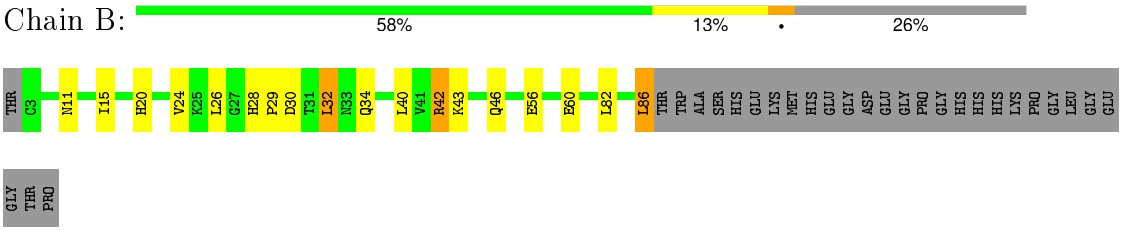
- Molecule 1: Migration Inhibitory Factor-Related Protein 14

Chain A:



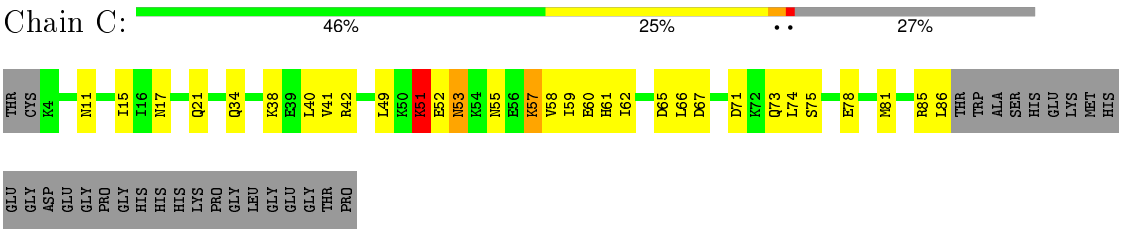
- Molecule 1: Migration Inhibitory Factor-Related Protein 14

Chain B:



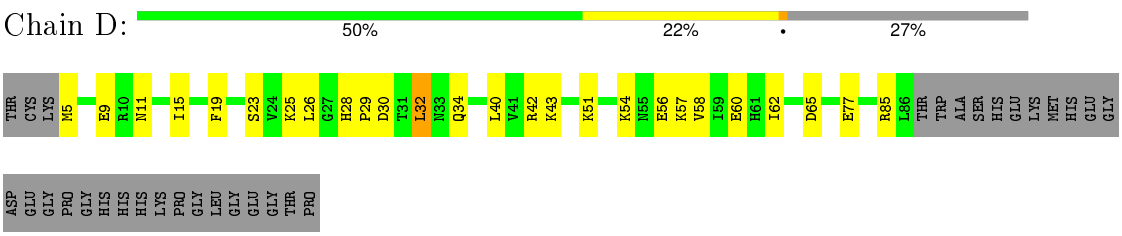
- Molecule 1: Migration Inhibitory Factor-Related Protein 14

Chain C:



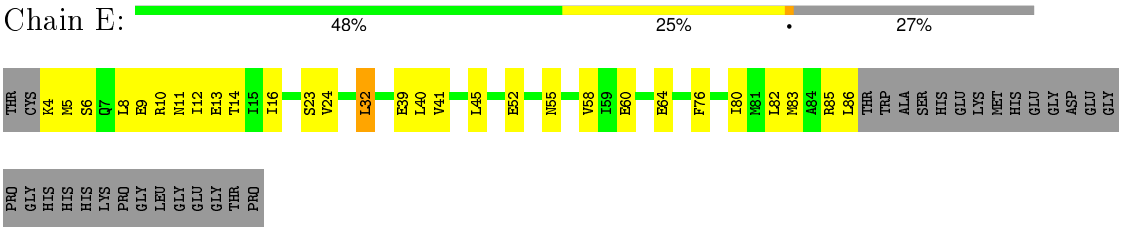
- Molecule 1: Migration Inhibitory Factor-Related Protein 14

Chain D:



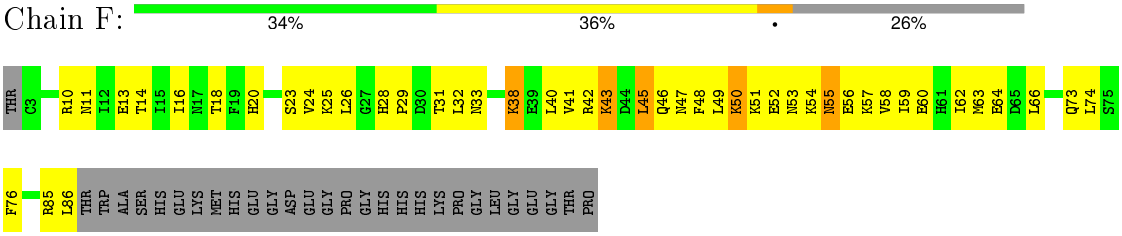
- Molecule 1: Migration Inhibitory Factor-Related Protein 14

Chain E:



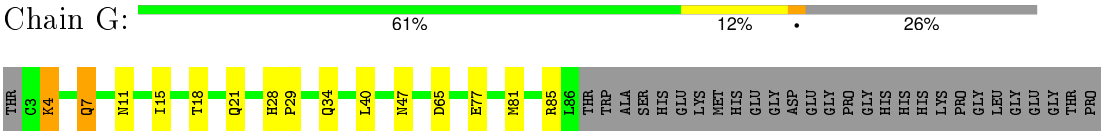
- Molecule 1: Migration Inhibitory Factor-Related Protein 14

Chain F:



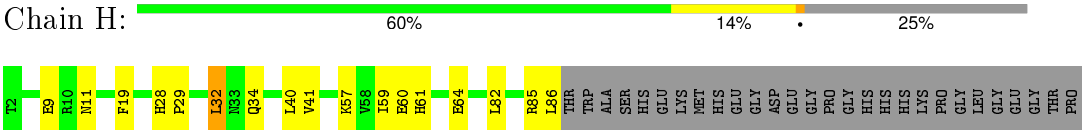
- Molecule 1: Migration Inhibitory Factor-Related Protein 14

Chain G:



- Molecule 1: Migration Inhibitory Factor-Related Protein 14

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 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	57.59Å 178.44Å 61.23Å 90.00° 113.17° 90.00°	Depositor
Resolution (Å)	10.00 – 2.10	Depositor
% Data completeness (in resolution range)	99.8 (10.00-2.10)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	0.07	Depositor
Refinement program	CNS	Depositor
R, R_{free}	0.245 , 0.274	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	5871	wwPDB-VP
Average B, all atoms (Å^2)	47.0	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: CA, CPS

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	0.43	0/716	0.58	0/957
1	B	0.43	0/709	0.64	1/947 (0.1%)
1	C	0.40	0/703	0.55	0/939
1	D	0.40	0/694	0.60	0/928
1	E	0.35	0/703	0.58	0/939
1	F	0.32	0/709	0.49	0/947
1	G	0.46	0/709	0.66	0/947
1	H	0.43	0/716	0.66	0/957
All	All	0.41	0/5659	0.60	1/7561 (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})
1	B	32	LEU	CA-CB-CG	5.36	127.64	115.30

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	707	0	709	18	0
1	B	700	0	702	20	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	C	694	0	697	33	0
1	D	685	0	684	21	0
1	E	694	0	697	51	0
1	F	700	0	702	77	0
1	G	700	0	702	15	0
1	H	707	0	709	12	0
2	A	2	0	0	0	0
2	B	2	0	0	0	0
2	C	2	0	0	0	0
2	D	2	0	0	0	0
2	E	2	0	0	0	0
2	F	2	0	0	0	0
2	G	2	0	0	0	0
2	H	2	0	0	0	0
3	B	32	0	42	5	0
3	D	64	0	84	12	0
3	G	32	0	42	6	0
4	A	19	0	0	1	0
4	B	28	0	0	0	0
4	C	6	0	0	0	0
4	D	20	0	0	0	0
4	E	9	0	0	0	0
4	F	2	0	0	0	0
4	G	30	0	0	2	0
4	H	26	0	0	0	0
All	All	5871	0	5770	241	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 21.

All (241) 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)
3:B:189:CPS:C5	3:B:189:CPS:C10	1.76	1.63
3:D:289:CPS:C10	3:D:289:CPS:C5	1.75	1.62
3:G:489:CPS:C5	3:G:489:CPS:C10	1.75	1.62
3:D:389:CPS:C5	3:D:389:CPS:C10	1.76	1.61
1:E:5:MET:CE	1:F:47:ASN:H	1.76	0.98
1:A:54:LYS:HE3	1:A:54:LYS:HA	1.48	0.96
1:E:5:MET:HE3	1:F:47:ASN:H	1.30	0.95
1:C:55:ASN:HD22	1:C:58:VAL:HG23	1.32	0.94

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:34:GLN:HE21	1:H:60:GLU:HG2	1.35	0.91
1:F:51:LYS:HA	1:F:54:LYS:HE3	1.53	0.90
1:E:5:MET:HG2	1:E:6:SER:H	1.34	0.90
1:E:5:MET:SD	1:E:9:GLU:HB2	2.12	0.90
1:B:28:HIS:HD2	1:B:30:ASP:H	1.15	0.89
3:D:289:CPS:C9	3:D:289:CPS:C10	2.51	0.88
1:C:57:LYS:HA	1:C:57:LYS:HE2	1.55	0.87
1:F:86:LEU:HD22	1:F:86:LEU:H	1.39	0.87
3:G:489:CPS:C9	3:G:489:CPS:C10	2.53	0.87
3:D:389:CPS:C9	3:D:389:CPS:C10	2.54	0.86
3:B:189:CPS:C10	3:B:189:CPS:C6	2.55	0.84
1:F:50:LYS:HD2	1:F:51:LYS:H	1.40	0.84
1:E:5:MET:HE2	1:F:46:GLN:H	1.40	0.84
1:E:5:MET:HG2	1:E:6:SER:N	1.89	0.84
3:B:189:CPS:C10	3:B:189:CPS:C9	2.55	0.83
3:G:489:CPS:C6	3:G:489:CPS:C10	2.56	0.82
1:E:83:MET:HA	1:E:86:LEU:HD12	1.61	0.82
3:D:389:CPS:C6	3:D:389:CPS:C10	2.58	0.81
3:D:389:CPS:C4	3:D:389:CPS:C10	2.58	0.81
3:D:289:CPS:C6	3:D:289:CPS:C10	2.58	0.81
3:G:489:CPS:C4	3:G:489:CPS:C10	2.59	0.79
3:D:289:CPS:C10	3:D:289:CPS:C4	2.60	0.79
3:B:189:CPS:C4	3:B:189:CPS:C10	2.59	0.79
1:E:5:MET:HB3	1:E:9:GLU:HG3	1.63	0.79
1:E:52:GLU:H	1:E:52:GLU:CD	1.85	0.79
1:B:56:GLU:O	1:B:60:GLU:HG3	1.84	0.78
1:F:62:ILE:HG12	1:F:85:ARG:HH22	1.49	0.76
1:F:50:LYS:CD	1:F:51:LYS:H	2.00	0.75
1:C:55:ASN:ND2	1:C:58:VAL:HG23	2.01	0.75
1:B:28:HIS:CD2	1:B:30:ASP:H	2.05	0.74
1:F:38:LYS:HE2	1:F:42:ARG:HD3	1.69	0.73
1:B:26:LEU:HD22	1:E:39:GLU:HG3	1.70	0.72
1:E:5:MET:HE3	1:F:47:ASN:N	2.04	0.72
1:F:26:LEU:HD12	1:F:33:ASN:HD21	1.55	0.70
1:E:4:LYS:HE3	1:E:10:ARG:NE	2.07	0.70
1:A:2:THR:HB	1:A:4:LYS:HG2	1.75	0.69
1:B:42:ARG:HB3	1:B:42:ARG:HH11	1.57	0.68
1:E:4:LYS:HE2	1:E:5:MET:O	1.93	0.68
1:F:50:LYS:HE3	1:F:51:LYS:HG2	1.75	0.68
1:C:55:ASN:HD21	1:C:57:LYS:HB3	1.58	0.68
1:A:2:THR:HG22	1:A:3:CYS:H	1.59	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:60:GLU:O	1:H:64:GLU:HG3	1.94	0.67
1:F:16:ILE:HG12	1:F:76:PHE:CZ	2.29	0.67
1:A:54:LYS:CE	1:A:54:LYS:HA	2.22	0.67
1:H:34:GLN:NE2	1:H:60:GLU:HG2	2.08	0.66
1:E:85:ARG:HH11	1:E:85:ARG:HG3	1.60	0.66
1:H:57:LYS:HE3	1:H:61:HIS:CE1	2.32	0.65
1:F:50:LYS:N	1:F:50:LYS:HE2	2.11	0.65
1:E:16:ILE:HG12	1:E:76:PHE:CE1	2.31	0.65
1:F:55:ASN:HD22	1:F:55:ASN:N	1.93	0.64
1:F:86:LEU:CD2	1:F:86:LEU:H	2.10	0.63
1:F:56:GLU:O	1:F:60:GLU:HG3	1.99	0.63
1:F:60:GLU:O	1:F:64:GLU:HG3	1.98	0.63
1:D:28:HIS:CD2	1:D:30:ASP:H	2.16	0.63
1:G:77:GLU:OE2	1:H:85:ARG:NH2	2.31	0.63
1:F:86:LEU:HD22	1:F:86:LEU:N	2.13	0.62
1:F:42:ARG:HA	1:F:53:ASN:OD1	2.00	0.62
1:C:49:LEU:HD22	1:C:52:GLU:HG3	1.82	0.61
1:F:31:THR:HB	1:F:73:GLN:CG	2.29	0.61
1:E:5:MET:HE1	1:F:45:LEU:HA	1.81	0.61
1:F:54:LYS:C	1:F:55:ASN:HD22	2.04	0.60
1:F:38:LYS:C	1:F:38:LYS:HD3	2.21	0.60
1:E:14:THR:HG21	1:F:11:ASN:ND2	2.17	0.59
1:B:42:ARG:NH1	1:B:43:LYS:HG3	2.18	0.59
1:F:31:THR:HB	1:F:73:GLN:HG3	1.84	0.59
1:E:5:MET:HE2	1:F:46:GLN:N	2.16	0.59
1:E:55:ASN:OD1	1:E:58:VAL:HG23	2.02	0.59
1:C:52:GLU:H	1:C:52:GLU:CD	2.04	0.58
1:E:82:LEU:O	1:E:86:LEU:HG	2.03	0.58
1:E:8:LEU:HD23	1:E:8:LEU:O	2.03	0.58
1:F:55:ASN:ND2	1:F:55:ASN:N	2.50	0.58
1:F:41:VAL:HG13	1:F:49:LEU:HD12	1.86	0.58
1:D:28:HIS:CD2	1:D:29:PRO:HD2	2.39	0.58
1:F:51:LYS:HA	1:F:54:LYS:CE	2.30	0.57
1:E:85:ARG:HG3	1:E:85:ARG:NH1	2.19	0.57
1:C:67:ASP:OD1	1:C:73:GLN:O	2.22	0.57
1:F:55:ASN:HB2	1:F:58:VAL:HG23	1.87	0.56
1:E:16:ILE:HG12	1:E:76:PHE:HE1	1.71	0.56
1:F:28:HIS:HD2	1:F:29:PRO:HD2	1.69	0.56
1:E:5:MET:CG	1:E:6:SER:H	2.13	0.56
1:F:47:ASN:O	1:F:50:LYS:HG3	2.05	0.56
1:C:75:SER:OG	1:C:78:GLU:HG3	2.06	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:60:GLU:O	1:E:64:GLU:HG3	2.05	0.56
1:C:42:ARG:HD2	1:C:42:ARG:O	2.06	0.56
1:C:51:LYS:HB3	1:C:51:LYS:HZ2	1.71	0.56
1:A:2:THR:HG22	1:A:3:CYS:N	2.20	0.56
1:B:42:ARG:HH12	1:B:43:LYS:HG3	1.70	0.55
1:A:82:LEU:O	1:A:86:LEU:HD13	2.06	0.55
1:E:4:LYS:HE3	1:E:10:ARG:CZ	2.37	0.55
1:D:28:HIS:HD2	1:D:30:ASP:H	1.53	0.55
1:C:49:LEU:O	1:C:53:ASN:HB2	2.06	0.55
1:B:28:HIS:HD2	1:B:30:ASP:N	1.96	0.55
1:G:65:ASP:CG	1:G:85:ARG:HH12	2.09	0.55
1:C:51:LYS:HB3	1:C:51:LYS:NZ	2.22	0.55
1:C:65:ASP:OD2	1:C:65:ASP:N	2.40	0.55
1:B:82:LEU:O	1:B:86:LEU:HD13	2.07	0.55
1:C:58:VAL:O	1:C:61:HIS:HB2	2.07	0.54
1:A:15:ILE:HD12	1:B:15:ILE:HD12	1.89	0.54
1:F:50:LYS:CE	1:F:51:LYS:H	2.21	0.54
1:C:55:ASN:ND2	1:C:57:LYS:HB3	2.22	0.54
1:F:41:VAL:HG21	1:F:59:ILE:HG21	1.90	0.53
1:F:46:GLN:O	1:F:50:LYS:HB3	2.09	0.53
1:H:82:LEU:O	1:H:86:LEU:HD23	2.09	0.53
1:D:5:MET:HA	1:D:9:GLU:OE1	2.08	0.53
1:D:19:PHE:CE1	1:D:32:LEU:HD22	2.43	0.53
1:F:23:SER:HB2	1:F:31:THR:O	2.09	0.53
1:D:56:GLU:O	1:D:60:GLU:HG3	2.09	0.52
1:E:5:MET:CE	1:F:46:GLN:H	2.17	0.52
1:F:49:LEU:O	1:F:53:ASN:HB2	2.10	0.52
1:C:57:LYS:HA	1:C:57:LYS:CE	2.34	0.52
1:G:34:GLN:NE2	4:G:511:HOH:O	2.41	0.52
1:F:50:LYS:CE	1:F:51:LYS:HG2	2.39	0.52
1:C:11:ASN:OD1	1:D:11:ASN:HA	2.09	0.52
1:F:62:ILE:HG23	1:F:85:ARG:NH2	2.24	0.52
1:F:10:ARG:NH1	1:F:13:GLU:OE1	2.43	0.52
1:C:41:VAL:HG11	1:C:59:ILE:HD12	1.91	0.51
1:F:41:VAL:HG13	1:F:49:LEU:CD1	2.41	0.51
1:C:74:LEU:HA	1:C:78:GLU:OE1	2.10	0.51
1:B:20:HIS:O	1:B:24:VAL:HG13	2.10	0.51
1:E:5:MET:HE3	1:F:47:ASN:HB2	1.92	0.51
1:G:65:ASP:OD1	1:G:85:ARG:NH1	2.41	0.51
1:D:28:HIS:HD2	1:D:29:PRO:HD2	1.76	0.50
1:F:28:HIS:HB3	1:F:31:THR:OG1	2.11	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:18:THR:HA	1:G:21:GLN:HG2	1.94	0.50
1:E:5:MET:HE3	1:F:47:ASN:CB	2.42	0.50
1:F:24:VAL:HG22	1:F:24:VAL:O	2.12	0.49
1:F:57:LYS:HA	1:F:60:GLU:OE1	2.12	0.49
1:D:57:LYS:HD2	1:E:64:GLU:OE1	2.13	0.49
1:G:7:GLN:HG2	4:G:509:HOH:O	2.12	0.49
1:F:41:VAL:HG21	1:F:59:ILE:CG2	2.43	0.49
1:D:65:ASP:OD2	1:D:85:ARG:NH1	2.46	0.49
1:F:18:THR:HG22	1:F:18:THR:O	2.13	0.49
1:F:38:LYS:O	1:F:38:LYS:HD3	2.12	0.49
1:A:15:ILE:HD12	1:B:15:ILE:CD1	2.43	0.49
1:H:41:VAL:HG11	1:H:59:ILE:HD12	1.94	0.49
1:B:34:GLN:HE21	1:B:60:GLU:HG2	1.76	0.49
1:A:25:LYS:NZ	1:A:39:GLU:OE1	2.46	0.49
1:E:9:GLU:HG2	1:F:48:PHE:CZ	2.47	0.48
1:E:5:MET:HB3	1:E:9:GLU:CG	2.41	0.48
1:E:23:SER:HB3	1:E:32:LEU:CD1	2.44	0.48
1:D:34:GLN:NE2	1:D:60:GLU:HG2	2.28	0.48
1:B:26:LEU:HB3	1:E:39:GLU:HG3	1.95	0.48
1:E:24:VAL:HG12	1:E:24:VAL:O	2.13	0.48
1:A:52:GLU:H	1:A:52:GLU:CD	2.17	0.48
1:E:6:SER:O	1:E:9:GLU:HB3	2.13	0.47
1:E:83:MET:O	1:E:86:LEU:HB2	2.14	0.47
1:D:42:ARG:HH11	1:D:43:LYS:HG3	1.79	0.47
1:C:86:LEU:C	1:C:86:LEU:HD13	2.34	0.47
1:E:5:MET:CE	1:F:46:GLN:N	2.76	0.47
1:C:15:ILE:HG13	1:D:11:ASN:HB3	1.96	0.47
1:F:40:LEU:C	1:F:40:LEU:HD23	2.34	0.47
1:G:28:HIS:HA	1:G:29:PRO:HD3	1.69	0.47
1:F:73:GLN:HA	1:F:73:GLN:NE2	2.30	0.47
1:G:4:LYS:HE2	1:G:4:LYS:HA	1.97	0.47
1:D:40:LEU:C	1:D:40:LEU:HD23	2.35	0.46
1:G:28:HIS:ND1	1:G:29:PRO:HD2	2.30	0.46
1:A:15:ILE:CD1	1:B:15:ILE:HD12	2.45	0.46
1:F:40:LEU:O	1:F:40:LEU:HD23	2.16	0.46
1:H:40:LEU:C	1:H:40:LEU:HD23	2.36	0.46
1:F:16:ILE:HG12	1:F:76:PHE:CE2	2.49	0.46
1:E:8:LEU:C	1:E:8:LEU:HD23	2.36	0.46
1:B:28:HIS:HA	1:B:29:PRO:HD3	1.79	0.46
1:C:34:GLN:CG	1:C:38:LYS:HE3	2.46	0.46
1:F:20:HIS:HA	1:F:23:SER:OG	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:55:ASN:HB2	1:F:58:VAL:CG2	2.45	0.46
1:C:40:LEU:C	1:C:40:LEU:HD23	2.37	0.45
1:C:81:MET:CE	1:D:77:GLU:HG3	2.47	0.45
1:B:40:LEU:C	1:B:40:LEU:HD23	2.37	0.45
1:C:51:LYS:C	1:C:51:LYS:HD2	2.37	0.45
1:E:5:MET:CE	1:F:45:LEU:HA	2.45	0.45
1:E:82:LEU:HG	1:E:86:LEU:HD11	1.99	0.45
1:C:53:ASN:HA	1:C:59:ILE:HD11	1.99	0.45
1:G:47:ASN:HB3	1:H:9:GLU:OE2	2.17	0.45
1:A:81:MET:O	1:A:85:ARG:HG2	2.17	0.45
1:A:34:GLN:OE1	1:A:60:GLU:HG2	2.16	0.45
3:D:289:CPS:C8	3:D:289:CPS:C10	2.95	0.44
1:C:62:ILE:O	1:C:65:ASP:OD2	2.34	0.44
1:C:62:ILE:O	1:C:66:LEU:HG	2.17	0.44
1:D:51:LYS:HD2	1:D:54:LYS:HE2	1.98	0.44
1:F:59:ILE:HD13	1:F:62:ILE:HD12	1.99	0.44
1:G:40:LEU:C	1:G:40:LEU:HD23	2.38	0.44
1:D:28:HIS:HA	1:D:29:PRO:HD3	1.85	0.44
1:E:9:GLU:OE2	1:E:13:GLU:HB2	2.18	0.44
1:E:16:ILE:HG12	1:E:76:PHE:CZ	2.53	0.44
1:F:25:LYS:O	1:F:26:LEU:HD23	2.18	0.43
1:E:52:GLU:CD	1:E:52:GLU:N	2.57	0.43
1:G:11:ASN:O	1:G:15:ILE:HG13	2.18	0.43
1:D:23:SER:HB3	1:D:32:LEU:HD13	2.00	0.43
1:F:26:LEU:HB2	1:F:33:ASN:ND2	2.33	0.43
1:B:34:GLN:NE2	1:B:60:GLU:HG2	2.34	0.43
1:F:62:ILE:O	1:F:66:LEU:HG	2.19	0.43
1:F:62:ILE:CD1	1:F:85:ARG:HH12	2.32	0.43
1:G:18:THR:O	1:G:21:GLN:HG2	2.18	0.43
1:E:5:MET:CE	1:F:48:PHE:H	2.32	0.43
1:F:50:LYS:CD	1:F:51:LYS:HG2	2.48	0.43
1:F:73:GLN:HA	1:F:73:GLN:HE21	1.83	0.43
1:D:58:VAL:O	1:D:62:ILE:HG13	2.19	0.43
1:H:19:PHE:CE1	1:H:32:LEU:HD13	2.53	0.42
1:F:43:LYS:C	1:F:43:LYS:HD3	2.39	0.42
1:G:11:ASN:OD1	1:H:11:ASN:HA	2.18	0.42
1:E:80:ILE:HA	1:E:83:MET:HE3	2.02	0.42
1:E:40:LEU:HD23	1:E:40:LEU:C	2.39	0.42
3:B:189:CPS:C7	3:B:189:CPS:C10	2.97	0.42
3:D:389:CPS:H21	3:D:389:CPS:H23A	1.82	0.42
1:F:73:GLN:CA	1:F:73:GLN:HE21	2.33	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:5:MET:HE3	1:F:47:ASN:CA	2.50	0.42
1:F:62:ILE:HG12	1:F:85:ARG:NH2	2.27	0.41
1:A:34:GLN:HA	1:A:63:MET:SD	2.59	0.41
1:E:41:VAL:HG22	1:E:45:LEU:HD12	2.01	0.41
1:F:50:LYS:HD2	1:F:51:LYS:N	2.22	0.41
1:E:8:LEU:O	1:E:12:ILE:HG13	2.20	0.41
1:C:85:ARG:HG2	1:C:85:ARG:HH11	1.85	0.41
3:G:489:CPS:C8	3:G:489:CPS:C10	2.97	0.41
1:D:11:ASN:O	1:D:15:ILE:HG12	2.20	0.41
1:A:14:THR:CG2	1:B:11:ASN:OD1	2.68	0.41
3:G:489:CPS:C7	3:G:489:CPS:C10	2.98	0.41
1:F:60:GLU:O	1:F:63:MET:HB3	2.20	0.41
1:H:28:HIS:HA	1:H:29:PRO:HD3	1.77	0.41
1:A:26:LEU:HD13	4:A:204:HOH:O	2.21	0.41
1:A:49:LEU:O	1:A:53:ASN:HB2	2.20	0.41
1:C:17:ASN:O	1:C:21:GLN:HG3	2.21	0.41
1:C:42:ARG:C	1:C:42:ARG:HD2	2.41	0.41
3:D:389:CPS:C8	3:D:389:CPS:C10	2.99	0.41
1:F:26:LEU:HB2	1:F:33:ASN:HD21	1.86	0.41
1:E:11:ASN:OD1	1:F:14:THR:CG2	2.69	0.41
3:D:289:CPS:C7	3:D:289:CPS:C10	2.98	0.41
1:G:81:MET:O	1:G:85:ARG:HG2	2.21	0.40
1:F:32:LEU:HB3	1:F:74:LEU:HB2	2.03	0.40
1:C:67:ASP:OD2	1:C:71:ASP:N	2.53	0.40
1:D:25:LYS:O	1:D:26:LEU:HD23	2.20	0.40
1:C:60:GLU:HG2	1:C:60:GLU:H	1.64	0.40
1:B:43:LYS:HE2	1:B:43:LYS:HB3	1.86	0.40
1:A:43:LYS:HB3	1:A:43:LYS:HE2	1.79	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	83/113 (74%)	80 (96%)	3 (4%)	0	100 100
1	B	82/113 (73%)	81 (99%)	1 (1%)	0	100 100
1	C	81/113 (72%)	74 (91%)	6 (7%)	1 (1%)	16 10
1	D	80/113 (71%)	80 (100%)	0	0	100 100
1	E	81/113 (72%)	76 (94%)	5 (6%)	0	100 100
1	F	82/113 (73%)	66 (80%)	13 (16%)	3 (4%)	4 1
1	G	82/113 (73%)	81 (99%)	1 (1%)	0	100 100
1	H	83/113 (74%)	83 (100%)	0	0	100 100
All	All	654/904 (72%)	621 (95%)	29 (4%)	4 (1%)	30 24

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	F	43	LYS
1	F	45	LEU
1	C	51	LYS
1	F	52	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	81/102 (79%)	80 (99%)	1 (1%)	78 84
1	B	80/102 (78%)	76 (95%)	4 (5%)	30 27
1	C	79/102 (78%)	76 (96%)	3 (4%)	40 40
1	D	78/102 (76%)	77 (99%)	1 (1%)	76 82
1	E	79/102 (78%)	78 (99%)	1 (1%)	76 82
1	F	80/102 (78%)	77 (96%)	3 (4%)	40 40
1	G	80/102 (78%)	78 (98%)	2 (2%)	55 59
1	H	81/102 (79%)	80 (99%)	1 (1%)	78 84
All	All	638/816 (78%)	622 (98%)	16 (2%)	55 59

All (16) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	54	LYS
1	B	32	LEU
1	B	42	ARG
1	B	46	GLN
1	B	86	LEU
1	C	51	LYS
1	C	53	ASN
1	C	57	LYS
1	D	32	LEU
1	E	32	LEU
1	F	38	LYS
1	F	50	LYS
1	F	55	ASN
1	G	4	LYS
1	G	7	GLN
1	H	32	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (23) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	73	GLN
1	B	28	HIS
1	B	34	GLN
1	C	21	GLN
1	C	47	ASN
1	C	55	ASN
1	C	73	GLN
1	D	28	HIS
1	D	34	GLN
1	D	73	GLN
1	E	7	GLN
1	E	28	HIS
1	E	73	GLN
1	F	17	ASN
1	F	21	GLN
1	F	28	HIS
1	F	55	ASN
1	F	73	GLN
1	G	34	GLN
1	H	21	GLN
1	H	34	GLN

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Mol	Chain	Res	Type
1	H	61	HIS
1	H	73	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

Of 20 ligands modelled in this entry, 16 are monoatomic - leaving 4 for Mogul analysis.

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	$\#\|Z\| > 2$
3	CPS	B	189	-	35,35,45	4.55	20 (57%)	54,54,70	3.65	25 (46%)
3	CPS	D	289	-	35,35,45	4.51	19 (54%)	54,54,70	3.71	29 (53%)
3	CPS	D	389	-	35,35,45	4.58	19 (54%)	54,54,70	3.88	29 (53%)
3	CPS	G	489	-	35,35,45	4.35	18 (51%)	54,54,70	3.69	27 (50%)

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
3	CPS	B	189	-	-	0/13/78/90	0/4/4/4
3	CPS	D	289	-	-	0/13/78/90	0/4/4/4
3	CPS	D	389	-	-	1/13/78/90	0/4/4/4
3	CPS	G	489	-	-	0/13/78/90	0/4/4/4

All (76) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	D	389	CPS	O4-C4	-12.73	1.21	1.43
3	B	189	CPS	O4-C4	-12.16	1.22	1.43
3	D	289	CPS	O4-C4	-11.77	1.23	1.43
3	G	489	CPS	O4-C4	-11.02	1.24	1.43
3	D	289	CPS	C5-C9	-7.52	1.42	1.55
3	B	189	CPS	C5-C9	-7.42	1.42	1.55
3	G	489	CPS	C5-C9	-7.11	1.43	1.55
3	D	389	CPS	C5-C9	-6.96	1.43	1.55
3	D	289	CPS	O3-C17	-5.33	1.31	1.43
3	D	389	CPS	O3-C17	-4.99	1.32	1.43
3	B	189	CPS	O3-C17	-4.93	1.32	1.43
3	G	489	CPS	O3-C17	-4.38	1.33	1.43
3	B	189	CPS	C23-C24	-4.25	1.43	1.51
3	D	289	CPS	C23-C24	-4.06	1.43	1.51
3	G	489	CPS	C16-C15	-3.54	1.47	1.53
3	D	389	CPS	C23-C24	-3.49	1.44	1.51
3	B	189	CPS	C16-C15	-3.38	1.47	1.53
3	G	489	CPS	C23-C24	-3.16	1.45	1.51
3	D	289	CPS	C16-C15	-2.99	1.48	1.53
3	D	389	CPS	C5-C4	-2.95	1.49	1.54
3	D	389	CPS	C16-C15	-2.94	1.48	1.53
3	B	189	CPS	C5-C4	-2.73	1.50	1.54
3	B	189	CPS	C5-C6	-2.43	1.51	1.55
3	D	289	CPS	C5-C4	-2.43	1.50	1.54
3	G	489	CPS	C5-C4	-2.33	1.50	1.54
3	D	289	CPS	C22-C23	-2.25	1.45	1.52
3	D	389	CPS	C22-C23	-2.24	1.45	1.52
3	B	189	CPS	C22-C23	-2.16	1.45	1.52
3	B	189	CPS	C20-C9	2.68	1.59	1.54
3	G	489	CPS	C11-C2	2.91	1.59	1.54
3	D	289	CPS	C20-C9	2.94	1.59	1.54
3	G	489	CPS	O2-C13	3.00	1.52	1.43
3	D	389	CPS	C14-C15	3.01	1.59	1.53
3	D	389	CPS	C11-C2	3.02	1.60	1.54
3	G	489	CPS	C20-C9	3.06	1.60	1.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	189	CPS	O2-C13	3.08	1.52	1.43
3	B	189	CPS	C14-C13	3.09	1.57	1.51
3	D	289	CPS	O2-C13	3.15	1.52	1.43
3	D	389	CPS	C14-C13	3.26	1.58	1.51
3	D	289	CPS	C14-C15	3.27	1.59	1.53
3	D	289	CPS	C11-C2	3.27	1.60	1.54
3	G	489	CPS	C14-C13	3.33	1.58	1.51
3	D	389	CPS	O2-C13	3.33	1.53	1.43
3	G	489	CPS	C8-C7	3.36	1.63	1.54
3	D	289	CPS	C8-C7	3.43	1.63	1.54
3	D	289	CPS	C14-C13	3.44	1.58	1.51
3	B	189	CPS	C11-C2	3.47	1.60	1.54
3	D	389	CPS	C20-C9	3.49	1.60	1.54
3	G	489	CPS	C14-C15	3.51	1.59	1.53
3	B	189	CPS	C8-C7	3.51	1.63	1.54
3	D	389	CPS	C8-C7	3.58	1.64	1.54
3	B	189	CPS	C14-C15	3.95	1.60	1.53
3	B	189	CPS	C8-C9	4.13	1.63	1.54
3	G	489	CPS	C8-C9	4.24	1.64	1.54
3	D	289	CPS	C8-C9	4.43	1.64	1.54
3	D	389	CPS	C8-C9	4.49	1.64	1.54
3	B	189	CPS	C3-C4	5.28	1.62	1.53
3	G	489	CPS	C3-C4	5.38	1.63	1.53
3	D	289	CPS	C3-C4	5.62	1.63	1.53
3	D	389	CPS	C3-C4	5.67	1.63	1.53
3	D	289	CPS	C24-N1	5.72	1.47	1.33
3	D	389	CPS	C24-N1	5.91	1.47	1.33
3	B	189	CPS	C24-N1	6.06	1.47	1.33
3	G	489	CPS	C24-N1	6.23	1.48	1.33
3	G	489	CPS	C18-C17	6.78	1.64	1.53
3	D	289	CPS	C18-C17	6.91	1.64	1.53
3	B	189	CPS	C18-C17	6.96	1.64	1.53
3	D	389	CPS	C18-C17	7.18	1.65	1.53
3	G	489	CPS	C18-C19	8.02	1.69	1.53
3	B	189	CPS	C18-C19	8.15	1.70	1.53
3	D	389	CPS	C18-C19	8.33	1.70	1.53
3	D	289	CPS	C18-C19	8.76	1.71	1.53
3	D	289	CPS	C10-C5	12.84	1.75	1.54
3	G	489	CPS	C10-C5	12.89	1.75	1.54
3	B	189	CPS	C10-C5	13.29	1.76	1.54
3	D	389	CPS	C10-C5	13.33	1.76	1.54

All (110) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	D	389	CPS	C19-C18-C17	-9.22	101.03	111.92
3	D	289	CPS	C19-C18-C17	-8.95	101.35	111.92
3	G	489	CPS	C19-C18-C17	-8.68	101.67	111.92
3	B	189	CPS	C19-C18-C17	-8.58	101.79	111.92
3	G	489	CPS	C7-C6-C18	-6.66	108.65	118.32
3	D	389	CPS	C7-C6-C18	-6.16	109.37	118.32
3	D	289	CPS	C7-C6-C18	-6.03	109.56	118.32
3	B	189	CPS	C7-C6-C18	-5.95	109.67	118.32
3	B	189	CPS	C3-C19-C18	-5.66	102.67	110.73
3	B	189	CPS	C10-C5-C6	-5.61	102.36	111.22
3	D	389	CPS	C3-C19-C18	-5.50	102.90	110.73
3	D	289	CPS	C3-C19-C18	-5.46	102.95	110.73
3	G	489	CPS	C10-C5-C6	-5.37	102.75	111.22
3	G	489	CPS	C3-C19-C18	-5.17	103.37	110.73
3	D	389	CPS	C10-C5-C6	-5.17	103.06	111.22
3	D	289	CPS	C10-C5-C6	-4.57	104.01	111.22
3	D	389	CPS	C10-C5-C4	-4.24	104.95	109.09
3	D	289	CPS	C10-C5-C9	-4.24	104.53	111.22
3	G	489	CPS	C10-C5-C9	-3.97	104.96	111.22
3	G	489	CPS	C10-C5-C4	-3.93	105.25	109.09
3	D	389	CPS	C25-N1-C24	-3.88	115.16	122.79
3	D	289	CPS	O4-C4-C5	-3.87	104.84	111.11
3	D	389	CPS	C10-C5-C9	-3.84	105.15	111.22
3	D	289	CPS	C25-N1-C24	-3.84	115.23	122.79
3	B	189	CPS	C10-C5-C4	-3.83	105.36	109.09
3	B	189	CPS	O4-C4-C5	-3.83	104.91	111.11
3	G	489	CPS	C25-N1-C24	-3.67	115.58	122.79
3	D	389	CPS	O4-C4-C5	-3.57	105.32	111.11
3	B	189	CPS	C25-N1-C24	-3.55	115.81	122.79
3	D	389	CPS	C15-C14-C13	-3.30	108.00	112.91
3	D	289	CPS	C10-C5-C4	-3.25	105.92	109.09
3	G	489	CPS	O4-C4-C5	-3.23	105.87	111.11
3	B	189	CPS	C15-C14-C13	-3.18	108.19	112.91
3	B	189	CPS	C10-C5-C9	-3.17	106.22	111.22
3	D	289	CPS	C15-C14-C13	-3.13	108.26	112.91
3	G	489	CPS	C8-C9-C20	-3.12	106.49	112.05
3	B	189	CPS	C19-C2-C15	-3.09	104.11	108.67
3	G	489	CPS	C15-C14-C13	-3.06	108.36	112.91
3	B	189	CPS	O3-C17-C18	-2.99	102.67	109.26
3	G	489	CPS	O3-C17-C18	-2.96	102.73	109.26
3	D	389	CPS	C11-C2-C19	-2.87	106.88	111.18
3	D	389	CPS	C8-C9-C20	-2.86	106.96	112.05
3	D	389	CPS	C3-C4-C5	-2.71	108.45	111.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	D	289	CPS	O3-C17-C18	-2.70	103.30	109.26
3	G	489	CPS	C3-C4-C5	-2.68	108.48	111.20
3	G	489	CPS	C19-C2-C15	-2.57	104.88	108.67
3	D	389	CPS	O3-C17-C18	-2.56	103.62	109.26
3	D	289	CPS	C19-C2-C15	-2.41	105.11	108.67
3	D	289	CPS	C16-C15-C14	-2.32	108.46	111.05
3	D	389	CPS	C16-C15-C14	-2.31	108.47	111.05
3	B	189	CPS	C16-C15-C14	-2.30	108.48	111.05
3	D	289	CPS	C11-C2-C19	-2.30	107.74	111.18
3	D	289	CPS	C3-C4-C5	-2.27	108.89	111.20
3	D	289	CPS	C8-C9-C20	-2.21	108.12	112.05
3	D	389	CPS	C19-C2-C15	-2.11	105.55	108.67
3	G	489	CPS	C16-C15-C14	-2.09	108.71	111.05
3	B	189	CPS	C1-C12-C13	2.28	114.13	110.43
3	B	189	CPS	C21-C20-C9	2.32	116.82	112.96
3	D	289	CPS	C5-C9-C20	2.35	122.36	119.50
3	G	489	CPS	C16-C17-C18	2.37	113.98	111.47
3	D	389	CPS	C1-C12-C13	2.39	114.31	110.43
3	D	289	CPS	C1-C12-C13	2.41	114.35	110.43
3	G	489	CPS	C5-C9-C20	2.43	122.46	119.50
3	G	489	CPS	C11-C2-C1	2.50	112.40	108.20
3	D	389	CPS	C5-C9-C20	2.57	122.63	119.50
3	B	189	CPS	C11-C2-C1	2.64	112.65	108.20
3	D	389	CPS	C11-C2-C1	2.82	112.94	108.20
3	D	289	CPS	C11-C2-C1	2.84	112.98	108.20
3	D	289	CPS	C21-C20-C9	2.85	117.71	112.96
3	D	389	CPS	C16-C17-C18	2.96	114.61	111.47
3	G	489	CPS	C21-C20-C9	3.02	117.98	112.96
3	B	189	CPS	C16-C17-C18	3.03	114.69	111.47
3	D	389	CPS	C21-C20-C9	3.26	118.39	112.96
3	D	289	CPS	C6-C5-C4	3.40	110.43	107.39
3	D	289	CPS	C16-C17-C18	3.61	115.30	111.47
3	D	389	CPS	C6-C5-C4	3.71	110.71	107.39
3	G	489	CPS	C6-C5-C4	3.74	110.74	107.39
3	G	489	CPS	C15-C16-C17	3.98	118.88	114.44
3	B	189	CPS	C6-C5-C4	4.05	111.02	107.39
3	D	389	CPS	C7-C6-C5	4.10	107.68	103.60
3	D	289	CPS	C7-C6-C5	4.20	107.78	103.60
3	G	489	CPS	C5-C6-C18	4.54	120.61	114.75
3	B	189	CPS	C7-C6-C5	4.56	108.13	103.60
3	D	389	CPS	C5-C6-C18	4.59	120.67	114.75
3	B	189	CPS	C15-C16-C17	4.77	119.75	114.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	B	189	CPS	C5-C6-C18	4.78	120.91	114.75
3	G	489	CPS	C7-C6-C5	4.80	108.37	103.60
3	D	389	CPS	C15-C16-C17	4.89	119.90	114.44
3	D	289	CPS	C5-C6-C18	4.93	121.10	114.75
3	D	289	CPS	C15-C16-C17	5.06	120.08	114.44
3	B	189	CPS	C9-C5-C6	5.79	105.90	100.05
3	D	289	CPS	C9-C5-C6	5.88	105.99	100.05
3	D	289	CPS	C2-C19-C18	6.07	118.55	111.88
3	G	489	CPS	C2-C19-C18	6.09	118.57	111.88
3	G	489	CPS	C9-C5-C6	6.15	106.27	100.05
3	B	189	CPS	C2-C19-C18	6.51	119.02	111.88
3	D	389	CPS	C2-C19-C18	6.54	119.06	111.88
3	D	389	CPS	C9-C5-C6	6.66	106.78	100.05
3	B	189	CPS	C9-C5-C4	6.99	123.88	117.68
3	D	389	CPS	C9-C5-C4	7.23	124.09	117.68
3	D	289	CPS	C9-C5-C4	7.28	124.13	117.68
3	G	489	CPS	C9-C5-C4	7.85	124.64	117.68
3	D	289	CPS	C19-C3-C4	8.72	125.37	114.36
3	G	489	CPS	C19-C3-C4	8.72	125.37	114.36
3	B	189	CPS	C19-C3-C4	8.99	125.72	114.36
3	D	389	CPS	C19-C3-C4	9.88	126.84	114.36
3	B	189	CPS	C6-C18-C17	10.52	126.33	111.74
3	G	489	CPS	C6-C18-C17	10.94	126.91	111.74
3	D	289	CPS	C6-C18-C17	11.44	127.60	111.74
3	D	389	CPS	C6-C18-C17	12.07	128.47	111.74

There are no chirality outliers.

All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	D	389	CPS	C23-C24-N1-C25

There are no ring outliers.

4 monomers are involved in 23 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	189	CPS	5	0
3	D	289	CPS	6	0
3	D	389	CPS	6	0
3	G	489	CPS	6	0

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.