Full wwPDB X-ray Structure Validation Report

Jan 31, 2016 – 06:29 PM GMT

PDB ID	:	1AXM
Title	:	HEPARIN-LINKED BIOLOGICALLY-ACTIVE DIMER OF FIBROBLAST GROWTH FACTOR
Authors	:	DiGabriele, A.D.; Lax, I.; Chen, D.I.; Svahn, C.M.; Jaye, M.; Schlessinger, J.; Hendrickson, W.A.
Deposited on	:	1997-10-16
Resolution	:	3.00 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.
We welcome your comments at validation@mail.wwpdb.org
A user guide is available at
http://wwpdb.org/validation/2016/XrayValidationReportHelp
with specific help available everywhere you see the ⓘ symbol.

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

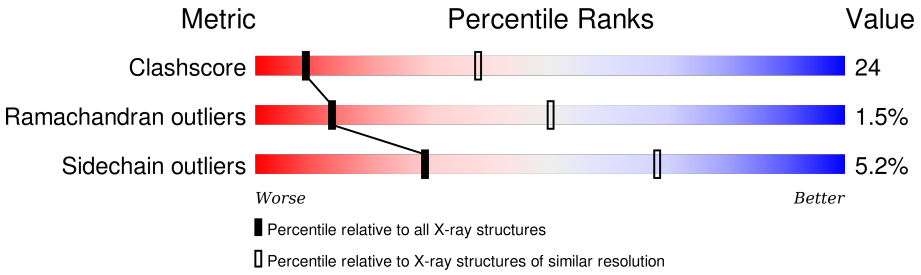
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)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

1 Overall quality at a glance

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

The reported resolution of this entry is 3.00 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	102246	1912 (3.00-3.00)
Ramachandran outliers	100387	1853 (3.00-3.00)
Sidechain outliers	100360	1856 (3.00-3.00)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5% The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	135	64% 31%
1	B	135	50% 41% 6%
1	C	135	50% 37% 7% 5%
1	D	135	49% 41% 6%
1	E	135	54% 38%
1	F	135	56% 39%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard

residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	IDS	F	506	X	-	-	-

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 6463 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 ACIDIC FIBROBLAST GROWTH FACTOR.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	130	Total	C	N	O	S	Se	0	0	0
			1029	649	180	196	3	1			
1	B	127	Total	C	N	O	S	Se	0	0	0
			1011	638	177	192	3	1			
1	C	128	Total	C	N	O	S	Se	0	0	0
			1018	643	178	193	3	1			
1	D	127	Total	C	N	O	S	Se	0	0	0
			1011	638	177	192	3	1			
1	E	129	Total	C	N	O	S	Se	0	0	0
			1028	649	180	195	3	1			
1	F	129	Total	C	N	O	S	Se	0	0	0
			1028	649	180	195	3	1			

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	67	MSE	MET	MODIFIED RESIDUE	UNP P05230
B	67	MSE	MET	MODIFIED RESIDUE	UNP P05230
C	67	MSE	MET	MODIFIED RESIDUE	UNP P05230
D	67	MSE	MET	MODIFIED RESIDUE	UNP P05230
E	67	MSE	MET	MODIFIED RESIDUE	UNP P05230
F	67	MSE	MET	MODIFIED RESIDUE	UNP P05230

- Molecule 2 is a polymer of unknown type called SUGAR (5-MER).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	B	5	Total	C	N	O	S	0	0
			90	30	3	49	8		
2	C	5	Total	C	N	O	S	0	0
			90	30	3	49	8		

- Molecule 3 is a polymer of unknown type called SUGAR (5-MER).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	F	5	Total	C	N	O	S	0	0
			87	30	2	48	7		

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	25	Total	O	0	0
			25	25		
4	B	10	Total	O	0	0
			10	10		
4	C	7	Total	O	0	0
			7	7		
4	D	13	Total	O	0	0
			13	13		
4	E	12	Total	O	0	0
			12	12		
4	F	4	Total	O	0	0
			4	4		

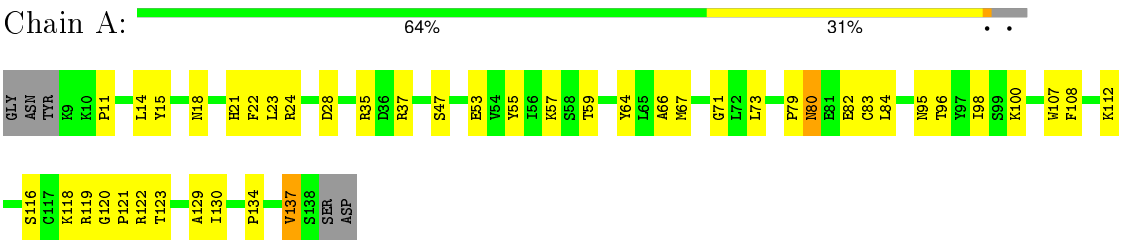
3 Residue-property plots (i)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of 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.

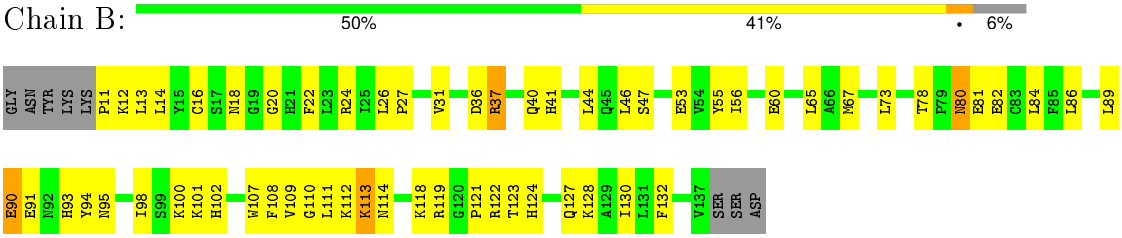
• Molecule 1: ACIDIC FIBROBLAST GROWTH FACTOR

Chain A:



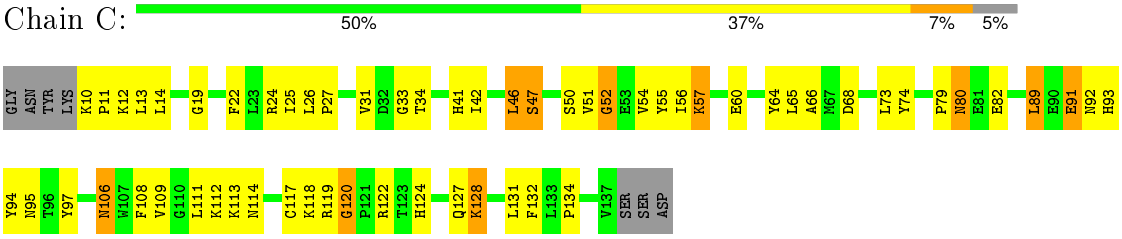
• Molecule 1: ACIDIC FIBROBLAST GROWTH FACTOR

Chain B:



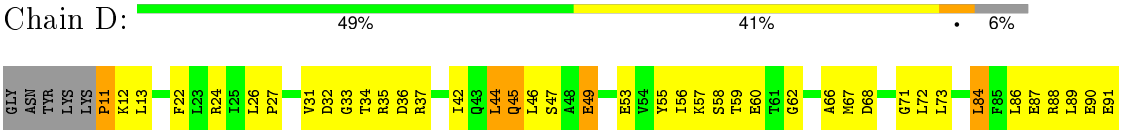
• Molecule 1: ACIDIC FIBROBLAST GROWTH FACTOR

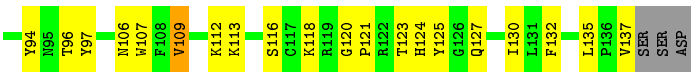
Chain C:



• Molecule 1: ACIDIC FIBROBLAST GROWTH FACTOR

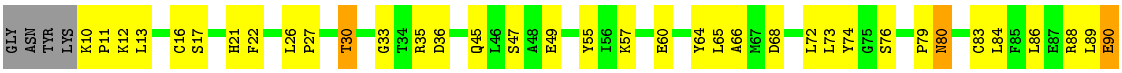
Chain D:





• Molecule 1: ACIDIC FIBROBLAST GROWTH FACTOR

Chain E:



• Molecule 1: ACIDIC FIBROBLAST GROWTH FACTOR

Chain F:

4 Data and refinement statistics (i)

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

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α, β, γ	87.69Å 158.05Å 190.58Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	14.00 – 3.00	Depositor
% Data completeness (in resolution range)	88.6 (14.00-3.00)	Depositor
R_{merge}	0.10	Depositor
R_{sym}	0.10	Depositor
Refinement program	X-PLOR 3.1	Depositor
R, R_{free}	0.217 , 0.304	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	6463	wwPDB-VP
Average B, all atoms (Å^2)	37.0	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: IDS, SGN

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	0.74	0/1051	0.77	0/1418
1	B	0.70	0/1032	0.82	1/1391 (0.1%)
1	C	0.68	0/1040	0.74	0/1403
1	D	0.68	0/1032	0.79	1/1391 (0.1%)
1	E	0.68	0/1050	0.78	0/1415
1	F	0.65	0/1050	0.77	0/1415
All	All	0.69	0/6255	0.78	2/8433 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
3	F	1	0

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	D	11	PRO	N-CA-CB	6.23	110.78	103.30
1	B	11	PRO	N-CA-CB	6.23	110.77	103.30

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
3	F	506	IDS	C1

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	1029	0	1003	32	0
1	B	1011	0	989	52	0
1	C	1018	0	996	57	0
1	D	1011	0	989	62	0
1	E	1028	0	1012	47	0
1	F	1028	0	1012	41	0
2	B	90	0	37	9	0
2	C	90	0	37	13	0
3	F	87	0	34	6	0
4	A	25	0	0	2	0
4	B	10	0	0	0	0
4	C	7	0	0	2	0
4	D	13	0	0	0	0
4	E	12	0	0	1	0
4	F	4	0	0	0	0
All	All	6463	0	6109	299	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 24.

All (299) 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:B:18:ASN:HB2	1:B:128:LYS:HG2	1.40	1.03
1:C:47:SER:HB2	1:C:57:LYS:HE2	1.54	0.90
1:D:118:LYS:HG2	1:D:123:THR:HG22	1.53	0.89
1:C:122:ARG:HH22	2:C:401:SGN:H2	1.42	0.85
1:A:64:TYR:CE1	1:A:79:PRO:HG3	2.13	0.82
1:E:86:LEU:HB3	1:E:88:ARG:HH21	1.46	0.81
1:D:22:PHE:HE1	1:D:135:LEU:HD23	1.47	0.79
1:E:80:ASN:ND2	1:E:83:CYS:SG	2.55	0.79
1:C:73:LEU:HD21	1:C:109:VAL:HG13	1.65	0.77
1:E:57:LYS:HB3	1:E:64:TYR:CD1	2.19	0.77
1:C:46:LEU:HD13	1:C:54:VAL:HG11	1.67	0.76
1:C:24:ARG:HH11	1:C:26:LEU:HD11	1.49	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:37:ARG:HG2	1:B:37:ARG:HH11	1.50	0.75
1:C:24:ARG:NH1	1:C:26:LEU:HD11	2.02	0.74
1:B:73:LEU:HD21	1:B:109:VAL:HG13	1.69	0.73
1:F:35:ARG:HG2	1:F:35:ARG:HH11	1.54	0.73
1:B:14:LEU:HB3	1:B:132:PHE:HD2	1.54	0.71
1:D:123:THR:HA	1:D:127:GLN:OE1	1.90	0.71
1:D:35:ARG:HH11	1:D:35:ARG:HG3	1.53	0.71
1:D:113:LYS:NZ	3:F:506:IDS:H2	2.06	0.70
1:D:90:GLU:HG2	1:D:96:THR:OG1	1.92	0.70
1:C:10:LYS:N	1:C:11:PRO:HD2	2.06	0.70
1:E:10:LYS:N	1:E:138:SER:HG	1.88	0.69
1:D:112:LYS:HD3	1:D:116:SER:HB2	1.75	0.69
1:E:111:LEU:HD23	1:E:117:CYS:HA	1.73	0.69
1:D:106:ASN:ND2	1:D:124:HIS:HA	2.08	0.69
1:F:43:GLN:HE22	1:F:137:VAL:HG21	1.60	0.67
1:C:12:LYS:HD3	1:C:134:PRO:HB2	1.76	0.67
1:A:96:THR:HG22	1:A:130:ILE:O	1.95	0.67
1:D:13:LEU:HD21	1:D:42:ILE:HG13	1.77	0.66
1:A:118:LYS:HD3	1:A:123:THR:HG22	1.76	0.66
1:D:97:TYR:O	1:D:109:VAL:HG23	1.96	0.66
1:C:106:ASN:ND2	1:C:108:PHE:HE1	1.93	0.66
1:E:74:TYR:HE1	1:E:76:SER:HB2	1.59	0.66
1:A:66:ALA:HB2	1:A:83:CYS:SG	2.36	0.66
1:C:118:LYS:HD2	2:C:404:IDS:O1S	1.96	0.65
1:D:22:PHE:CE1	1:D:135:LEU:HD23	2.31	0.65
1:F:35:ARG:HG2	1:F:35:ARG:NH1	2.11	0.65
1:F:66:ALA:HB3	1:F:74:TYR:CE1	2.32	0.64
1:D:35:ARG:NH1	1:D:35:ARG:HG3	2.10	0.64
1:F:15:TYR:HB2	1:F:135:LEU:HD22	1.79	0.64
1:F:65:LEU:HG	1:F:85:PHE:HE2	1.63	0.64
1:D:24:ARG:HD2	1:D:32:ASP:OD1	1.97	0.64
1:C:106:ASN:ND2	1:C:108:PHE:CE1	2.66	0.64
1:E:94:TYR:CD2	1:E:131:LEU:HB3	2.33	0.64
1:F:74:TYR:HE1	1:F:76:SER:HB2	1.62	0.64
1:C:122:ARG:NH2	2:C:401:SGN:H2	2.11	0.63
1:A:21:HIS:CD2	1:A:35:ARG:HG3	2.33	0.63
1:B:14:LEU:HB3	1:B:132:PHE:CD2	2.33	0.63
1:C:66:ALA:HB3	1:C:74:TYR:CE1	2.33	0.63
1:B:122:ARG:HH22	2:B:301:SGN:H4	1.63	0.63
1:F:14:LEU:HG	1:F:44:LEU:HD12	1.81	0.63
1:E:12:LYS:HE2	1:E:134:PRO:HB2	1.81	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:57:LYS:HB3	1:E:64:TYR:CE1	2.35	0.62
1:B:37:ARG:CG	1:B:37:ARG:HH11	2.11	0.62
1:B:16:CYS:O	1:B:20:GLY:HA2	2.00	0.62
1:B:37:ARG:HD3	1:B:37:ARG:O	2.01	0.61
1:D:12:LYS:NZ	1:D:46:LEU:HD22	2.16	0.61
1:E:90:GLU:HA	4:E:654:HOH:O	2.01	0.60
1:F:57:LYS:HB3	1:F:64:TYR:CD1	2.37	0.59
1:B:114:ASN:HB3	2:B:303:SGN:S2	2.42	0.59
1:C:91:GLU:HB2	1:C:94:TYR:HD2	1.67	0.59
1:D:86:LEU:HD22	1:D:88:ARG:NH2	2.17	0.59
1:B:122:ARG:NH2	2:B:301:SGN:H2	2.18	0.59
1:A:80:ASN:HD22	1:A:82:GLU:N	2.01	0.59
1:B:110:GLY:O	1:B:111:LEU:HD23	2.02	0.59
1:D:113:LYS:HZ2	3:F:506:IDS:H2	1.66	0.59
1:D:45:GLN:NE2	1:D:59:THR:HG22	2.18	0.59
1:E:13:LEU:O	1:E:134:PRO:HA	2.04	0.58
1:B:80:ASN:HD21	1:B:82:GLU:HB2	1.67	0.58
1:E:47:SER:HB2	1:E:55:TYR:HB2	1.86	0.58
1:C:106:ASN:HD21	1:C:108:PHE:HE1	1.50	0.58
1:C:128:LYS:HA	1:C:131:LEU:HD12	1.85	0.58
1:E:66:ALA:HB3	1:E:74:TYR:CE1	2.39	0.58
2:C:404:IDS:O61	2:C:405:SGN:H5	2.05	0.57
1:E:98:ILE:HD11	1:E:103:ALA:HA	1.86	0.57
1:B:40:GLN:O	1:B:60:GLU:HG3	2.05	0.57
1:F:26:LEU:HD12	1:F:30:THR:HB	1.87	0.57
1:F:120:GLY:N	1:F:121:PRO:HD2	2.19	0.57
1:F:65:LEU:HG	1:F:85:PHE:CE2	2.40	0.57
1:B:114:ASN:HB3	2:B:303:SGN:O6S	2.05	0.57
1:A:95:ASN:HD22	1:A:134:PRO:HG2	1.70	0.57
1:B:123:THR:HA	1:B:127:GLN:OE1	2.05	0.56
1:C:14:LEU:HB3	1:C:132:PHE:CD2	2.40	0.56
1:D:57:LYS:HG2	1:D:58:SER:O	2.05	0.56
1:D:120:GLY:N	1:D:121:PRO:HD2	2.21	0.56
1:C:27:PRO:HD3	1:C:41:HIS:CE1	2.41	0.56
1:F:85:PHE:HD1	1:F:99:SER:HA	1.70	0.56
1:C:55:TYR:CE2	1:C:79:PRO:HB3	2.42	0.55
1:E:80:ASN:H	1:E:80:ASN:ND2	2.04	0.55
1:B:26:LEU:HB3	1:B:27:PRO:HD2	1.89	0.55
1:E:123:THR:HA	1:E:127:GLN:OE1	2.07	0.55
1:A:53:GLU:OE1	1:A:84:LEU:HD21	2.07	0.55
1:A:57:LYS:HB3	4:A:620:HOH:O	2.06	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:80:ASN:ND2	1:B:82:GLU:HB2	2.21	0.55
1:C:10:LYS:N	1:C:11:PRO:CD	2.70	0.55
1:B:122:ARG:HH22	2:B:301:SGN:H2	1.71	0.55
1:F:24:ARG:NE	1:F:26:LEU:HD21	2.22	0.55
1:D:67:MSE:HE2	1:D:71:GLY:O	2.07	0.54
1:B:47:SER:HB2	1:B:55:TYR:HB2	1.88	0.54
1:C:57:LYS:HD2	1:C:64:TYR:CE2	2.43	0.54
1:B:119:ARG:HG2	1:B:121:PRO:HD2	1.90	0.54
1:E:64:TYR:CE2	1:E:79:PRO:HB3	2.43	0.54
1:D:106:ASN:ND2	1:D:124:HIS:CD2	2.76	0.54
1:C:14:LEU:HB3	1:C:132:PHE:HD2	1.72	0.54
1:F:37:ARG:HH11	1:F:37:ARG:HG2	1.72	0.54
1:A:37:ARG:HH22	1:A:137:VAL:HG23	1.73	0.54
1:A:80:ASN:HD22	1:A:82:GLU:H	1.56	0.53
1:D:107:TRP:NE1	1:D:121:PRO:HA	2.23	0.53
1:D:106:ASN:HD21	1:D:125:TYR:H	1.54	0.53
1:B:53:GLU:HB3	1:B:84:LEU:HD11	1.91	0.53
1:C:122:ARG:HH12	2:C:401:SGN:H2	1.74	0.53
1:D:49:GLU:HB2	1:D:55:TYR:CE1	2.43	0.52
1:D:24:ARG:NH2	1:D:34:THR:HB	2.24	0.52
1:C:47:SER:CB	1:C:57:LYS:HE2	2.35	0.52
1:E:21:HIS:ND1	1:E:115:GLY:HA2	2.24	0.52
1:D:57:LYS:HG3	1:D:62:GLY:O	2.10	0.52
1:D:113:LYS:HD2	3:F:506:IDS:O3	2.10	0.52
1:D:106:ASN:HD21	1:D:124:HIS:HA	1.75	0.52
2:B:301:SGN:H61	2:B:302:IDS:H2	1.91	0.52
1:D:49:GLU:HB2	1:D:55:TYR:HE1	1.75	0.52
1:B:89:LEU:HA	1:B:94:TYR:O	2.09	0.52
1:E:106:ASN:HD21	1:E:125:TYR:H	1.57	0.52
1:F:24:ARG:HB3	1:F:32:ASP:OD1	2.10	0.52
1:B:24:ARG:HG3	1:B:41:HIS:HB2	1.91	0.52
1:C:95:ASN:HB3	1:C:97:TYR:CE1	2.45	0.52
1:F:64:TYR:CE2	1:F:79:PRO:HD3	2.45	0.51
1:A:67:MSE:HE2	1:A:71:GLY:O	2.11	0.51
1:B:113:LYS:HZ1	2:B:305:SGN:H3	1.75	0.51
1:E:49:GLU:OE1	1:E:84:LEU:HD11	2.11	0.51
1:F:86:LEU:HB2	1:F:98:ILE:HG23	1.92	0.51
1:A:98:ILE:HB	1:A:108:PHE:CE2	2.46	0.51
1:B:98:ILE:HG13	1:B:107:TRP:O	2.11	0.51
1:B:67:MSE:HG3	1:B:73:LEU:HD12	1.93	0.51
1:A:64:TYR:CZ	1:A:79:PRO:HG3	2.46	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:15:TYR:HB2	1:A:22:PHE:CE1	2.45	0.50
1:F:112:LYS:CE	1:F:116:SER:HB2	2.41	0.50
1:C:91:GLU:O	1:C:93:HIS:N	2.44	0.50
1:C:112:LYS:HG2	2:C:404:IDS:O1S	2.12	0.50
1:D:22:PHE:O	1:D:33:GLY:HA2	2.11	0.50
1:B:80:ASN:HD22	1:B:82:GLU:H	1.59	0.50
1:E:119:ARG:HD2	1:E:122:ARG:NH2	2.26	0.50
1:D:12:LYS:CE	1:D:46:LEU:HD22	2.42	0.50
1:A:112:LYS:HD2	1:A:116:SER:HB2	1.93	0.50
1:B:101:LYS:HE3	1:B:102:HIS:CE1	2.47	0.50
2:B:304:IDS:C6	2:B:305:SGN:H5	2.42	0.49
1:E:80:ASN:H	1:E:80:ASN:HD22	1.59	0.49
1:C:54:VAL:CG1	1:C:55:TYR:N	2.75	0.49
1:D:87:GLU:HG3	1:D:97:TYR:CE2	2.47	0.49
1:E:90:GLU:HG2	1:E:131:LEU:HD21	1.95	0.49
1:C:113:LYS:HG3	2:C:404:IDS:O2S	2.12	0.49
1:B:24:ARG:CZ	1:B:26:LEU:HD21	2.42	0.49
1:C:19:GLY:N	4:C:653:HOH:O	2.40	0.48
1:C:122:ARG:NH2	2:C:401:SGN:O1S	2.46	0.48
1:B:55:TYR:CE1	1:B:84:LEU:HD13	2.49	0.48
1:D:94:TYR:HA	1:D:132:PHE:O	2.13	0.48
1:D:113:LYS:HZ3	3:F:506:IDS:H2	1.78	0.48
1:D:89:LEU:HG	1:D:91:GLU:O	2.13	0.48
1:D:13:LEU:HB2	1:D:135:LEU:O	2.13	0.48
1:C:111:LEU:HD23	1:C:117:CYS:HA	1.95	0.48
1:C:47:SER:HB3	1:C:55:TYR:HB2	1.96	0.48
1:B:31:VAL:HG11	1:B:73:LEU:HD23	1.95	0.47
1:F:21:HIS:CE1	1:F:35:ARG:HE	2.32	0.47
1:A:95:ASN:HD22	1:A:134:PRO:CG	2.27	0.47
1:E:22:PHE:O	1:E:33:GLY:HA2	2.13	0.47
1:F:54:VAL:HG22	1:F:85:PHE:O	2.15	0.47
1:B:24:ARG:NE	1:B:26:LEU:HD21	2.30	0.47
1:C:50:SER:C	1:C:52:GLY:H	2.17	0.47
1:A:47:SER:HB3	1:A:55:TYR:HB2	1.96	0.47
1:C:46:LEU:HD22	1:C:56:ILE:HG12	1.96	0.47
1:E:73:LEU:HD11	1:E:109:VAL:HG13	1.94	0.47
1:D:112:LYS:CD	1:D:116:SER:HB2	2.43	0.47
1:E:26:LEU:N	1:E:26:LEU:HD22	2.28	0.47
1:C:80:ASN:C	1:C:80:ASN:HD22	2.17	0.47
1:E:17:SER:HB3	1:E:94:TYR:HE2	1.79	0.47
1:D:97:TYR:HB2	1:D:109:VAL:CG2	2.45	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:124:HIS:O	1:B:127:GLN:HG3	2.14	0.47
1:C:22:PHE:O	1:C:33:GLY:HA2	2.15	0.47
1:F:74:TYR:CE1	1:F:76:SER:HB2	2.47	0.47
1:A:11:PRO:HB3	1:A:59:THR:HG21	1.97	0.47
1:A:98:ILE:HG13	1:A:107:TRP:O	2.14	0.46
1:C:91:GLU:HB2	1:C:94:TYR:CD2	2.49	0.46
1:F:112:LYS:HE2	1:F:116:SER:HB2	1.97	0.46
3:F:506:IDS:O1S	3:F:506:IDS:H3	2.16	0.46
1:A:84:LEU:HD23	1:A:100:LYS:HD2	1.97	0.46
1:D:44:LEU:HD22	1:D:56:ILE:HG22	1.96	0.46
1:D:90:GLU:HG3	1:D:96:THR:HG21	1.97	0.46
1:C:24:ARG:HD3	1:C:26:LEU:CD2	2.46	0.46
1:B:91:GLU:C	1:B:93:HIS:H	2.19	0.46
1:E:89:LEU:HD12	1:E:94:TYR:O	2.16	0.46
1:F:47:SER:HB3	1:F:55:TYR:HB2	1.96	0.45
1:E:86:LEU:HD13	1:E:88:ARG:NH2	2.31	0.45
1:E:26:LEU:HB3	1:E:27:PRO:HD2	1.99	0.45
1:E:11:PRO:HD3	1:E:45:GLN:HE22	1.81	0.45
1:A:107:TRP:NE1	1:A:121:PRO:HA	2.31	0.45
1:D:26:LEU:HB3	1:D:27:PRO:HD2	1.99	0.45
1:B:118:LYS:HG2	1:B:123:THR:HG22	1.99	0.45
1:D:107:TRP:HE1	1:D:121:PRO:HA	1.81	0.44
1:B:89:LEU:HD23	1:B:95:ASN:OD1	2.17	0.44
1:E:26:LEU:HD23	1:E:30:THR:HG22	1.99	0.44
1:A:122:ARG:HD3	1:A:122:ARG:HA	1.64	0.44
1:A:23:LEU:HD12	1:A:24:ARG:H	1.82	0.44
1:B:14:LEU:O	1:B:22:PHE:HA	2.18	0.44
1:E:106:ASN:HD21	1:E:125:TYR:N	2.15	0.44
1:E:26:LEU:HD23	1:E:30:THR:O	2.18	0.44
1:C:118:LYS:HE2	1:C:122:ARG:O	2.17	0.44
1:E:98:ILE:HD11	1:E:103:ALA:CA	2.47	0.44
1:D:11:PRO:O	1:D:137:VAL:HG12	2.18	0.44
1:D:13:LEU:HD23	1:D:42:ILE:O	2.17	0.44
1:C:66:ALA:O	1:C:73:LEU:HA	2.17	0.44
1:C:24:ARG:HD3	1:C:26:LEU:HD21	1.99	0.44
1:C:25:ILE:HD11	1:C:65:LEU:HB2	1.99	0.44
1:A:18:ASN:HD22	1:A:129:ALA:HB2	1.82	0.44
1:F:27:PRO:HD3	1:F:41:HIS:CE1	2.52	0.44
1:B:18:ASN:HA	1:B:128:LYS:HD3	1.99	0.44
1:B:91:GLU:HA	1:B:91:GLU:OE1	2.17	0.44
1:F:80:ASN:ND2	1:F:83:CYS:SG	2.90	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:112:LYS:NZ	1:B:114:ASN:HD21	2.15	0.44
1:C:13:LEU:HD21	1:C:42:ILE:HG13	2.00	0.44
1:F:86:LEU:HB3	1:F:88:ARG:NH2	2.32	0.44
1:E:80:ASN:N	1:E:80:ASN:HD22	2.16	0.44
1:F:128:LYS:HA	1:F:131:LEU:CD1	2.48	0.44
1:E:21:HIS:HD2	1:E:35:ARG:HG2	1.83	0.44
1:C:80:ASN:HD21	1:C:82:GLU:HB2	1.83	0.44
1:C:91:GLU:CB	1:C:94:TYR:HD2	2.30	0.43
1:B:80:ASN:HD22	1:B:82:GLU:N	2.16	0.43
1:E:68:ASP:OD2	1:E:72:LEU:HB3	2.18	0.43
1:F:37:ARG:HG2	1:F:37:ARG:NH1	2.33	0.43
1:B:81:GLU:HG3	1:B:101:LYS:HD3	2.00	0.43
1:A:14:LEU:HD12	1:A:23:LEU:HD23	2.00	0.43
1:D:73:LEU:HD11	1:D:109:VAL:CG1	2.48	0.43
1:D:97:TYR:HB2	1:D:109:VAL:HG23	2.00	0.43
1:D:91:GLU:OE1	1:D:91:GLU:HA	2.17	0.43
2:C:402:IDS:O1S	1:E:129:ALA:HB2	2.18	0.43
2:C:402:IDS:O61	2:C:403:SGN:H5	2.18	0.43
1:E:72:LEU:HB2	1:E:119:ARG:HH21	1.84	0.43
1:C:24:ARG:HH11	1:C:26:LEU:CD1	2.24	0.43
1:E:120:GLY:N	1:E:121:PRO:HD2	2.33	0.43
1:D:37:ARG:NH2	1:D:137:VAL:HA	2.33	0.43
1:D:67:MSE:HA	1:D:72:LEU:O	2.18	0.43
1:A:67:MSE:HE3	1:A:73:LEU:CD2	2.48	0.43
1:F:85:PHE:CD1	1:F:99:SER:HA	2.53	0.43
1:F:46:LEU:HA	1:F:55:TYR:O	2.18	0.42
1:C:114:ASN:ND2	2:C:403:SGN:S2	2.92	0.42
1:F:15:TYR:HB3	1:F:135:LEU:HD13	2.00	0.42
1:C:31:VAL:HG21	1:C:65:LEU:HD23	2.00	0.42
3:F:502:IDS:O61	3:F:503:SGN:H62	2.20	0.42
1:F:67:MSE:SE	1:F:107:TRP:HE3	2.51	0.42
1:D:13:LEU:CD2	1:D:42:ILE:HG13	2.47	0.42
1:D:53:GLU:HB3	1:D:84:LEU:HD23	2.01	0.42
1:D:37:ARG:HH21	1:D:137:VAL:HG23	1.84	0.42
1:D:37:ARG:O	1:D:42:ILE:HD11	2.19	0.42
1:E:64:TYR:CE2	1:E:79:PRO:HD3	2.55	0.42
1:F:108:PHE:CD2	1:F:130:ILE:HD12	2.55	0.42
1:B:127:GLN:O	1:B:130:ILE:HG12	2.19	0.42
1:A:95:ASN:ND2	1:A:134:PRO:HG2	2.35	0.42
1:F:97:TYR:CD1	1:F:97:TYR:N	2.87	0.42
1:E:10:LYS:HB3	1:E:10:LYS:HE2	1.82	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:80:ASN:ND2	1:A:82:GLU:HB2	2.35	0.41
1:C:55:TYR:HE2	1:C:79:PRO:HB3	1.82	0.41
1:E:86:LEU:HB2	1:E:98:ILE:HG23	2.01	0.41
1:E:79:PRO:HA	1:E:83:CYS:SG	2.60	0.41
1:D:49:GLU:CB	1:D:55:TYR:HE1	2.32	0.41
1:D:96:THR:HG22	1:D:130:ILE:O	2.21	0.41
1:C:24:ARG:HH21	1:C:34:THR:HB	1.85	0.41
1:E:10:LYS:N	1:E:11:PRO:HD2	2.36	0.41
1:D:127:GLN:O	1:D:130:ILE:HG12	2.20	0.41
1:F:43:GLN:OE1	1:F:137:VAL:HG11	2.20	0.41
1:B:86:LEU:HD21	1:B:100:LYS:HG3	2.02	0.41
1:B:12:LYS:O	1:B:13:LEU:HD12	2.21	0.41
1:F:15:TYR:CE1	1:F:20:GLY:HA2	2.56	0.41
1:D:47:SER:HB3	1:D:55:TYR:HB2	2.02	0.41
1:B:90:GLU:OE1	1:B:94:TYR:HD2	2.04	0.41
1:D:66:ALA:O	1:D:73:LEU:HA	2.21	0.41
1:A:119:ARG:O	1:A:120:GLY:C	2.58	0.41
1:A:107:TRP:HE1	1:A:121:PRO:HA	1.85	0.41
1:B:44:LEU:HD23	1:B:56:ILE:CG2	2.51	0.41
1:F:111:LEU:HD23	1:F:117:CYS:HA	2.03	0.41
1:D:24:ARG:O	1:D:31:VAL:HA	2.20	0.41
1:D:24:ARG:HD3	1:D:26:LEU:CD2	2.51	0.41
1:D:24:ARG:HD3	1:D:26:LEU:HD21	2.01	0.41
1:B:46:LEU:N	1:B:46:LEU:HD12	2.35	0.41
1:B:98:ILE:HA	1:B:108:PHE:HA	2.03	0.41
1:F:24:ARG:CZ	1:F:26:LEU:HD21	2.51	0.40
1:A:73:LEU:HG	4:A:622:HOH:O	2.20	0.40
1:C:26:LEU:HB3	1:C:27:PRO:HD2	2.03	0.40
1:F:14:LEU:HD12	1:F:23:LEU:HD23	2.02	0.40
1:C:89:LEU:HA	1:C:94:TYR:O	2.21	0.40
1:B:111:LEU:HA	1:B:111:LEU:HD23	1.85	0.40
2:B:304:IDS:O62	2:B:305:SGN:H5	2.21	0.40
1:F:124:HIS:ND1	1:F:125:TYR:N	2.68	0.40
1:C:119:ARG:O	1:C:120:GLY:C	2.59	0.40
1:C:124:HIS:O	1:C:127:GLN:HG3	2.21	0.40
1:C:109:VAL:HA	4:C:648:HOH:O	2.22	0.40
1:D:106:ASN:ND2	1:D:106:ASN:O	2.54	0.40
1:B:90:GLU:OE1	1:B:94:TYR:HB2	2.20	0.40
1:C:122:ARG:NH1	2:C:401:SGN:H2	2.34	0.40
2:C:402:IDS:C6	2:C:403:SGN:H5	2.51	0.40
1:E:16:CYS:HB2	1:E:132:PHE:CE1	2.56	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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	128/135 (95%)	117 (91%)	11 (9%)	0	100	100
1	B	125/135 (93%)	112 (90%)	12 (10%)	1 (1%)	24	66
1	C	126/135 (93%)	106 (84%)	15 (12%)	5 (4%)	4	21
1	D	125/135 (93%)	109 (87%)	14 (11%)	2 (2%)	12	48
1	E	127/135 (94%)	116 (91%)	9 (7%)	2 (2%)	12	48
1	F	127/135 (94%)	113 (89%)	13 (10%)	1 (1%)	24	66
All	All	758/810 (94%)	673 (89%)	74 (10%)	11 (2%)	13	50

All (11) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	92	ASN
1	B	36	ASP
1	D	36	ASP
1	E	90	GLU
1	F	50	SER
1	C	68	ASP
1	D	68	ASP
1	E	36	ASP
1	C	51	VAL
1	C	52	GLY
1	C	120	GLY

5.3.2 Protein sidechains

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	112/117 (96%)	109 (97%)	3 (3%)	52 85
1	B	110/117 (94%)	104 (94%)	6 (6%)	27 65
1	C	111/117 (95%)	102 (92%)	9 (8%)	15 47
1	D	110/117 (94%)	104 (94%)	6 (6%)	27 65
1	E	113/117 (97%)	107 (95%)	6 (5%)	28 67
1	F	113/117 (97%)	108 (96%)	5 (4%)	35 74
All	All	669/702 (95%)	634 (95%)	35 (5%)	29 68

All (35) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	28	ASP
1	A	80	ASN
1	A	137	VAL
1	B	37	ARG
1	B	65	LEU
1	B	78	THR
1	B	80	ASN
1	B	90	GLU
1	B	113	LYS
1	C	46	LEU
1	C	47	SER
1	C	57	LYS
1	C	60	GLU
1	C	80	ASN
1	C	89	LEU
1	C	91	GLU
1	C	106	ASN
1	C	128	LYS
1	D	44	LEU
1	D	45	GLN
1	D	49	GLU
1	D	60	GLU
1	D	84	LEU
1	D	109	VAL
1	E	30	THR
1	E	60	GLU
1	E	65	LEU

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Mol	Chain	Res	Type
1	E	80	ASN
1	E	98	ILE
1	E	119	ARG
1	F	13	LEU
1	F	35	ARG
1	F	80	ASN
1	F	92	ASN
1	F	113	LYS

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	21	HIS
1	A	43	GLN
1	A	80	ASN
1	A	95	ASN
1	A	102	HIS
1	B	21	HIS
1	B	43	GLN
1	B	80	ASN
1	B	114	ASN
1	C	41	HIS
1	C	80	ASN
1	C	95	ASN
1	C	106	ASN
1	D	41	HIS
1	D	45	GLN
1	D	106	ASN
1	D	124	HIS
1	E	80	ASN
1	E	93	HIS
1	E	106	ASN
1	F	41	HIS
1	F	63	GLN
1	F	80	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)

15 carbohydrates 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	SGN	B	301	2	18,20,20	1.83	3 (16%)	20,31,31	1.49	3 (15%)
2	IDS	B	302	2	13,16,17	1.80	2 (15%)	17,24,26	1.19	2 (11%)
2	SGN	B	303	2	17,19,20	1.11	2 (11%)	19,29,31	1.18	2 (10%)
2	IDS	B	304	2	13,16,17	1.91	2 (15%)	17,24,26	1.11	2 (11%)
2	SGN	B	305	2	17,19,20	0.83	0	19,29,31	1.16	2 (10%)
2	SGN	C	401	2	18,20,20	1.39	3 (16%)	20,31,31	0.88	0
2	IDS	C	402	2	13,16,17	1.52	1 (7%)	17,24,26	1.16	1 (5%)
2	SGN	C	403	2	17,19,20	1.30	2 (11%)	19,29,31	1.32	2 (10%)
2	IDS	C	404	2	13,16,17	1.37	3 (23%)	17,24,26	1.46	3 (17%)
2	SGN	C	405	2	17,19,20	1.09	2 (11%)	19,29,31	1.39	5 (26%)
3	IDS	F	502	3	13,17,17	1.04	1 (7%)	19,26,26	1.33	1 (5%)
3	SGN	F	503	3	17,19,20	1.64	2 (11%)	19,29,31	1.00	0
3	IDS	F	504	3	13,16,17	1.33	3 (23%)	17,24,26	0.97	1 (5%)
3	SGN	F	505	3	17,19,20	1.41	2 (11%)	19,29,31	1.57	5 (26%)
3	IDS	F	506	3	13,16,17	1.77	2 (15%)	17,24,26	1.15	2 (11%)

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	SGN	B	301	2	-	0/11/31/31	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	IDS	B	302	2	-	0/5/26/29	0/1/1/1
2	SGN	B	303	2	-	0/11/28/31	0/1/1/1
2	IDS	B	304	2	-	0/5/26/29	0/1/1/1
2	SGN	B	305	2	-	0/11/28/31	0/1/1/1
2	SGN	C	401	2	-	0/11/31/31	0/1/1/1
2	IDS	C	402	2	-	0/5/26/29	0/1/1/1
2	SGN	C	403	2	-	0/11/28/31	0/1/1/1
2	IDS	C	404	2	-	0/5/26/29	0/1/1/1
2	SGN	C	405	2	-	0/11/28/31	0/1/1/1
3	IDS	F	502	3	-	0/5/29/29	0/1/1/1
3	SGN	F	503	3	-	0/11/28/31	0/1/1/1
3	IDS	F	504	3	-	0/5/26/29	0/1/1/1
3	SGN	F	505	3	-	0/11/28/31	0/1/1/1
3	IDS	F	506	3	1/1/6/7	0/5/26/29	0/1/1/1

All (30) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	402	IDS	O2-C2	-4.47	1.40	1.47
2	B	304	IDS	O2-C2	-4.31	1.40	1.47
3	F	506	IDS	O5-C5	-4.25	1.39	1.43
2	B	304	IDS	O5-C5	-4.07	1.39	1.43
2	B	302	IDS	O5-C5	-3.92	1.39	1.43
3	F	506	IDS	O2-C2	-3.61	1.41	1.47
2	B	302	IDS	O2-C2	-3.53	1.42	1.47
3	F	504	IDS	O2-C2	-2.83	1.43	1.47
3	F	502	IDS	O2-C2	-2.66	1.40	1.46
2	C	404	IDS	O2-C2	-2.38	1.43	1.47
3	F	504	IDS	O5-C5	-2.23	1.41	1.43
2	C	404	IDS	O5-C5	-2.19	1.41	1.43
2	B	301	SGN	O6-C6	-2.11	1.37	1.46
2	C	401	SGN	O2S-S1	2.02	1.44	1.42
2	B	303	SGN	C4-C3	2.08	1.57	1.52
2	C	405	SGN	O1S-S1	2.22	1.44	1.42
2	C	403	SGN	O1S-S1	2.31	1.44	1.42
3	F	504	IDS	C3-C2	2.40	1.58	1.53
2	C	405	SGN	O2S-S1	2.47	1.44	1.42
2	B	303	SGN	O1S-S1	2.51	1.44	1.42
2	C	404	IDS	C1-C2	2.54	1.55	1.51
2	C	401	SGN	C2-N	2.59	1.51	1.47
3	F	505	SGN	O2S-S1	2.62	1.44	1.42
3	F	505	SGN	O1S-S1	2.98	1.45	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	403	SGN	O2S-S1	3.26	1.45	1.42
3	F	503	SGN	O1S-S1	3.27	1.45	1.42
2	C	401	SGN	O1S-S1	3.28	1.45	1.42
2	B	301	SGN	O2S-S1	3.36	1.45	1.42
3	F	503	SGN	O2S-S1	4.45	1.46	1.42
2	B	301	SGN	O1S-S1	5.43	1.47	1.42

All (31) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	301	SGN	C4-C3-C2	-4.40	104.33	110.43
3	F	505	SGN	C4-C3-C2	-3.57	105.67	111.23
2	B	301	SGN	C3-C4-C5	-3.13	104.74	110.20
2	B	303	SGN	O2S-S1-N	-2.73	104.85	108.50
3	F	505	SGN	O2S-S1-N	-2.68	104.92	108.50
2	C	405	SGN	C3-C4-C5	-2.53	105.79	110.20
2	C	403	SGN	O2S-S1-N	-2.47	105.19	108.50
2	B	303	SGN	C2-N-S1	-2.47	116.36	121.35
2	B	301	SGN	O2S-S1-N	-2.38	105.32	108.50
2	B	305	SGN	C4-C3-C2	-2.36	107.56	111.23
2	C	405	SGN	C4-C3-C2	-2.17	107.86	111.23
2	C	405	SGN	O2S-S1-N	-2.08	105.72	108.50
2	C	405	SGN	O1S-S1-N	-2.06	105.75	108.50
3	F	505	SGN	C3-C4-C5	-2.06	106.61	110.20
2	B	305	SGN	C2-N-S1	-2.04	117.22	121.35
3	F	506	IDS	C4-C3-C2	2.02	113.72	110.20
3	F	504	IDS	C1-C2-C3	2.06	112.46	109.39
2	B	302	IDS	C4-C3-C2	2.08	113.83	110.20
3	F	505	SGN	C3-C2-N	2.10	115.34	110.50
2	C	404	IDS	C4-C3-C2	2.19	114.01	110.20
2	C	404	IDS	C3-C4-C5	2.22	112.97	108.66
2	B	304	IDS	O5-C5-C4	2.27	112.63	108.79
3	F	505	SGN	O4-C4-C3	2.32	115.56	110.34
2	B	304	IDS	C1-C2-C3	2.36	112.90	109.39
2	C	405	SGN	C1-O5-C5	2.45	115.36	112.25
3	F	506	IDS	C1-C2-C3	2.64	113.33	109.39
2	C	403	SGN	C1-O5-C5	2.97	116.01	112.25
2	C	402	IDS	C1-C2-C3	3.03	113.91	109.39
2	B	302	IDS	C1-C2-C3	3.32	114.33	109.39
2	C	404	IDS	C1-C2-C3	3.47	114.56	109.39
3	F	502	IDS	C2-O2-S	4.71	127.75	118.77

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
3	F	506	IDS	C1

There are no torsion outliers.

There are no ring outliers.

13 monomers are involved in 28 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	301	SGN	4	0
2	B	302	IDS	1	0
2	B	303	SGN	2	0
2	B	304	IDS	2	0
2	B	305	SGN	3	0
2	C	401	SGN	5	0
2	C	402	IDS	3	0
2	C	403	SGN	3	0
2	C	404	IDS	4	0
2	C	405	SGN	1	0
3	F	502	IDS	1	0
3	F	503	SGN	1	0
3	F	506	IDS	5	0

5.6 Ligand geometry (i)

There are no ligands in this entry.

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data

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.