Full wwPDB X-ray Structure Validation Report (i)

Jan 31, 2016 – 06:27 PM GMT

PDB ID	:	1AWH
Title	:	NOVEL COVALENT THROMBIN INHIBITOR FROM PLANT EXTRACT
Authors	:	Jhoti, H.; Cleasby, A.; Wonacott, A.
Deposited on	:	1997-10-02
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 (i) symbol.

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

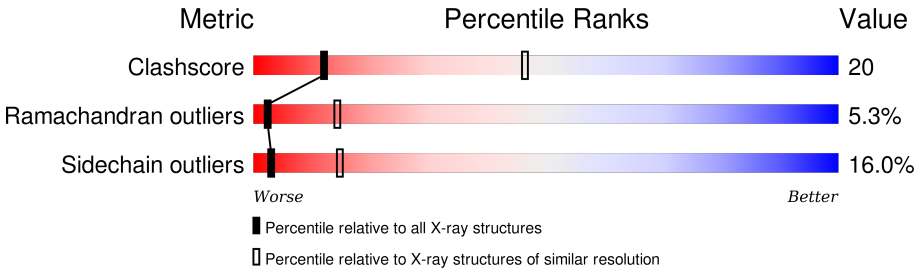
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)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

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 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	36	28% 42% 25% 6%
1	C	36	33% 47% 6% 14%
2	B	259	49% 36% 12% •
2	D	259	43% 43% 12% •

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 4840 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.

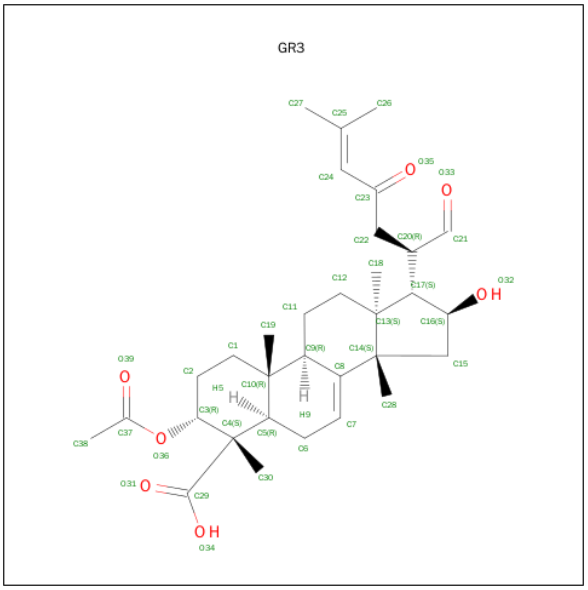
- Molecule 1 is a protein called ALPHA THROMBIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	36	Total	C	N	O	S	0	0	0
			287	177	48	61	1			
1	C	36	Total	C	N	O	S	0	0	0
			287	177	48	61	1			

- Molecule 2 is a protein called ALPHA THROMBIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	259	Total	C	N	O	S	0	0	0
			2093	1334	370	375	14			
2	D	259	Total	C	N	O	S	0	0	0
			2093	1334	370	375	14			

- Molecule 3 is 3-ACETOXY-17-(1-FORMYL-5-METHYL-3-OXO-HEX-4-ENYL)-16-HYDROXY-4,10,13,14-TETRAMETHYL-2,3,4,5,6,9,10,11,12,13,14,15,16,17-TETRADECAHYDRO-1H-CYCLOPENTA[A]PHENANTHRENE-4-CARBOXYLIC ACID (three-letter code: GR3) (formula: $C_{32}H_{46}O_7$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	B	1	Total C O 39 32 7	0	0
3	D	1	Total C O 39 32 7	0	0

- Molecule 4 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	B	1	Total O 1 1	0	0
4	D	1	Total O 1 1	0	0

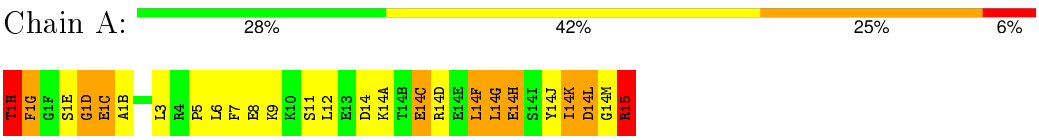
3 Residue-property plots (i)

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: ALPHA THROMBIN

Chain A:

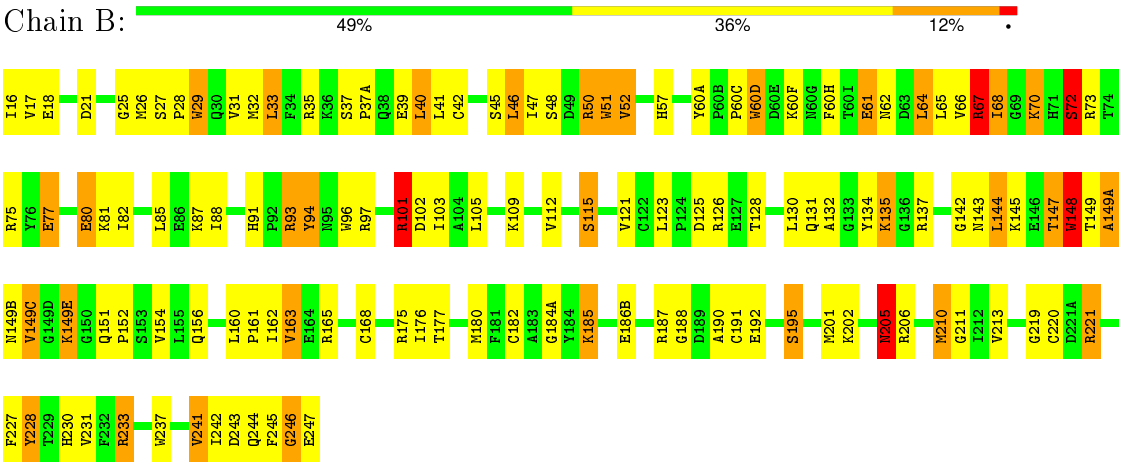


- Molecule 1: ALPHA THROMBIN

Chain C:

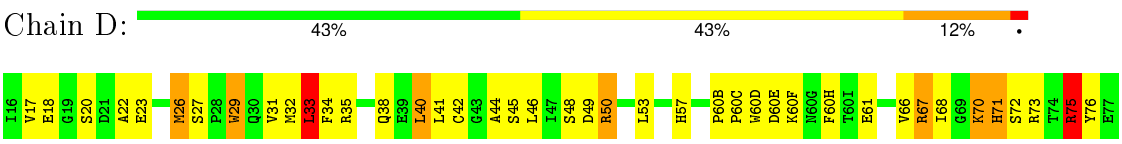
- Molecule 2: ALPHA THROMBIN

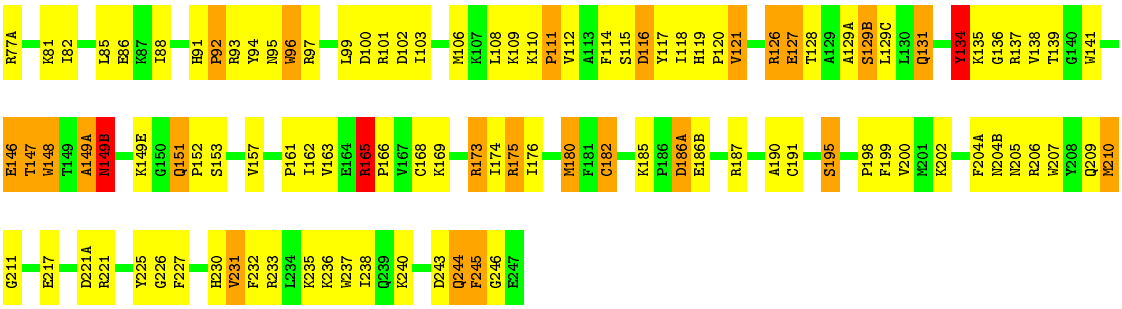
Chain B:



- Molecule 2: ALPHA THROMBIN

Chain D:




R77A
K81
I82
L85
E86
K87
I88
H91
P92
R93
Y94
N95
W96
R97
L99
D100
R101
D102
I103
M106
K107
L108
K109
K110
P111
V112
A113
F114
S115
D116
Y117
I118
H119
P120
V121
R126
E127
T128
A129
A129A
S129B
L129C
L130
Q131
Y134
K135
G136
R137
V138
T139
G140
W141
E146
T147
W148
T149
A149A
N149B
K149E
G150
Q151
P152
S153
V157
P161
I162
V163
E164
R165
P166
V167
C168
K169
R173
I174
R175
I176
M180
F181
C182
K185
P186
D186A
E186B
R187
A190
C191
S195
P198
F199
V200
M201
K202
F204A
N204B
N205
R206
W207
Y208
Q209
M210
G211
E217
D221A
R221
Y225
G226
F227
H230
V231
F232
R233
L234
K235
K236
W237
I238
Q239
K240
D243
Q244
F245
G246
E247

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 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	65.60Å 102.80Å 119.70Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	10.00 – 3.00	Depositor
% Data completeness (in resolution range)	(Not available) (10.00-3.00)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	0.12	Depositor
Refinement program	X-PLOR 3.1	Depositor
R, R_{free}	0.202 , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	4840	wwPDB-VP
Average B, all atoms (Å^2)	25.0	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: GR3

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	1.05	0/290	1.89	3/384 (0.8%)
1	C	1.10	0/290	1.83	6/384 (1.6%)
2	B	1.01	5/2148 (0.2%)	1.77	26/2903 (0.9%)
2	D	1.01	5/2148 (0.2%)	1.79	32/2903 (1.1%)
All	All	1.02	10/4876 (0.2%)	1.79	67/6574 (1.0%)

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
1	A	0	7
1	C	0	4
2	B	0	9
2	D	0	9
All	All	0	29

All (10) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	195	SER	CB-OG	-9.10	1.30	1.42
2	D	195	SER	CB-OG	-8.60	1.31	1.42
2	B	148	TRP	CD2-CE2	6.58	1.49	1.41
2	D	96	TRP	CD2-CE2	6.03	1.48	1.41
2	B	237	TRP	CD2-CE2	5.95	1.48	1.41
2	D	29	TRP	CD2-CE2	5.90	1.48	1.41
2	B	29	TRP	CD2-CE2	5.67	1.48	1.41
2	D	148	TRP	CD2-CE2	5.25	1.47	1.41
2	B	51	TRP	CD2-CE2	5.07	1.47	1.41
2	D	60(D)	TRP	CD2-CE2	5.04	1.47	1.41

All (67) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	134	TYR	CB-CG-CD2	-13.41	112.96	121.00
2	B	134	TYR	CB-CG-CD1	12.84	128.70	121.00
1	A	15	ARG	NE-CZ-NH1	12.81	126.70	120.30
2	D	67	ARG	NE-CZ-NH1	8.03	124.31	120.30
2	B	221	ARG	NE-CZ-NH1	7.66	124.13	120.30
2	D	165	ARG	CD-NE-CZ	-7.64	112.91	123.60
2	D	126	ARG	NE-CZ-NH1	7.46	124.03	120.30
2	D	50	ARG	NE-CZ-NH2	-7.39	116.61	120.30
2	B	75	ARG	CA-CB-CG	7.24	129.32	113.40
2	B	220	CYS	CA-CB-SG	-7.23	100.99	114.00
2	D	175	ARG	NE-CZ-NH2	-7.05	116.77	120.30
2	D	151	GLN	CB-CA-C	-7.05	96.30	110.40
2	D	165	ARG	NE-CZ-NH2	-6.96	116.82	120.30
2	D	131	GLN	CA-CB-CG	-6.81	98.42	113.40
2	B	67	ARG	CD-NE-CZ	-6.65	114.28	123.60
2	B	97	ARG	NE-CZ-NH1	6.63	123.61	120.30
2	B	233	ARG	NE-CZ-NH1	6.58	123.59	120.30
2	D	134	TYR	CB-CG-CD2	-6.46	117.12	121.00
1	A	14(G)	LEU	CA-CB-CG	6.36	129.92	115.30
2	B	144	LEU	CA-CB-CG	-6.20	101.04	115.30
2	B	101	ARG	NE-CZ-NH2	-6.15	117.22	120.30
2	D	75	ARG	N-CA-CB	-6.13	99.56	110.60
1	C	14(G)	LEU	N-CA-CB	-6.07	98.26	110.40
1	C	14(K)	ILE	N-CA-CB	6.05	124.71	110.80
2	B	244	GLN	C-N-CA	-5.98	106.74	121.70
2	D	173	ARG	NE-CZ-NH1	5.95	123.27	120.30
2	D	33	LEU	CB-CA-C	-5.88	99.04	110.20
2	D	175	ARG	CB-CA-C	-5.81	98.78	110.40
1	C	14(G)	LEU	CB-CA-C	5.73	121.09	110.20
2	D	148	TRP	CB-CA-C	-5.73	98.94	110.40
2	D	35	ARG	NE-CZ-NH2	-5.70	117.45	120.30
2	D	165	ARG	NE-CZ-NH1	5.70	123.15	120.30
2	D	182	CYS	CA-CB-SG	5.69	124.25	114.00
2	B	65	LEU	CA-CB-CG	5.69	128.39	115.30
2	D	149(A)	ALA	N-CA-C	5.67	126.31	111.00
2	B	65	LEU	N-CA-CB	-5.54	99.32	110.40
2	D	77(A)	ARG	CA-CB-CG	5.51	125.53	113.40
1	A	14(M)	GLY	C-N-CA	5.48	135.39	121.70
2	B	205	ASN	CA-CB-CG	-5.46	101.40	113.40
2	D	221(A)	ASP	C-N-CA	-5.45	108.07	121.70
2	B	210	MET	CA-CB-CG	5.42	122.52	113.30
2	B	182	CYS	CA-CB-SG	5.42	123.75	114.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	14(K)	ILE	CB-CA-C	-5.32	100.96	111.60
2	D	76	TYR	C-N-CA	-5.32	108.40	121.70
2	D	180	MET	N-CA-CB	-5.31	101.04	110.60
2	D	115	SER	C-N-CA	-5.31	108.43	121.70
2	B	68	ILE	C-N-CA	-5.30	111.17	122.30
2	B	75	ARG	NE-CZ-NH1	5.28	122.94	120.30
2	B	149(A)	ALA	C-N-CA	-5.27	108.52	121.70
2	D	126	ARG	CB-CG-CD	5.25	125.26	111.60
2	B	94	TYR	CB-CG-CD2	-5.25	117.85	121.00
2	D	137	ARG	CD-NE-CZ	-5.25	116.26	123.60
2	D	116	ASP	CB-CA-C	5.23	120.86	110.40
1	C	14(H)	GLU	CA-CB-CG	5.22	124.88	113.40
2	D	175	ARG	NE-CZ-NH1	5.21	122.90	120.30
2	B	149(A)	ALA	CB-CA-C	5.16	117.84	110.10
2	D	112	VAL	CG1-CB-CG2	5.15	119.14	110.90
2	D	153	SER	CB-CA-C	-5.13	100.36	110.10
2	D	38	GLN	CA-C-N	-5.12	105.93	117.20
2	B	228	TYR	CB-CG-CD1	-5.10	117.94	121.00
2	B	52	VAL	CG1-CB-CG2	-5.10	102.74	110.90
2	D	77(A)	ARG	C-N-CA	-5.09	108.97	121.70
2	B	72	SER	CB-CA-C	-5.08	100.45	110.10
1	C	1(C)	GLU	CA-CB-CG	5.05	124.50	113.40
2	B	149(E)	LYS	C-N-CA	-5.04	111.71	122.30
2	B	233	ARG	NE-CZ-NH2	-5.03	117.78	120.30
2	D	71	HIS	CA-CB-CG	5.01	122.11	113.60

There are no chirality outliers.

All (29) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	1(D)	GLY	Peptide
1	A	1(G)	PHE	Peptide
1	A	1(H)	THR	Peptide
1	A	14(J)	TYR	Sidechain,Peptide
1	A	14(L)	ASP	Peptide
1	A	15	ARG	Sidechain
2	B	137	ARG	Sidechain
2	B	142	GLY	Peptide
2	B	148	TRP	Peptide
2	B	149(A)	ALA	Peptide
2	B	187	ARG	Sidechain
2	B	221	ARG	Sidechain

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Mol	Chain	Res	Type	Group
2	B	246	GLY	Peptide
2	B	67	ARG	Sidechain
2	B	77	GLU	Peptide
1	C	1(F)	GLY	Peptide
1	C	1(G)	PHE	Peptide
1	C	14(J)	TYR	Sidechain
1	C	14(M)	GLY	Peptide
2	D	134	TYR	Sidechain
2	D	146	GLU	Peptide
2	D	147	THR	Peptide
2	D	165	ARG	Sidechain
2	D	173	ARG	Sidechain
2	D	186(A)	ASP	Peptide
2	D	246	GLY	Peptide
2	D	81	LYS	Peptide
2	D	93	ARG	Sidechain

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	287	0	278	22	0
1	C	287	0	278	19	0
2	B	2093	0	2063	80	0
2	D	2093	0	2063	86	0
3	B	39	0	44	5	0
3	D	39	0	44	4	0
4	B	1	0	0	0	0
4	D	1	0	0	0	0
All	All	4840	0	4770	191	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 20.

All (191) 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)
2:B:60(F):LYS:HG3	2:B:60(H):PHE:HE1	1.33	0.94
1:A:14(G):LEU:HB3	1:A:15:ARG:NE	1.90	0.87
2:D:230:HIS:CD2	2:D:233:ARG:HG2	2.16	0.80
2:D:200:VAL:HG12	2:D:209:GLN:HA	1.62	0.80
2:D:190:ALA:HB3	3:D:1:GR3:H262	1.64	0.80
2:D:67:ARG:HG2	2:D:82:ILE:HG12	1.64	0.79
2:B:185:LYS:HB2	2:B:186(B):GLU:HG3	1.65	0.77
2:B:60(F):LYS:HG3	2:B:60(H):PHE:CE1	2.20	0.74
1:C:14(G):LEU:HB3	1:C:15:ARG:CZ	2.18	0.73
2:B:144:LEU:HD11	2:B:152:PRO:HB3	1.72	0.71
2:D:163:VAL:HG21	2:D:225:TYR:CD2	2.28	0.68
2:D:49:ASP:HB3	2:D:114:PHE:CZ	2.28	0.68
2:B:130:LEU:HD23	2:B:162:ILE:HD13	1.75	0.68
1:C:14(G):LEU:O	1:C:15:ARG:HD3	1.95	0.67
2:D:163:VAL:HG21	2:D:225:TYR:CE2	2.31	0.65
1:C:14(G):LEU:HB3	1:C:15:ARG:NH1	2.10	0.65
2:B:35:ARG:HH21	2:B:37(A):PRO:HD2	1.62	0.65
1:A:1(G):PHE:CD1	1:A:1(E):SER:HB2	2.34	0.63
1:A:3:LEU:HD11	2:B:206:ARG:NH1	2.14	0.63
2:B:154:VAL:O	2:B:156:GLN:HG3	1.98	0.62
2:B:91:HIS:HB2	2:B:103:ILE:HG22	1.80	0.62
2:B:144:LEU:HD13	2:B:149(E):LYS:HB3	1.82	0.61
2:B:60(A):TYR:HD2	2:B:60(D):TRP:HB2	1.67	0.60
2:B:51:TRP:CE2	2:B:242:ILE:HG12	2.37	0.60
2:B:60(A):TYR:CD2	2:B:60(D):TRP:HB2	2.36	0.60
2:B:81:LYS:HD3	2:B:112:VAL:HG23	1.83	0.59
2:D:128:THR:HG23	2:D:129(C):LEU:HD12	1.85	0.58
2:D:33:LEU:O	2:D:40:LEU:HD23	2.03	0.58
1:A:14(G):LEU:HD21	2:B:202:LYS:HD3	1.84	0.58
1:C:14(F):LEU:HD21	2:D:207:TRP:HH2	1.68	0.57
2:D:68:ILE:HG22	2:D:118:ILE:HG12	1.87	0.57
2:B:57:HIS:O	2:B:60(F):LYS:HE2	2.04	0.57
1:C:4:ARG:HD3	2:D:26:MET:O	2.05	0.57
2:D:17:VAL:HG12	2:D:18:GLU:HG2	1.87	0.57
2:B:67:ARG:HG2	2:B:82:ILE:HG12	1.86	0.57
2:B:147:THR:HA	2:B:149:THR:O	2.04	0.57
1:C:1(H):THR:HA	2:D:243:ASP:HA	1.87	0.56
2:D:165:ARG:HH22	2:D:176:ILE:HG22	1.69	0.56
2:D:91:HIS:ND1	2:D:101:ARG:HD3	2.20	0.56
2:B:42:CYS:HB3	2:B:195:SER:O	2.06	0.56
1:C:14:ASP:HB2	2:D:23:GLU:OE1	2.05	0.55
3:D:1:GR3:H192	3:D:1:GR3:H303	1.88	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:211:GLY:HA2	2:B:231:VAL:HG23	1.89	0.55
2:D:180:MET:HG2	2:D:227:PHE:HD2	1.72	0.54
2:B:190:ALA:HB3	3:B:1:GR3:H262	1.90	0.54
1:C:1(H):THR:N	2:D:243:ASP:HA	2.23	0.53
2:B:61:GLU:CD	2:B:61:GLU:H	2.11	0.53
2:D:91:HIS:CE1	2:D:101:ARG:HD3	2.44	0.53
2:D:182:CYS:HB2	2:D:226:GLY:O	2.09	0.53
2:B:94:TYR:CZ	2:B:96:TRP:HB3	2.44	0.53
2:D:32:MET:HE2	2:D:34:PHE:HE1	1.74	0.53
2:B:73:ARG:CZ	2:B:151:GLN:HG2	2.40	0.52
1:C:1(H):THR:HA	2:D:243:ASP:OD1	2.10	0.52
2:D:22:ALA:O	2:D:71:HIS:HE1	1.94	0.51
2:B:35:ARG:HE	2:B:37(A):PRO:HD2	1.75	0.51
2:B:70:LYS:HB2	2:B:70:LYS:NZ	2.26	0.51
2:B:21:ASP:HA	2:B:156:GLN:HG2	1.92	0.51
2:B:144:LEU:CD1	2:B:149(E):LYS:HB3	2.41	0.51
3:B:1:GR3:H303	3:B:1:GR3:H192	1.92	0.51
2:D:204(B):ASN:ND2	2:D:206:ARG:HD2	2.26	0.51
2:D:165:ARG:HG2	2:D:169:LYS:HE2	1.93	0.51
1:A:14(F):LEU:HB3	1:A:14(G):LEU:HD22	1.94	0.50
1:A:14(G):LEU:HB3	1:A:15:ARG:CZ	2.41	0.50
2:B:176:ILE:HD11	2:B:227:PHE:CE2	2.46	0.50
2:D:60(B):PRO:HB2	2:D:60(C):PRO:HD3	1.93	0.50
2:B:213:VAL:HG22	2:B:228:TYR:CE2	2.47	0.50
2:D:135:LYS:HA	2:D:161:PRO:HA	1.93	0.50
1:C:5:PRO:HA	1:C:9:LYS:HB2	1.94	0.49
1:A:1(G):PHE:HD1	1:A:1(E):SER:HB2	1.76	0.49
2:D:185:LYS:HB2	2:D:186(B):GLU:HG3	1.93	0.49
2:B:77:GLU:HB2	2:B:80:GLU:HG2	1.95	0.49
2:D:73:ARG:HD3	2:D:152:PRO:O	2.12	0.48
2:D:126:ARG:HA	2:D:232:PHE:CZ	2.48	0.48
1:A:3:LEU:HD11	2:B:206:ARG:HH12	1.77	0.48
2:D:50:ARG:HD3	2:D:111:PRO:HD3	1.95	0.48
1:A:15:ARG:HB2	1:A:15:ARG:HH11	1.78	0.48
2:B:70:LYS:HZ3	2:B:70:LYS:HB2	1.79	0.47
2:D:96:TRP:CH2	2:D:97:ARG:HG3	2.49	0.47
2:B:201:MET:SD	2:B:210:MET:HG3	2.55	0.47
1:A:1(H):THR:H3	2:B:246:GLY:HA3	1.79	0.47
2:B:41:LEU:O	2:B:42:CYS:SG	2.72	0.47
2:D:73:ARG:HG3	2:D:141:TRP:CD1	2.50	0.47
2:B:17:VAL:O	2:B:188:GLY:HA2	2.13	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:20:SER:O	2:D:157:VAL:HG12	2.15	0.47
2:D:32:MET:HE2	2:D:34:PHE:CE1	2.48	0.47
1:C:14(K):ILE:HG13	2:D:134:TYR:CE1	2.49	0.47
2:D:165:ARG:N	2:D:166:PRO:HD2	2.30	0.47
2:B:145:LYS:HE3	2:B:149(C):VAL:N	2.31	0.46
2:D:202:LYS:HE2	2:D:205:ASN:HB2	1.98	0.46
2:B:32:MET:HG3	2:B:40:LEU:HD23	1.97	0.46
2:D:168:CYS:HB3	2:D:227:PHE:CZ	2.50	0.46
1:A:3:LEU:O	1:A:5:PRO:HD3	2.15	0.46
2:D:211:GLY:HA2	2:D:231:VAL:HG23	1.98	0.46
1:A:14(G):LEU:HD12	1:A:15:ARG:HH21	1.81	0.46
2:D:60(B):PRO:HG2	2:D:96:TRP:CE2	2.51	0.46
2:D:94:TYR:CZ	2:D:96:TRP:HB3	2.51	0.46
2:D:199:PHE:O	2:D:210:MET:N	2.49	0.46
1:A:7:PHE:CE2	2:B:26:MET:HA	2.51	0.46
1:C:1(G):PHE:CE1	1:C:1(C):GLU:HB3	2.51	0.46
2:D:85:LEU:HD13	2:D:88:ILE:HD11	1.97	0.46
2:B:60(A):TYR:CZ	2:B:60(C):PRO:HG2	2.50	0.45
2:D:243:ASP:O	2:D:245:PHE:N	2.49	0.45
2:D:91:HIS:HD2	2:D:237:TRP:CD2	2.34	0.45
1:A:5:PRO:HG2	2:B:115:SER:O	2.15	0.45
2:B:47:ILE:HD12	2:B:123:LEU:HD11	1.98	0.45
2:D:191:CYS:HA	3:D:1:GR3:H273	1.98	0.45
1:C:14(G):LEU:C	1:C:15:ARG:HD3	2.37	0.45
2:D:95:ASN:HB3	2:D:100:ASP:HB3	1.98	0.45
2:B:151:GLN:CD	2:B:151:GLN:H	2.19	0.45
2:D:136:GLY:HA3	2:D:199:PHE:CZ	2.51	0.45
2:B:163:VAL:HG12	2:B:168:CYS:SG	2.56	0.45
2:B:185:LYS:HD3	2:B:186(B):GLU:OE2	2.17	0.45
1:A:1(H):THR:N	2:B:246:GLY:HA3	2.32	0.45
2:D:146:GLU:O	2:D:149(B):ASN:OD1	2.35	0.45
2:B:105:LEU:HD13	2:B:241:VAL:HG22	1.99	0.44
2:B:135:LYS:HA	2:B:161:PRO:HA	1.98	0.44
1:A:14(G):LEU:HB3	1:A:15:ARG:CD	2.46	0.44
3:B:1:GR3:C12	3:B:1:GR3:H221	2.48	0.44
2:D:42:CYS:SG	2:D:195:SER:HB2	2.57	0.44
2:B:213:VAL:HG22	2:B:228:TYR:HE2	1.83	0.44
2:D:60(C):PRO:HD3	2:D:96:TRP:CZ3	2.52	0.44
2:D:91:HIS:HA	2:D:92:PRO:HD2	1.85	0.44
2:D:18:GLU:HG3	2:D:187:ARG:HB2	2.00	0.43
2:D:50:ARG:NH1	2:D:111:PRO:HG3	2.32	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:29:TRP:CG	2:B:121:VAL:HB	2.52	0.43
1:C:6:LEU:HD21	2:D:116:ASP:O	2.18	0.43
2:B:177:THR:O	2:B:180:MET:HG2	2.17	0.43
1:A:1(G):PHE:HD1	1:A:1(E):SER:CB	2.32	0.43
2:B:70:LYS:HB2	2:B:77:GLU:OE1	2.17	0.43
2:D:149(E):LYS:HE2	2:D:151:GLN:O	2.17	0.43
2:D:101:ARG:O	2:D:103:ILE:N	2.51	0.43
2:D:110:LYS:HA	2:D:111:PRO:HD2	1.75	0.43
2:B:160:LEU:HD22	2:B:184(A):GLY:HA2	2.01	0.43
2:D:60(C):PRO:HD3	2:D:96:TRP:CE3	2.53	0.43
2:B:91:HIS:HB2	2:B:103:ILE:CG2	2.48	0.43
2:B:39:GLU:OE2	2:D:169:LYS:HE3	2.18	0.43
2:D:180:MET:HB2	2:D:180:MET:HE3	1.91	0.43
2:D:162:ILE:HD13	2:D:162:ILE:HG21	1.78	0.43
2:B:148:TRP:CZ3	2:B:219:GLY:HA2	2.54	0.43
2:D:138:VAL:CG2	2:D:199:PHE:HD1	2.32	0.43
2:B:25:GLY:O	2:B:28:PRO:HD3	2.19	0.42
1:C:14(K):ILE:HG13	2:D:134:TYR:HE1	1.84	0.42
2:B:64:LEU:HD23	2:B:85:LEU:CD1	2.49	0.42
2:B:72:SER:HA	2:B:154:VAL:HG23	2.02	0.42
2:D:60(F):LYS:HG2	2:D:60(H):PHE:CE2	2.54	0.42
1:C:14(J):TYR:CD2	1:C:15:ARG:HD2	2.53	0.42
2:B:50:ARG:HG2	2:B:51:TRP:CD1	2.54	0.42
1:A:14:ASP:OD1	1:A:14(C):GLU:HB2	2.20	0.42
2:D:129(B):SER:HA	2:D:131:GLN:NE2	2.34	0.42
2:B:31:VAL:HG13	2:B:66:VAL:HG13	2.02	0.42
1:A:1(G):PHE:HE1	1:A:1(C):GLU:HB3	1.84	0.42
2:B:101:ARG:O	2:B:103:ILE:N	2.52	0.42
2:D:237:TRP:O	2:D:238:ILE:C	2.57	0.42
2:B:191:CYS:HA	3:B:1:GR3:H273	2.02	0.42
2:B:64:LEU:HD23	2:B:85:LEU:HD12	2.02	0.42
2:B:202:LYS:NZ	2:B:205:ASN:HD21	2.18	0.42
2:B:144:LEU:HA	2:B:144:LEU:HD23	1.79	0.42
2:B:33:LEU:HD13	2:B:41:LEU:HD12	2.01	0.42
1:A:1(G):PHE:CE1	1:A:1(E):SER:HB2	2.55	0.41
2:B:37:SER:HA	2:B:37(A):PRO:HA	1.75	0.41
2:B:37(A):PRO:HG3	2:D:165:ARG:HD2	2.02	0.41
2:D:232:PHE:HA	2:D:235:LYS:HB2	2.03	0.41
2:B:131:GLN:O	2:B:132:ALA:C	2.59	0.41
2:D:182:CYS:SG	2:D:225:TYR:HB3	2.60	0.41
2:D:88:ILE:HD13	2:D:106:MET:HB3	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:125:ASP:O	2:B:126:ARG:C	2.58	0.41
2:D:198:PRO:HB2	2:D:200:VAL:HG13	2.03	0.41
1:C:1(H):THR:CA	2:D:243:ASP:HA	2.51	0.41
3:B:1:GR3:H111	3:B:1:GR3:H283	2.03	0.41
2:D:88:ILE:CD1	2:D:106:MET:HE2	2.51	0.41
2:D:41:LEU:HA	2:D:41:LEU:HD23	1.88	0.41
2:B:31:VAL:HG11	2:B:52:VAL:HG11	2.02	0.41
1:C:3:LEU:HD23	1:C:8:GLU:HG2	2.02	0.41
2:D:31:VAL:O	2:D:44:ALA:N	2.53	0.41
2:B:147:THR:C	2:B:148:TRP:HD1	2.23	0.41
2:D:70:LYS:HE3	2:D:72:SER:O	2.21	0.41
2:B:230:HIS:ND1	2:B:233:ARG:HB2	2.35	0.41
2:B:46:LEU:HD22	2:B:48:SER:O	2.21	0.41
2:B:68:ILE:HD13	2:B:112:VAL:HG21	2.03	0.40
1:A:7:PHE:HB3	1:A:12:LEU:O	2.21	0.40
2:B:191:CYS:SG	2:B:192:GLU:N	2.94	0.40
2:B:145:LYS:HB2	2:B:145:LYS:HE2	1.66	0.40
1:A:14(D):ARG:O	1:A:14(H):GLU:HB2	2.22	0.40
2:D:127:GLU:O	2:D:129(A):ALA:HB3	2.22	0.40
2:D:230:HIS:O	2:D:231:VAL:C	2.59	0.40
2:D:121:VAL:HG11	2:D:209:GLN:HB2	2.04	0.40
2:D:57:HIS:NE2	3:D:1:GR3:H281	2.37	0.40
2:B:60(A):TYR:CE2	2:B:60(C):PRO:HG2	2.57	0.40
1:C:14(F):LEU:HD21	2:D:207:TRP:CH2	2.52	0.40
2:D:174:ILE:O	2:D:176:ILE:N	2.55	0.40
2:D:119:HIS:HA	2:D:120:PRO:HD3	1.98	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	34/36 (94%)	16 (47%)	10 (29%)	8 (24%)	0 0
1	C	34/36 (94%)	20 (59%)	9 (26%)	5 (15%)	0 1
2	B	257/259 (99%)	220 (86%)	32 (12%)	5 (2%)	10 43
2	D	257/259 (99%)	210 (82%)	34 (13%)	13 (5%)	2 15
All	All	582/590 (99%)	466 (80%)	85 (15%)	31 (5%)	2 14

All (31) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	1(B)	ALA
1	A	14(K)	ILE
1	A	14(L)	ASP
2	B	62	ASN
2	B	93	ARG
2	B	102	ASP
2	D	102	ASP
2	D	149(A)	ALA
2	D	149(B)	ASN
2	D	244	GLN
1	A	1(D)	GLY
1	A	1(C)	GLU
1	A	14(C)	GLU
1	C	1(E)	SER
1	C	1(B)	ALA
1	C	14(H)	GLU
1	C	14(K)	ILE
2	D	60(E)	ASP
2	D	61	GLU
2	D	148	TRP
2	D	175	ARG
2	B	61	GLU
1	C	1(G)	PHE
2	D	75	ARG
2	D	231	VAL
2	B	147	THR
2	D	117	TYR
1	A	14(A)	LYS
1	A	8	GLU
2	D	92	PRO
2	D	111	PRO

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	31/31 (100%)	23 (74%)	8 (26%)	0 3
1	C	31/31 (100%)	22 (71%)	9 (29%)	0 2
2	B	225/225 (100%)	192 (85%)	33 (15%)	4 18
2	D	225/225 (100%)	193 (86%)	32 (14%)	4 19
All	All	512/512 (100%)	430 (84%)	82 (16%)	3 15

All (82) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1(H)	THR
1	A	6	LEU
1	A	9	LYS
1	A	11	SER
1	A	14(F)	LEU
1	A	14(H)	GLU
1	A	14(K)	ILE
1	A	15	ARG
2	B	16	ILE
2	B	18	GLU
2	B	27	SER
2	B	33	LEU
2	B	40	LEU
2	B	45	SER
2	B	46	LEU
2	B	50	ARG
2	B	60(D)	TRP
2	B	64	LEU
2	B	70	LYS
2	B	72	SER
2	B	80	GLU
2	B	87	LYS
2	B	88	ILE
2	B	93	ARG

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Mol	Chain	Res	Type
2	B	101	ARG
2	B	109	LYS
2	B	115	SER
2	B	128	THR
2	B	135	LYS
2	B	143	ASN
2	B	149(B)	ASN
2	B	149(C)	VAL
2	B	163	VAL
2	B	165	ARG
2	B	175	ARG
2	B	185	LYS
2	B	205	ASN
2	B	241	VAL
2	B	243	ASP
2	B	245	PHE
2	B	247	GLU
1	C	1(H)	THR
1	C	1(G)	PHE
1	C	1(C)	GLU
1	C	1(A)	ASP
1	C	12	LEU
1	C	14(D)	ARG
1	C	14(H)	GLU
1	C	14(I)	SER
1	C	14(J)	TYR
2	D	26	MET
2	D	27	SER
2	D	29	TRP
2	D	33	LEU
2	D	40	LEU
2	D	45	SER
2	D	46	LEU
2	D	48	SER
2	D	53	LEU
2	D	66	VAL
2	D	70	LYS
2	D	75	ARG
2	D	86	GLU
2	D	99	LEU
2	D	108	LEU
2	D	109	LYS

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Mol	Chain	Res	Type
2	D	121	VAL
2	D	127	GLU
2	D	129(B)	SER
2	D	139	THR
2	D	147	THR
2	D	149(B)	ASN
2	D	165	ARG
2	D	186(A)	ASP
2	D	204(A)	PHE
2	D	210	MET
2	D	217	GLU
2	D	221	ARG
2	D	236	LYS
2	D	240	LYS
2	D	244	GLN
2	D	245	PHE

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (9) such sidechains are listed below:

Mol	Chain	Res	Type
2	B	205	ASN
2	B	244	GLN
2	D	71	HIS
2	D	91	HIS
2	D	131	GLN
2	D	143	ASN
2	D	151	GLN
2	D	159	ASN
2	D	230	HIS

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no carbohydrates in this entry.

5.6 Ligand geometry (i)

2 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
3	GR3	B	1	2	40,42,42	1.04	3 (7%)	55,68,68	1.27	8 (14%)
3	GR3	D	1	2	40,42,42	1.02	2 (5%)	55,68,68	1.57	6 (10%)

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	GR3	B	1	2	-	0/17/99/99	0/4/4/4
3	GR3	D	1	2	-	0/17/99/99	0/4/4/4

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	D	1	GR3	C14-C8	-2.66	1.48	1.53
3	B	1	GR3	C4-C3	-2.35	1.51	1.56
3	D	1	GR3	C4-C3	-2.05	1.52	1.56
3	B	1	GR3	C10-C5	-2.05	1.53	1.56
3	B	1	GR3	C4-C29	2.59	1.55	1.50

All (14) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	D	1	GR3	C28-C14-C8	-5.34	101.65	107.61
3	B	1	GR3	C28-C14-C8	-2.98	104.28	107.61

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	D	1	GR3	C28-C14-C15	-2.72	104.76	112.21
3	B	1	GR3	C19-C10-C5	-2.07	109.06	112.95
3	B	1	GR3	C28-C14-C15	-2.06	106.58	112.21
3	B	1	GR3	C1-C10-C5	2.01	110.71	108.06
3	B	1	GR3	C18-C13-C14	2.02	115.10	110.99
3	B	1	GR3	C11-C12-C13	2.04	116.28	112.80
3	B	1	GR3	O36-C37-O39	2.07	127.05	122.92
3	D	1	GR3	O36-C37-O39	2.13	127.17	122.92
3	D	1	GR3	O36-C3-C4	2.53	111.33	107.10
3	B	1	GR3	C3-O36-C37	3.25	123.10	117.91
3	D	1	GR3	C3-O36-C37	4.08	124.42	117.91
3	D	1	GR3	C15-C14-C8	4.80	120.99	117.20

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 9 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	1	GR3	5	0
3	D	1	GR3	4	0

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

EDS was not executed - this section will therefore be empty.

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

EDS was not executed - this section will therefore be empty.

6.3 Carbohydrates

EDS was not executed - this section will therefore be empty.

6.4 Ligands

EDS was not executed - this section will therefore be empty.

6.5 Other polymers

EDS was not executed - this section will therefore be empty.