Full wwPDB X-ray Structure Validation Report (i)

Jan 31, 2016 – 09:36 PM GMT

PDB ID	:	1PST
Title	:	CRYSTALLOGRAPHIC ANALYSES OF SITE-DIRECTED MUTANTS OF THE PHOTOSYNTHETIC REACTION CENTER FROM RHODOBACTER SPHAEROIDES
Authors	:	Chirino, A.J.; Feher, G.; Rees, D.C.
Deposited on	:	1993-12-13
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:

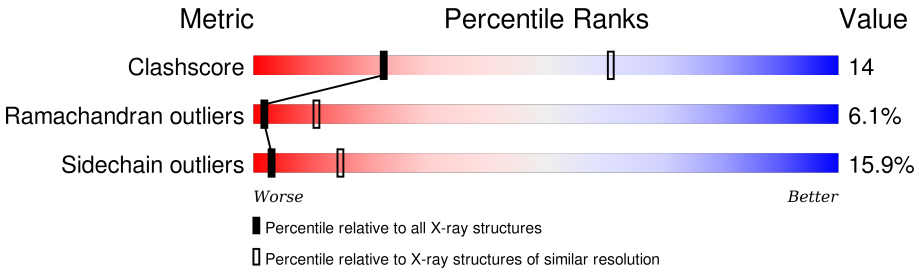
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
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	L	266	62% 30% 8%
2	M	296	56% 32% 9%
3	H	237	53% 33% 10%

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
6	BPH	M	5	X	-	-	-

2 Entry composition

There are 8 unique types of molecules in this entry. The entry contains 6786 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 PHOTOSYNTHETIC REACTION CENTER.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	L	266	Total	C	N	O	S	0	0	0
			2121	1433	336	344	8			

- Molecule 2 is a protein called PHOTOSYNTHETIC REACTION CENTER.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	M	296	Total	C	N	O	S	0	0	0
			2360	1579	384	387	10			

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
M	202	LEU	HIS	CONFLICT	UNP P02953

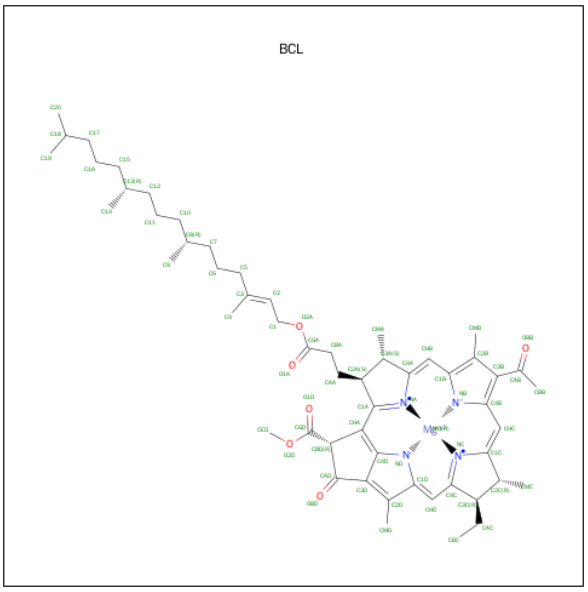
- Molecule 3 is a protein called PHOTOSYNTHETIC REACTION CENTER.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	H	237	Total	C	N	O	S	0	0	0
			1807	1156	310	332	9			

- Molecule 4 is FE (III) ION (three-letter code: FE) (formula: Fe).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	M	1	Total	Fe	0	0
			1	1		

- Molecule 5 is BACTERIOCHLOROPHYLL A (three-letter code: BCL) (formula: $C_{55}H_{74}MgN_4O_6$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
5	M	1	Total	C	Mg	N	O	0	0
			51	40	1	4	6		
5	L	1	Total	C	Mg	N	O	0	0
			66	55	1	4	6		
5	L	1	Total	C	Mg	N	O	0	0
			51	40	1	4	6		

- Molecule 6 is BACTERIOPHEOPHYTIN A (three-letter code: BPH) (formula: $C_{55}H_{76}N_4O_6$).

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
6	M	1	Total	C	N	O	0	0
			65	55	4	6		

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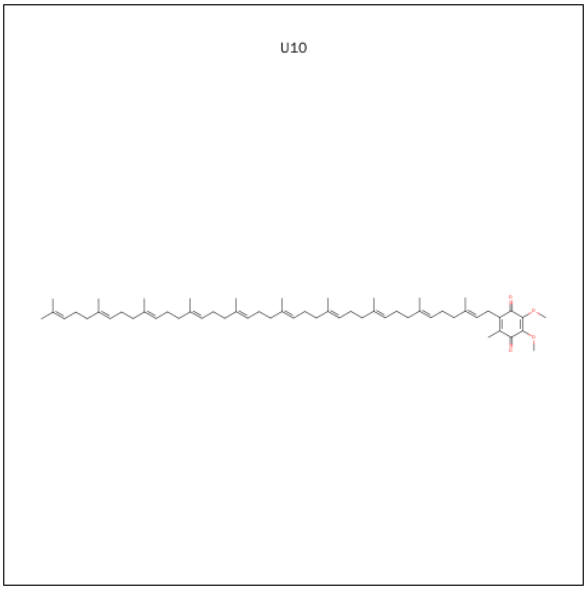
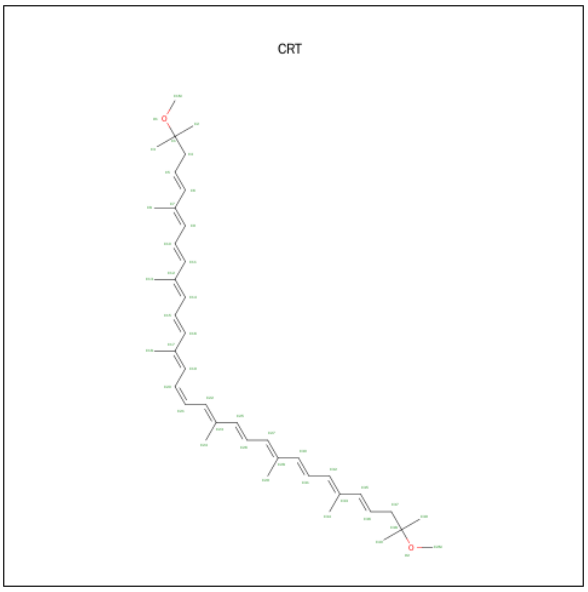
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
6	M	1	Total	C	N	O	0	0
			65	55	4	6		
6	L	1	Total	C	N	O	0	0
			65	55	4	6		

- Molecule 7 is UBIQUINONE-10 (three-letter code: U10) (formula: $C_{59}H_{90}O_4$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	M	1	Total	C	O	0	0
			51	47	4		
7	L	1	Total	C	O	0	0
			41	37	4		

- Molecule 8 is SPIRILLOXANTHIN (three-letter code: CRT) (formula: $C_{42}H_{60}O_2$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	C	O		
8	M	1	42	41	1	0	0

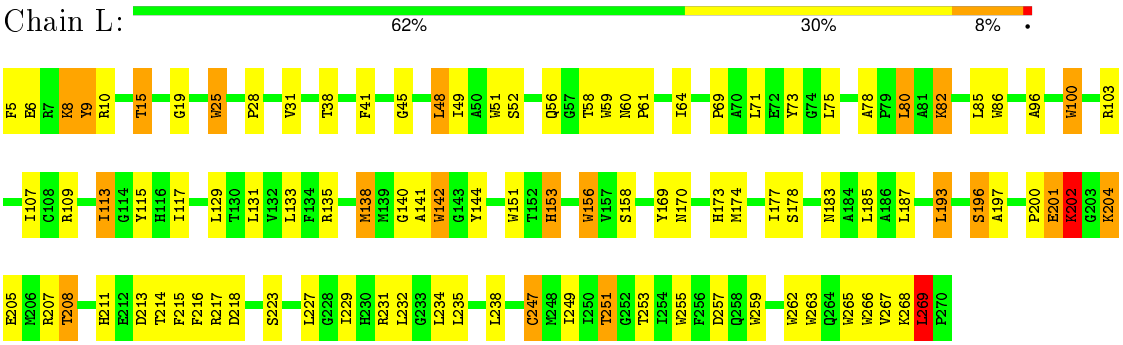
3 Residue-property plots (i)

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.

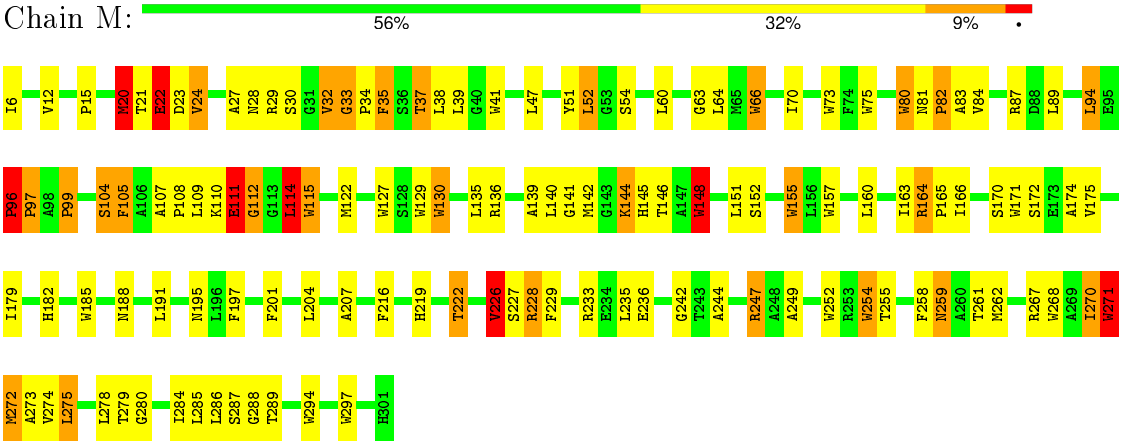
- Molecule 1: PHOTOSYNTHETIC REACTION CENTER

Chain L:



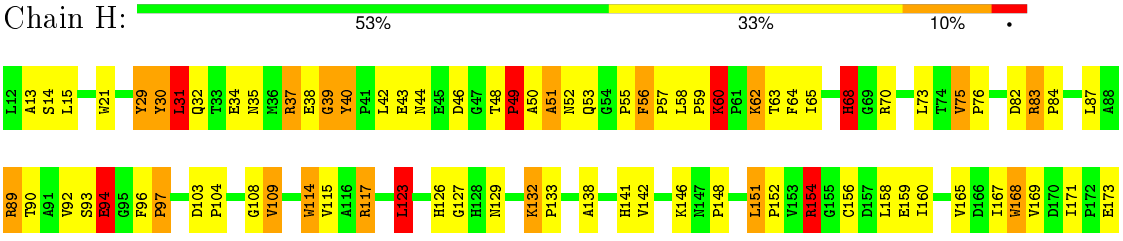
- Molecule 2: PHOTOSYNTHETIC REACTION CENTER

Chain M:



- Molecule 3: PHOTOSYNTHETIC REACTION CENTER

Chain H:




R177
F178
K184
D185
T188
R189
L190
L191
P192
M193
R202
V205
N206
A207
L208
S209
S210
D211
L212
F213
A214
G215
I216
P217
T218
I219
K220
S221
E224
L228
I233
V237
L241
P246
K247
R248

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	138.00Å 77.50Å 141.80Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	(Not available) – 3.00	Depositor
% Data completeness (in resolution range)	(Not available) ((Not available)-3.00)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	X-PLOR	Depositor
R, R_{free}	0.218 , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	6786	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: BCL, BPH, FE, CRT, U10

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	L	0.83	0/2204	1.66	54/3014 (1.8%)
2	M	0.90	0/2450	1.77	81/3344 (2.4%)
3	H	0.80	0/1855	1.56	30/2523 (1.2%)
All	All	0.85	0/6509	1.67	165/8881 (1.9%)

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	L	0	1
2	M	0	2
3	H	0	4
All	All	0	7

There are no bond length outliers.

All (165) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	L	100	TRP	CD1-CG-CD2	10.03	114.33	106.30
3	H	168	TRP	CD1-CG-CD2	9.15	113.62	106.30
2	M	171	TRP	CD1-CG-CD2	9.08	113.56	106.30
1	L	86	TRP	CD1-CG-CD2	9.04	113.53	106.30
2	M	157	TRP	CD1-CG-CD2	8.71	113.27	106.30
2	M	185	TRP	CD1-CG-CD2	8.65	113.22	106.30
1	L	25	TRP	CD1-CG-CD2	8.51	113.11	106.30
1	L	151	TRP	CD1-CG-CD2	8.51	113.10	106.30
2	M	171	TRP	CE2-CD2-CG	-8.49	100.51	107.30
2	M	294	TRP	CD1-CG-CD2	8.44	113.05	106.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	M	297	TRP	CD1-CG-CD2	8.44	113.05	106.30
1	L	59	TRP	CD1-CG-CD2	8.27	112.92	106.30
1	L	262	TRP	CD1-CG-CD2	8.27	112.91	106.30
1	L	86	TRP	CE2-CD2-CG	-8.19	100.75	107.30
3	H	21	TRP	CD1-CG-CD2	8.17	112.83	106.30
2	M	66	TRP	CD1-CG-CD2	8.15	112.82	106.30
2	M	41	TRP	CD1-CG-CD2	8.12	112.80	106.30
2	M	185	TRP	CE2-CD2-CG	-8.11	100.81	107.30
1	L	142	TRP	CD1-CG-CD2	8.07	112.75	106.30
1	L	100	TRP	CE2-CD2-CG	-8.03	100.87	107.30
1	L	51	TRP	CD1-CG-CD2	8.03	112.72	106.30
2	M	252	TRP	CD1-CG-CD2	8.01	112.71	106.30
2	M	22	GLU	N-CA-C	7.93	132.41	111.00
1	L	142	TRP	CE2-CD2-CG	-7.86	101.01	107.30
2	M	129	TRP	CD1-CG-CD2	7.85	112.58	106.30
1	L	151	TRP	CE2-CD2-CG	-7.84	101.03	107.30
1	L	25	TRP	CE2-CD2-CG	-7.84	101.03	107.30
2	M	294	TRP	CE2-CD2-CG	-7.83	101.04	107.30
2	M	268	TRP	CE2-CD2-CG	-7.79	101.07	107.30
2	M	297	TRP	CE2-CD2-CG	-7.73	101.11	107.30
2	M	115	TRP	CD1-CG-CD2	7.72	112.47	106.30
1	L	266	TRP	CD1-CG-CD2	7.72	112.47	106.30
1	L	259	TRP	CD1-CG-CD2	7.71	112.47	106.30
3	H	168	TRP	CE2-CD2-CG	-7.71	101.14	107.30
2	M	41	TRP	CE2-CD2-CG	-7.70	101.14	107.30
2	M	252	TRP	CE2-CD2-CG	-7.70	101.14	107.30
2	M	254	TRP	CD1-CG-CD2	7.67	112.43	106.30
1	L	263	TRP	CD1-CG-CD2	7.63	112.40	106.30
2	M	268	TRP	CD1-CG-CD2	7.61	112.39	106.30
1	L	59	TRP	CE2-CD2-CG	-7.58	101.24	107.30
1	L	259	TRP	CE2-CD2-CG	-7.55	101.26	107.30
2	M	157	TRP	CE2-CD2-CG	-7.51	101.29	107.30
2	M	271	TRP	CD1-CG-CD2	7.47	112.28	106.30
1	L	255	TRP	CD1-CG-CD2	7.47	112.27	106.30
2	M	80	TRP	CD1-CG-CD2	7.46	112.27	106.30
2	M	75	TRP	CD1-CG-CD2	7.45	112.26	106.30
3	H	211	ASP	CA-C-N	-7.45	100.81	117.20
3	H	21	TRP	CE2-CD2-CG	-7.44	101.35	107.30
2	M	66	TRP	CE2-CD2-CG	-7.44	101.35	107.30
1	L	255	TRP	CE2-CD2-CG	-7.44	101.35	107.30
2	M	155	TRP	CD1-CG-CD2	7.44	112.25	106.30
3	H	31	LEU	N-CA-C	-7.43	90.93	111.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	L	263	TRP	CE2-CD2-CG	-7.43	101.36	107.30
2	M	75	TRP	CE2-CD2-CG	-7.37	101.40	107.30
2	M	129	TRP	CE2-CD2-CG	-7.35	101.42	107.30
1	L	262	TRP	CE2-CD2-CG	-7.32	101.45	107.30
1	L	51	TRP	CE2-CD2-CG	-7.25	101.50	107.30
2	M	73	TRP	CD1-CG-CD2	7.23	112.08	106.30
2	M	148	TRP	CA-CB-CG	7.22	127.42	113.70
2	M	254	TRP	CE2-CD2-CG	-7.21	101.53	107.30
1	L	266	TRP	CE2-CD2-CG	-7.19	101.55	107.30
2	M	148	TRP	N-CA-C	-7.19	91.60	111.00
2	M	271	TRP	CE2-CD2-CG	-7.15	101.58	107.30
3	H	114	TRP	CE2-CD2-CG	-7.14	101.59	107.30
2	M	155	TRP	CE2-CD2-CG	-7.11	101.61	107.30
1	L	265	TRP	CE2-CD2-CG	-7.06	101.65	107.30
1	L	169	TYR	CB-CG-CD2	-7.04	116.78	121.00
1	L	156	TRP	CE2-CD2-CG	-7.02	101.68	107.30
2	M	130	TRP	CE2-CD2-CG	-7.02	101.69	107.30
2	M	80	TRP	CE2-CD2-CG	-7.01	101.69	107.30
2	M	73	TRP	CE2-CD2-CG	-7.00	101.70	107.30
1	L	265	TRP	CD1-CG-CD2	6.94	111.85	106.30
2	M	115	TRP	CE2-CD2-CG	-6.94	101.75	107.30
2	M	127	TRP	CE2-CD2-CG	-6.94	101.75	107.30
2	M	270	ILE	CB-CA-C	-6.91	97.78	111.60
1	L	156	TRP	CD1-CG-CD2	6.84	111.77	106.30
3	H	173	GLU	N-CA-C	-6.75	92.77	111.00
2	M	127	TRP	CD1-CG-CD2	6.68	111.64	106.30
2	M	130	TRP	CD1-CG-CD2	6.63	111.60	106.30
2	M	294	TRP	CG-CD2-CE3	6.47	139.73	133.90
1	L	10	ARG	NE-CZ-NH2	-6.46	117.07	120.30
2	M	114	LEU	CA-CB-CG	6.44	130.12	115.30
2	M	171	TRP	CG-CD2-CE3	6.39	139.65	133.90
3	H	114	TRP	CD1-CG-CD2	6.29	111.33	106.30
1	L	259	TRP	CG-CD2-CE3	6.28	139.55	133.90
2	M	148	TRP	CD1-CG-CD2	6.23	111.29	106.30
3	H	37	ARG	NE-CZ-NH1	6.18	123.39	120.30
1	L	153	HIS	CA-CB-CG	6.16	124.08	113.60
2	M	171	TRP	CB-CG-CD1	-6.15	119.00	127.00
2	M	252	TRP	CG-CD2-CE3	6.12	139.41	133.90
3	H	49	PRO	N-CA-C	6.12	128.01	112.10
2	M	66	TRP	CG-CD2-CE3	6.11	139.40	133.90
1	L	59	TRP	CB-CG-CD1	-6.10	119.06	127.00
2	M	226	VAL	N-CA-CB	-6.05	98.19	111.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	M	268	TRP	CG-CD2-CE3	6.04	139.34	133.90
2	M	185	TRP	CB-CG-CD1	-6.01	119.19	127.00
1	L	59	TRP	CG-CD2-CE3	6.01	139.31	133.90
1	L	255	TRP	CB-CG-CD1	-6.00	119.20	127.00
3	H	168	TRP	CG-CD1-NE1	-5.94	104.16	110.10
3	H	177	ARG	NE-CZ-NH2	-5.94	117.33	120.30
2	M	148	TRP	CE2-CD2-CG	-5.92	102.57	107.30
1	L	231	ARG	NE-CZ-NH1	5.91	123.25	120.30
2	M	155	TRP	CB-CG-CD1	-5.90	119.33	127.00
1	L	100	TRP	CG-CD1-NE1	-5.88	104.22	110.10
3	H	212	LEU	CA-C-N	5.88	130.13	117.20
3	H	154	ARG	NE-CZ-NH1	5.86	123.23	120.30
2	M	29	ARG	CA-C-N	-5.84	104.35	117.20
3	H	228	LEU	CA-CB-CG	5.79	128.63	115.30
1	L	25	TRP	CG-CD2-CE3	5.79	139.11	133.90
1	L	10	ARG	NE-CZ-NH1	5.78	123.19	120.30
2	M	185	TRP	CG-CD2-CE3	5.76	139.09	133.90
2	M	252	TRP	CB-CG-CD1	-5.76	119.52	127.00
3	H	46	ASP	N-CA-C	-5.74	95.50	111.00
2	M	6	ILE	N-CA-C	-5.73	95.52	111.00
2	M	104	SER	N-CA-CB	-5.73	101.90	110.50
1	L	142	TRP	CG-CD2-CE3	5.73	139.06	133.90
2	M	297	TRP	CB-CG-CD1	-5.70	119.59	127.00
1	L	25	TRP	CB-CG-CD1	-5.68	119.62	127.00
2	M	226	VAL	CA-CB-CG2	-5.65	102.42	110.90
1	L	138	MET	CG-SD-CE	-5.63	91.19	100.20
3	H	165	VAL	CA-CB-CG2	-5.62	102.47	110.90
3	H	37	ARG	NE-CZ-NH2	-5.53	117.53	120.30
2	M	272	MET	CG-SD-CE	-5.52	91.37	100.20
3	H	123	LEU	CA-CB-CG	5.51	127.97	115.30
2	M	164	ARG	NE-CZ-NH1	5.50	123.05	120.30
1	L	86	TRP	CG-CD1-NE1	-5.50	104.60	110.10
2	M	233	ARG	NE-CZ-NH1	5.47	123.03	120.30
3	H	90	THR	N-CA-C	-5.46	96.25	111.00
2	M	20	MET	CG-SD-CE	5.45	108.92	100.20
2	M	297	TRP	CG-CD2-CE3	5.42	138.78	133.90
2	M	254	TRP	CG-CD2-CE3	5.40	138.76	133.90
1	L	142	TRP	CB-CG-CD1	-5.39	120.00	127.00
3	H	248	ARG	NE-CZ-NH1	5.37	122.98	120.30
1	L	9	TYR	CB-CG-CD1	-5.36	117.78	121.00
2	M	247	ARG	NE-CZ-NH1	5.33	122.96	120.30
1	L	86	TRP	CG-CD2-CE3	5.33	138.69	133.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	M	171	TRP	CG-CD1-NE1	-5.32	104.78	110.10
2	M	80	TRP	N-CA-C	-5.31	96.67	111.00
2	M	294	TRP	CB-CG-CD1	-5.31	120.10	127.00
2	M	226	VAL	CB-CA-C	5.29	121.46	111.40
3	H	51	ALA	N-CA-C	5.28	125.26	111.00
2	M	270	ILE	N-CA-CB	5.28	122.94	110.80
2	M	157	TRP	CG-CD1-NE1	-5.26	104.84	110.10
3	H	94	GLU	N-CA-C	5.22	125.09	111.00
3	H	21	TRP	CG-CD2-CE3	5.21	138.59	133.90
3	H	168	TRP	CG-CD2-CE3	5.18	138.56	133.90
3	H	30	TYR	CA-CB-CG	-5.18	103.56	113.40
1	L	25	TRP	CG-CD1-NE1	-5.15	104.95	110.10
2	M	294	TRP	CG-CD1-NE1	-5.15	104.95	110.10
2	M	268	TRP	CB-CG-CD1	-5.14	120.31	127.00
3	H	117	ARG	O-C-N	-5.14	114.47	122.70
2	M	75	TRP	CG-CD2-CE3	5.14	138.52	133.90
3	H	21	TRP	CB-CG-CD1	-5.13	120.33	127.00
1	L	80	LEU	CA-CB-CG	5.11	127.05	115.30
1	L	255	TRP	CG-CD2-CE3	5.10	138.49	133.90
2	M	297	TRP	CG-CD1-NE1	-5.10	105.00	110.10
1	L	151	TRP	CG-CD2-CE3	5.10	138.49	133.90
3	H	141	HIS	CA-C-N	-5.08	106.02	117.20
2	M	52	LEU	N-CA-C	5.07	124.68	111.00
1	L	259	TRP	CB-CG-CD1	-5.04	120.45	127.00
1	L	217	ARG	NE-CZ-NH2	-5.03	117.79	120.30
2	M	185	TRP	CG-CD1-NE1	-5.03	105.07	110.10
1	L	59	TRP	CG-CD1-NE1	-5.02	105.08	110.10
1	L	156	TRP	CG-CD2-CE3	5.01	138.41	133.90
2	M	66	TRP	CB-CG-CD1	-5.00	120.50	127.00

There are no chirality outliers.

All (7) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
3	H	40	TYR	Peptide
3	H	56	PHE	Peptide
3	H	58	LEU	Peptide
3	H	83	ARG	Peptide
1	L	269	LEU	Peptide
2	M	81	ASN	Peptide
2	M	96	PRO	Peptide

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	L	2121	0	2077	53	0
2	M	2360	0	2285	75	0
3	H	1807	0	1814	60	0
4	M	1	0	0	0	0
5	L	117	0	115	11	0
5	M	51	0	41	8	0
6	L	65	0	76	7	0
6	M	130	0	152	7	0
7	L	41	0	52	5	0
7	M	51	0	68	5	0
8	M	42	0	57	2	0
All	All	6786	0	6737	187	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 14.

All (187) 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:H:154:ARG:HD2	3:H:160:ILE:HG12	1.52	0.92
2:M:229:PHE:HB2	2:M:244:ALA:HB2	1.58	0.84
1:L:205:GLU:HA	3:H:65:ILE:HG13	1.63	0.79
2:M:261:THR:HG22	3:H:40:TYR:HD1	1.49	0.76
2:M:27:ALA:HB2	2:M:51:TYR:HD1	1.50	0.74
5:M:1:BCL:HBB3	6:M:3:BPH:H4C1	1.69	0.73
2:M:20:MET:SD	2:M:22:GLU:HG2	2.29	0.73
3:H:189:ARG:HD2	3:H:216:ILE:HB	1.71	0.72
3:H:89:ARG:HE	3:H:89:ARG:H	1.38	0.72
2:M:236:GLU:HG3	3:H:117:ARG:HH21	1.55	0.71
2:M:97:PRO:HA	2:M:111:GLU:O	1.92	0.70
2:M:27:ALA:HB2	2:M:51:TYR:CD1	2.27	0.69
6:L:271:BPH:HED1	7:M:303:U10:H171	1.74	0.67
2:M:144:LYS:HZ3	2:M:148:TRP:HB2	1.59	0.67
6:M:3:BPH:HBB2	6:M:3:BPH:HHC	1.77	0.67
3:H:148:PRO:HD2	3:H:167:ILE:HD11	1.78	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:100:TRP:HZ3	7:M:303:U10:H33	1.61	0.66
3:H:168:TRP:HB2	3:H:178:PHE:HB2	1.78	0.65
3:H:158:LEU:HD23	3:H:202:ARG:HH22	1.62	0.64
1:L:52:SER:OG	1:L:85:LEU:HD23	1.97	0.63
3:H:39:GLY:HA2	3:H:42:LEU:HG	1.81	0.63
3:H:154:ARG:HG3	3:H:202:ARG:NE	2.14	0.63
2:M:107:ALA:HB3	2:M:112:GLY:HA3	1.80	0.63
3:H:132:LYS:HE3	3:H:171:ILE:HD11	1.81	0.62
1:L:229:ILE:HG21	7:L:272:U10:H3M2	1.80	0.62
2:M:204:LEU:HB2	2:M:279:THR:HG21	1.82	0.62
5:L:2:BCL:HBB3	5:L:2:BCL:HMB1	1.82	0.62
2:M:130:TRP:CZ3	2:M:151:LEU:HG	2.35	0.61
2:M:12:VAL:HG11	3:H:169:VAL:HG11	1.81	0.61
2:M:271:TRP:HA	2:M:274:VAL:HG22	1.82	0.61
2:M:27:ALA:HA	2:M:51:TYR:HA	1.81	0.61
2:M:89:LEU:HD11	8:M:304:CRT:H81	1.83	0.60
3:H:63:THR:HA	3:H:73:LEU:O	2.02	0.59
2:M:63:GLY:HA3	6:M:5:BPH:H5C2	1.84	0.59
1:L:197:ALA:HB1	2:M:235:LEU:HD21	1.83	0.59
2:M:110:LYS:HD2	2:M:114:LEU:HD13	1.84	0.58
7:L:272:U10:H121	7:L:272:U10:H1M1	1.84	0.58
1:L:80:LEU:HB3	1:L:85:LEU:HD13	1.86	0.58
3:H:60:LYS:O	3:H:76:PRO:HD3	2.04	0.57
5:L:2:BCL:H122	6:L:271:BPH:HBA1	1.87	0.57
5:L:4:BCL:O1A	2:M:207:ALA:HA	2.05	0.57
2:M:145:HIS:O	2:M:148:TRP:HB3	2.05	0.57
2:M:21:THR:HB	2:M:27:ALA:CB	2.35	0.56
1:L:173:HIS:HB2	1:L:247:CYS:SG	2.46	0.56
3:H:30:TYR:OH	3:H:56:PHE:HB3	2.06	0.56
3:H:154:ARG:HG3	3:H:202:ARG:HE	1.69	0.55
1:L:187:LEU:HD23	2:M:273:ALA:HB2	1.88	0.55
2:M:226:VAL:HG13	2:M:244:ALA:HB1	1.87	0.55
5:L:2:BCL:HAA2	5:L:4:BCL:HBC1	1.87	0.55
1:L:117:ILE:HD11	2:M:222:THR:HG23	1.88	0.55
2:M:94:LEU:HD13	2:M:114:LEU:HG	1.87	0.55
1:L:41:PHE:HB3	1:L:96:ALA:HB2	1.88	0.55
1:L:15:THR:HG21	1:L:19:GLY:O	2.06	0.55
3:H:93:SER:HB2	3:H:96:PHE:CZ	2.43	0.54
1:L:60:ASN:O	1:L:64:ILE:HG13	2.08	0.54
2:M:228:ARG:HD2	2:M:228:ARG:H	1.72	0.54
1:L:170:ASN:O	1:L:173:HIS:HB3	2.07	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:M:21:THR:HB	2:M:27:ALA:HB3	1.88	0.54
5:M:1:BCL:HHC	5:M:1:BCL:HBB2	1.89	0.53
2:M:164:ARG:HH21	2:M:288:GLY:HA3	1.73	0.53
5:L:2:BCL:H171	6:L:271:BPH:H2	1.90	0.53
3:H:62:LYS:HG2	3:H:75:VAL:HG23	1.91	0.53
2:M:236:GLU:HG3	3:H:117:ARG:NH2	2.22	0.52
1:L:75:LEU:HG	1:L:140:GLY:O	2.10	0.52
3:H:233:ILE:O	3:H:237:VAL:HG23	2.09	0.52
1:L:229:ILE:HD13	7:L:272:U10:H1M2	1.92	0.52
2:M:35:PHE:HB2	2:M:47:LEU:HD21	1.91	0.51
2:M:249:ALA:HB3	3:H:40:TYR:CE2	2.46	0.51
1:L:131:LEU:HD22	1:L:156:TRP:HH2	1.76	0.51
1:L:174:MET:HB3	5:M:1:BCL:O1D	2.10	0.51
5:L:4:BCL:HMB1	5:L:4:BCL:HBB2	1.93	0.50
3:H:59:PRO:HB2	3:H:60:LYS:HD3	1.93	0.50
2:M:275:LEU:CD1	2:M:278:LEU:HD23	2.41	0.50
3:H:241:LEU:HA	3:H:247:LYS:HE2	1.94	0.50
2:M:179:ILE:HG23	5:M:1:BCL:HED1	1.93	0.50
5:L:2:BCL:O2D	5:L:2:BCL:HBA1	2.12	0.49
2:M:22:GLU:CB	2:M:139:ALA:HB1	2.43	0.49
1:L:69:PRO:HB3	1:L:78:ALA:HB2	1.93	0.49
1:L:218:ASP:HB3	2:M:136:ARG:HD3	1.94	0.49
1:L:135:ARG:NH1	1:L:251:THR:HG22	2.28	0.49
3:H:133:PRO:HA	3:H:168:TRP:HA	1.94	0.49
3:H:29:TYR:HB3	3:H:30:TYR:CE2	2.48	0.49
7:L:272:U10:H3M3	7:L:272:U10:H4M2	1.95	0.49
1:L:215:PHE:CZ	2:M:146:THR:HG21	2.48	0.49
2:M:285:LEU:O	2:M:289:THR:HB	2.13	0.48
1:L:73:TYR:HE2	1:L:82:LYS:HD2	1.78	0.48
3:H:37:ARG:HH21	3:H:43:GLU:H	1.61	0.48
6:M:3:BPH:CBB	6:M:3:BPH:HHC	2.44	0.48
1:L:107:ILE:HD13	2:M:255:THR:CG2	2.44	0.48
2:M:22:GLU:HB3	2:M:139:ALA:HB1	1.95	0.48
2:M:165:PRO:HG2	2:M:174:ALA:HB2	1.96	0.47
1:L:113:ILE:HD13	2:M:247:ARG:HG3	1.96	0.47
1:L:113:ILE:CD1	2:M:247:ARG:HG3	2.44	0.47
3:H:50:ALA:HB1	3:H:55:PRO:HG2	1.94	0.47
2:M:22:GLU:HG3	2:M:139:ALA:O	2.14	0.47
2:M:219:HIS:HA	7:M:303:U10:O2	2.14	0.47
1:L:208:THR:OG1	1:L:211:HIS:HD2	1.98	0.47
1:L:201:GLU:O	1:L:204:LYS:HE2	2.15	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:H:220:LYS:HG2	3:H:221:SER:N	2.30	0.47
5:L:2:BCL:H112	5:L:4:BCL:HBB2	1.97	0.46
3:H:212:LEU:O	3:H:214:ALA:N	2.46	0.46
2:M:140:LEU:HB2	2:M:142:MET:HG2	1.97	0.46
1:L:267:VAL:O	2:M:87:ARG:HD2	2.15	0.46
3:H:247:LYS:HG2	3:H:248:ARG:N	2.31	0.46
3:H:129:ASN:ND2	3:H:224:GLU:HB2	2.29	0.46
5:L:4:BCL:CBB	5:L:4:BCL:HMB1	2.44	0.46
3:H:68:HIS:HE1	3:H:123:LEU:HB2	1.80	0.46
2:M:170:SER:HB3	2:M:172:SER:OG	2.16	0.46
1:L:238:LEU:HD23	6:L:271:BPH:HBC1	1.97	0.45
6:L:271:BPH:HHC	6:L:271:BPH:OBB	2.15	0.45
1:L:178:SER:HA	5:M:1:BCL:O1A	2.16	0.45
2:M:280:GLY:HA2	6:M:3:BPH:HED3	1.99	0.45
2:M:242:GLY:HA2	3:H:115:VAL:HG11	1.98	0.45
3:H:154:ARG:HB2	3:H:202:ARG:HH21	1.81	0.45
3:H:210:SER:HA	3:H:213:PHE:HD2	1.82	0.45
1:L:153:HIS:CE1	6:L:271:BPH:H191	2.51	0.45
3:H:191:LEU:HD21	3:H:205:VAL:HG21	1.98	0.45
2:M:163:ILE:HA	2:M:166:ILE:HG12	1.98	0.45
1:L:48:LEU:HD12	1:L:85:LEU:HD11	2.00	0.44
3:H:48:THR:HA	3:H:49:PRO:HD2	1.64	0.44
2:M:33:GLY:H	2:M:34:PRO:HD3	1.82	0.44
2:M:188:ASN:HA	2:M:191:LEU:HD22	1.99	0.44
3:H:152:PRO:HB2	3:H:154:ARG:HD3	1.98	0.44
3:H:104:PRO:HB3	3:H:109:VAL:HG12	1.99	0.44
7:M:303:U10:H3M3	7:M:303:U10:H4M2	1.99	0.44
1:L:268:LYS:O	1:L:269:LEU:HB2	2.16	0.44
3:H:247:LYS:HB3	3:H:247:LYS:HE3	1.95	0.44
1:L:214:THR:HG21	2:M:20:MET:O	2.18	0.44
2:M:96:PRO:HA	2:M:115:TRP:CG	2.52	0.44
2:M:261:THR:HA	3:H:40:TYR:CD1	2.53	0.43
2:M:94:LEU:HA	2:M:94:LEU:HD22	1.84	0.43
2:M:82:PRO:O	2:M:84:VAL:N	2.51	0.43
2:M:160:LEU:HD23	2:M:284:ILE:HG21	1.98	0.43
3:H:64:PHE:HB2	3:H:73:LEU:HB3	2.00	0.43
2:M:109:LEU:O	2:M:114:LEU:HD22	2.18	0.43
1:L:107:ILE:HG23	2:M:254:TRP:HE3	1.83	0.43
1:L:25:TRP:HZ3	3:H:97:PRO:HG3	1.84	0.43
2:M:148:TRP:HZ2	2:M:271:TRP:CH2	2.36	0.43
1:L:177:ILE:HD13	5:M:1:BCL:HMD1	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:M:1:BCL:HMB1	5:M:1:BCL:OBB	2.19	0.43
7:L:272:U10:H101	7:L:272:U10:H172	2.01	0.43
1:L:213:ASP:HA	1:L:223:SER:OG	2.19	0.43
1:L:60:ASN:HA	1:L:61:PRO:HD3	1.78	0.43
1:L:56:GLN:HG3	1:L:58:THR:HG22	2.00	0.43
3:H:104:PRO:O	3:H:108:GLY:N	2.52	0.42
6:M:3:BPH:HBC2	6:M:3:BPH:H2C	1.90	0.42
3:H:148:PRO:HA	3:H:151:LEU:HD23	1.99	0.42
2:M:201:PHE:HD1	2:M:279:THR:HG23	1.84	0.42
2:M:164:ARG:HB3	2:M:165:PRO:HD3	2.01	0.42
1:L:107:ILE:HD13	2:M:255:THR:HG23	2.01	0.42
3:H:103:ASP:HA	3:H:104:PRO:HD3	1.73	0.42
5:L:2:BCL:H2C	6:M:3:BPH:HBC2	2.00	0.42
2:M:201:PHE:HA	2:M:204:LEU:HD12	2.02	0.42
1:L:38:THR:HG21	1:L:100:TRP:CE3	2.55	0.42
2:M:22:GLU:HB3	2:M:23:ASP:H	1.63	0.42
2:M:242:GLY:HA3	3:H:117:ARG:HD2	2.01	0.42
3:H:82:ASP:O	3:H:84:PRO:HA	2.20	0.42
2:M:261:THR:HG22	3:H:40:TYR:CD1	2.40	0.42
1:L:38:THR:HG21	1:L:100:TRP:HE3	1.84	0.42
1:L:28:PRO:O	2:M:254:TRP:HA	2.20	0.42
2:M:35:PHE:HB3	2:M:39:LEU:HB2	2.02	0.42
3:H:210:SER:HA	3:H:213:PHE:CD2	2.55	0.42
2:M:152:SER:O	2:M:155:TRP:HB3	2.20	0.41
2:M:66:TRP:CD1	2:M:122:MET:HB2	2.55	0.41
2:M:66:TRP:NE1	2:M:70:ILE:HD11	2.35	0.41
5:L:2:BCL:H142	5:L:4:BCL:HMB1	2.03	0.41
5:M:1:BCL:C3B	8:M:304:CRT:H20	2.50	0.41
1:L:141:ALA:HB3	1:L:144:TYR:CE2	2.56	0.41
2:M:259:ASN:ND2	3:H:40:TYR:HB3	2.36	0.41
3:H:132:LYS:CE	3:H:171:ILE:HD11	2.47	0.41
1:L:69:PRO:HG2	1:L:142:TRP:HB2	2.02	0.41
1:L:207:ARG:NH2	2:M:141:GLY:HA3	2.34	0.41
1:L:131:LEU:HD22	1:L:156:TRP:CH2	2.56	0.41
3:H:159:GLU:O	3:H:210:SER:HB3	2.21	0.41
6:L:271:BPH:HMB1	6:L:271:BPH:HHB	1.87	0.41
3:H:108:GLY:HA3	3:H:114:TRP:CE3	2.56	0.41
1:L:200:PRO:O	1:L:202:LYS:N	2.54	0.41
1:L:75:LEU:HA	1:L:142:TRP:CD1	2.57	0.40
1:L:45:GLY:O	1:L:49:ILE:HG13	2.21	0.40
3:H:89:ARG:H	3:H:89:ARG:NE	2.11	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:H:156:CYS:HB3	3:H:206:ASN:O	2.22	0.40
3:H:31:LEU:HD22	3:H:31:LEU:HA	1.87	0.40
7:M:303:U10:H401	7:M:303:U10:H421	1.77	0.40
3:H:184:LYS:O	3:H:185:ASP:HB3	2.21	0.40
3:H:68:HIS:CE1	3:H:123:LEU:HB2	2.55	0.40
1:L:8:LYS:HE2	1:L:9:TYR:CE2	2.57	0.40
1:L:193:LEU:O	1:L:196:SER:HB2	2.21	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	L	264/266 (99%)	237 (90%)	20 (8%)	7 (3%)	6 32
2	M	294/296 (99%)	242 (82%)	30 (10%)	22 (8%)	1 6
3	H	235/237 (99%)	188 (80%)	28 (12%)	19 (8%)	1 5
All	All	793/799 (99%)	667 (84%)	78 (10%)	48 (6%)	2 11

All (48) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	L	71	LEU
1	L	115	TYR
1	L	201	GLU
1	L	269	LEU
2	M	22	GLU
2	M	52	LEU
2	M	54	SER
2	M	99	PRO
2	M	104	SER
2	M	105	PHE

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Mol	Chain	Res	Type
2	M	111	GLU
2	M	144	LYS
3	H	13	ALA
3	H	51	ALA
3	H	60	LYS
3	H	94	GLU
3	H	127	GLY
3	H	138	ALA
3	H	185	ASP
3	H	212	LEU
2	M	37	THR
2	M	83	ALA
2	M	287	SER
3	H	44	ASN
3	H	57	PRO
3	H	68	HIS
3	H	92	VAL
3	H	142	VAL
3	H	214	ALA
1	L	15	THR
2	M	82	PRO
2	M	96	PRO
3	H	32	GLN
3	H	39	GLY
3	H	49	PRO
2	M	30	SER
2	M	33	GLY
2	M	80	TRP
3	H	31	LEU
3	H	246	PRO
1	L	31	VAL
1	L	202	LYS
2	M	24	VAL
2	M	195	ASN
2	M	97	PRO
2	M	112	GLY
2	M	15	PRO
2	M	32	VAL

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	L	210/210 (100%)	180 (86%)	30 (14%)	4 19
2	M	232/232 (100%)	197 (85%)	35 (15%)	3 17
3	H	192/192 (100%)	156 (81%)	36 (19%)	2 10
All	All	634/634 (100%)	533 (84%)	101 (16%)	3 15

All (101) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	L	5	PHE
1	L	6	GLU
1	L	8	LYS
1	L	48	LEU
1	L	82	LYS
1	L	103	ARG
1	L	109	ARG
1	L	113	ILE
1	L	129	LEU
1	L	133	LEU
1	L	138	MET
1	L	158	SER
1	L	183	ASN
1	L	185	LEU
1	L	193	LEU
1	L	196	SER
1	L	202	LYS
1	L	204	LYS
1	L	208	THR
1	L	216	PHE
1	L	227	LEU
1	L	232	LEU
1	L	234	LEU
1	L	235	LEU
1	L	247	CYS
1	L	249	ILE

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Mol	Chain	Res	Type
1	L	251	THR
1	L	253	THR
1	L	257	ASP
1	L	269	LEU
2	M	20	MET
2	M	22	GLU
2	M	24	VAL
2	M	28	ASN
2	M	32	VAL
2	M	35	PHE
2	M	37	THR
2	M	38	LEU
2	M	60	LEU
2	M	64	LEU
2	M	94	LEU
2	M	99	PRO
2	M	105	PHE
2	M	108	PRO
2	M	111	GLU
2	M	114	LEU
2	M	135	LEU
2	M	148	TRP
2	M	175	VAL
2	M	182	HIS
2	M	197	PHE
2	M	216	PHE
2	M	222	THR
2	M	226	VAL
2	M	227	SER
2	M	228	ARG
2	M	258	PHE
2	M	259	ASN
2	M	262	MET
2	M	267	ARG
2	M	270	ILE
2	M	271	TRP
2	M	272	MET
2	M	275	LEU
2	M	286	LEU
3	H	14	SER
3	H	15	LEU
3	H	29	TYR

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Mol	Chain	Res	Type
3	H	34	GLU
3	H	35	ASN
3	H	38	GLU
3	H	52	ASN
3	H	53	GLN
3	H	60	LYS
3	H	62	LYS
3	H	68	HIS
3	H	70	ARG
3	H	75	VAL
3	H	83	ARG
3	H	87	LEU
3	H	89	ARG
3	H	94	GLU
3	H	97	PRO
3	H	109	VAL
3	H	123	LEU
3	H	126	HIS
3	H	132	LYS
3	H	146	LYS
3	H	151	LEU
3	H	154	ARG
3	H	188	THR
3	H	193	MET
3	H	208	LEU
3	H	212	LEU
3	H	213	PHE
3	H	218	THR
3	H	219	ILE
3	H	220	LYS
3	H	228	LEU
3	H	247	LYS
3	H	248	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
1	L	173	HIS
1	L	211	HIS
2	M	11	GLN
3	H	141	HIS
3	H	204	HIS

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 10 ligands modelled in this entry, 1 is monoatomic - leaving 9 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	$\#\|Z\| > 2$
5	BCL	L	2	1	53,74,74	1.12	6 (11%)	57,115,115	1.56	10 (17%)
6	BPH	L	271	-	64,70,70	1.09	6 (9%)	73,101,101	1.83	8 (10%)
7	U10	L	272	-	41,41,63	1.85	10 (24%)	49,52,79	1.70	12 (24%)
5	BCL	L	4	1	38,59,74	1.30	5 (13%)	40,97,115	2.22	9 (22%)
5	BCL	M	1	2	38,59,74	1.21	4 (10%)	40,97,115	2.02	10 (25%)
6	BPH	M	3	-	64,70,70	1.17	7 (10%)	73,101,101	1.70	12 (16%)
7	U10	M	303	-	51,51,63	1.69	13 (25%)	61,64,79	1.77	16 (26%)
8	CRT	M	304	-	40,41,43	4.05	26 (65%)	44,50,54	2.91	16 (36%)
6	BPH	M	5	-	64,70,70	1.15	8 (12%)	73,101,101	1.71	9 (12%)

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
5	BCL	L	2	1	-	0/37/137/137	0/0/9/9
6	BPH	L	271	-	-	0/54/105/105	0/1/6/6
7	U10	L	272	-	-	0/37/61/87	0/1/1/1
5	BCL	L	4	1	-	0/19/119/137	0/0/9/9
5	BCL	M	1	2	-	0/19/119/137	0/0/9/9
6	BPH	M	3	-	-	0/54/105/105	0/1/6/6
7	U10	M	303	-	-	0/49/73/87	0/1/1/1
8	CRT	M	304	-	-	1/47/47/51	0/0/0/0
6	BPH	M	5	-	2/2/18/22	1/54/105/105	0/1/6/6

All (85) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	M	304	CRT	C37-C38	-5.21	1.37	1.54
6	M	3	BPH	C3D-CAD	-4.39	1.37	1.46
7	L	272	U10	C7-C8	-4.13	1.44	1.50
8	M	304	CRT	C25-C23	-4.12	1.36	1.45
8	M	304	CRT	C30-C28	-3.97	1.37	1.45
8	M	304	CRT	C11-C12	-3.88	1.37	1.45
5	L	2	BCL	O2D-CGD	-3.68	1.23	1.33
6	L	271	BPH	O2D-CGD	-3.46	1.24	1.33
6	L	271	BPH	C3D-CAD	-3.40	1.39	1.46
8	M	304	CRT	C16-C17	-3.39	1.38	1.45
5	L	4	BCL	O2D-CGD	-3.35	1.24	1.33
5	M	1	BCL	O2D-CGD	-3.34	1.24	1.33
5	L	4	BCL	O2A-CGA	-3.32	1.23	1.33
6	M	5	BPH	C3D-CAD	-3.31	1.40	1.46
6	M	5	BPH	O2A-CGA	-3.25	1.23	1.33
6	M	5	BPH	O2D-CGD	-3.25	1.24	1.33
6	M	3	BPH	C1B-C2B	-3.24	1.38	1.45
8	M	304	CRT	C6-C7	-3.18	1.38	1.45
6	M	3	BPH	O2D-CGD	-3.17	1.25	1.33
7	M	303	U10	C7-C8	-3.17	1.45	1.50
7	M	303	U10	C3-C2	-3.16	1.39	1.48
6	M	3	BPH	O2A-CGA	-3.11	1.23	1.33
7	M	303	U10	C4-C5	-3.10	1.40	1.48
5	L	2	BCL	O2A-CGA	-3.02	1.24	1.33
5	M	1	BCL	O2A-CGA	-2.97	1.24	1.33
7	L	272	U10	C3-C2	-2.93	1.40	1.48
6	L	271	BPH	O2A-CGA	-2.89	1.24	1.33
6	M	5	BPH	C1B-C2B	-2.88	1.39	1.45
7	L	272	U10	C4-C5	-2.83	1.40	1.48
6	L	271	BPH	C1B-C2B	-2.78	1.39	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	M	1	BCL	C3D-CAD	-2.72	1.38	1.45
5	L	4	BCL	C3D-CAD	-2.72	1.38	1.45
5	M	1	BCL	C3B-CAB	-2.61	1.41	1.49
5	L	4	BCL	C3B-CAB	-2.52	1.42	1.49
5	L	2	BCL	C3B-CAB	-2.51	1.42	1.49
5	L	2	BCL	C3D-CAD	-2.41	1.38	1.45
6	M	5	BPH	C3A-C2A	-2.33	1.47	1.54
6	M	5	BPH	C3B-C4B	-2.26	1.38	1.43
6	L	271	BPH	C3A-C2A	-2.24	1.47	1.54
5	L	2	BCL	CAA-C2A	-2.15	1.49	1.54
6	M	5	BPH	C3B-CAB	-2.13	1.40	1.46
7	M	303	U10	C22-C23	-2.07	1.44	1.50
6	M	3	BPH	C2C-C3C	-2.06	1.48	1.54
6	M	3	BPH	C4A-NA	2.06	1.39	1.34
8	M	304	CRT	C3-C1	2.11	1.57	1.52
8	M	304	CRT	C4-C1	2.17	1.56	1.53
8	M	304	CRT	C9-C7	2.17	1.38	1.35
8	M	304	CRT	C8-C7	2.19	1.55	1.50
5	L	4	BCL	C2-C3	2.28	1.39	1.32
8	M	304	CRT	C19-C17	2.29	1.38	1.35
7	M	303	U10	C6-C1	2.36	1.40	1.35
7	M	303	U10	C44-C43	2.42	1.45	1.28
7	L	272	U10	C34-C33	2.64	1.47	1.28
7	M	303	U10	C8-C9	2.65	1.38	1.33
6	M	3	BPH	C2-C3	2.65	1.38	1.33
7	L	272	U10	C6-C1	2.69	1.41	1.35
6	M	5	BPH	C2-C3	2.84	1.38	1.33
7	L	272	U10	C8-C9	2.94	1.38	1.33
7	M	303	U10	C13-C14	3.00	1.38	1.33
6	L	271	BPH	C2-C3	3.01	1.38	1.33
7	M	303	U10	C38-C39	3.07	1.39	1.33
7	M	303	U10	C23-C24	3.10	1.39	1.33
7	M	303	U10	C28-C29	3.10	1.39	1.33
7	L	272	U10	C13-C14	3.15	1.39	1.33
7	M	303	U10	C18-C19	3.17	1.39	1.33
8	M	304	CRT	C10-C9	3.19	1.53	1.43
5	L	2	BCL	C2-C3	3.33	1.39	1.33
8	M	304	CRT	C4-C5	3.33	1.54	1.50
8	M	304	CRT	C35-C33	3.34	1.53	1.45
7	M	303	U10	C33-C34	3.40	1.39	1.33
7	L	272	U10	C28-C29	3.45	1.39	1.33
8	M	304	CRT	C26-C27	3.48	1.54	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	M	304	CRT	C21-C22	3.54	1.54	1.43
7	L	272	U10	C18-C19	3.60	1.40	1.33
8	M	304	CRT	C20-C19	3.67	1.55	1.43
8	M	304	CRT	C15-C14	3.73	1.55	1.43
8	M	304	CRT	C31-C32	3.75	1.55	1.43
7	L	272	U10	C23-C24	3.78	1.40	1.33
8	M	304	CRT	C21-C20	7.00	1.54	1.35
8	M	304	CRT	C35-C36	7.02	1.51	1.31
8	M	304	CRT	C15-C16	7.51	1.54	1.34
8	M	304	CRT	C31-C30	7.67	1.54	1.34
8	M	304	CRT	C10-C11	7.69	1.54	1.34
8	M	304	CRT	C26-C25	7.95	1.55	1.34
8	M	304	CRT	C6-C5	8.48	1.55	1.31

All (102) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
8	M	304	CRT	C37-C36-C35	-8.56	106.03	125.67
6	L	271	BPH	O1D-CGD-CBD	-6.67	115.06	124.62
8	M	304	CRT	C36-C35-C33	-6.58	115.70	125.75
5	L	4	BCL	O1D-CGD-CBD	-6.32	115.57	124.62
8	M	304	CRT	C26-C27-C28	-6.09	118.41	127.20
6	M	5	BPH	C4D-C3D-C2D	-6.04	99.28	107.08
8	M	304	CRT	C5-C6-C7	-6.01	116.58	125.75
6	M	3	BPH	C4D-C3D-C2D	-5.36	100.17	107.08
6	M	5	BPH	O1D-CGD-CBD	-5.31	117.01	124.62
6	L	271	BPH	C4D-C3D-C2D	-5.01	100.62	107.08
8	M	304	CRT	C20-C19-C17	-4.63	120.51	127.20
8	M	304	CRT	C21-C22-C23	-4.50	120.69	127.20
7	M	303	U10	C30-C29-C28	-4.47	114.73	123.50
5	M	1	BCL	O1D-CGD-CBD	-4.41	118.31	124.62
8	M	304	CRT	C8-C7-C9	-4.03	116.95	122.90
8	M	304	CRT	C34-C33-C35	-3.84	111.70	118.10
5	L	4	BCL	CMB-C2B-C1B	-3.79	122.09	128.36
6	M	3	BPH	C1C-NC-C4C	-3.73	106.62	110.44
7	L	272	U10	C10-C9-C8	-3.67	116.30	123.50
5	L	2	BCL	CMB-C2B-C1B	-3.61	122.40	128.36
5	L	2	BCL	CBA-CAA-C2A	-3.46	103.97	113.73
7	M	303	U10	C40-C39-C38	-3.45	116.73	123.50
7	L	272	U10	C15-C14-C13	-3.42	116.80	123.50
7	L	272	U10	C20-C19-C18	-3.32	116.98	123.50
8	M	304	CRT	C9-C10-C11	-3.29	113.09	123.13

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	M	1	BCL	C1-C2-C3	-3.26	121.37	126.71
5	L	2	BCL	OBD-CAD-C3D	-3.15	121.93	128.35
5	L	4	BCL	OBD-CAD-C3D	-3.12	121.98	128.35
7	M	303	U10	C10-C9-C8	-3.08	117.45	123.50
7	M	303	U10	C20-C19-C18	-3.00	117.62	123.50
5	M	1	BCL	OBD-CAD-C3D	-2.97	122.29	128.35
8	M	304	CRT	C15-C14-C12	-2.96	122.92	127.20
7	L	272	U10	C7-C8-C9	-2.81	121.94	126.70
6	L	271	BPH	OBD-CAD-C3D	-2.77	122.69	128.35
7	L	272	U10	C30-C29-C28	-2.74	118.12	123.50
7	M	303	U10	C25-C24-C23	-2.72	118.17	123.50
7	M	303	U10	C15-C14-C13	-2.69	118.21	123.50
5	L	4	BCL	CAA-C2A-C3A	-2.57	105.82	113.22
5	L	2	BCL	CAA-C2A-C3A	-2.49	106.07	113.22
6	L	271	BPH	C17-C16-C15	-2.43	100.92	112.99
6	M	3	BPH	CGD-CBD-CAD	-2.41	102.46	110.62
7	M	303	U10	C35-C34-C33	-2.40	118.79	123.50
6	M	3	BPH	O1D-CGD-CBD	-2.38	121.21	124.62
6	M	5	BPH	CBB-CAB-C3B	-2.34	115.31	120.52
7	M	303	U10	C36-C37-C38	-2.30	105.66	111.69
6	M	3	BPH	C4-C3-C2	-2.29	119.01	123.50
8	M	304	CRT	C30-C28-C27	-2.25	115.36	118.98
6	M	5	BPH	OBD-CAD-CBD	-2.24	122.55	125.94
8	M	304	CRT	C29-C28-C27	-2.21	119.63	122.90
7	L	272	U10	C25-C24-C23	-2.20	119.19	123.50
6	M	3	BPH	CHC-C4B-NB	-2.17	120.77	124.91
7	L	272	U10	C27-C28-C29	-2.15	123.08	127.76
8	M	304	CRT	C18-C17-C16	-2.15	114.52	118.10
5	M	1	BCL	CAA-C2A-C3A	-2.13	107.08	113.22
6	M	3	BPH	CAC-C3C-C4C	-2.12	107.23	112.67
8	M	304	CRT	C32-C31-C30	-2.10	116.73	123.13
5	M	1	BCL	CAC-C3C-C4C	-2.09	107.94	112.58
5	M	1	BCL	CMB-C2B-C1B	-2.07	124.95	128.36
7	M	303	U10	C12-C13-C14	-2.04	123.32	127.76
7	M	303	U10	C22-C23-C24	-2.01	123.38	127.76
5	L	2	BCL	CED-O2D-CGD	2.01	120.71	115.99
7	M	303	U10	C16-C14-C13	2.02	124.87	121.05
5	M	1	BCL	CAA-CBA-CGA	2.02	119.24	113.32
5	L	2	BCL	O2D-CGD-CBD	2.07	114.14	111.30
5	M	1	BCL	CMB-C2B-C3B	2.09	129.18	125.09
5	L	4	BCL	C5-C3-C4	2.15	119.91	114.64
6	M	5	BPH	C4-C3-C5	2.15	118.70	115.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
8	M	304	CRT	C10-C9-C7	2.16	130.32	127.20
5	L	2	BCL	C3A-C2A-C1A	2.18	105.19	101.50
7	M	303	U10	C35-C34-C36	2.20	118.77	115.41
7	L	272	U10	C22-C21-C19	2.23	119.97	112.71
7	M	303	U10	C25-C24-C26	2.27	118.88	115.41
7	L	272	U10	C15-C14-C16	2.33	118.97	115.41
6	M	3	BPH	C4-C3-C5	2.61	119.40	115.41
6	M	3	BPH	CED-O2D-CGD	2.76	122.46	115.99
6	L	271	BPH	CBA-CAA-C2A	2.94	122.03	113.73
7	L	272	U10	C30-C29-C31	2.99	119.98	115.41
5	L	2	BCL	CBC-CAC-C3C	3.28	121.60	113.57
5	L	4	BCL	CAA-CBA-CGA	3.28	122.93	113.32
6	M	3	BPH	C3D-CAD-CBD	3.31	112.27	107.60
7	L	272	U10	C10-C9-C11	3.34	120.51	115.41
7	M	303	U10	C30-C29-C31	3.44	120.67	115.41
5	L	4	BCL	C3D-CAD-CBD	3.44	112.46	107.60
7	M	303	U10	C40-C39-C41	3.45	120.68	115.41
5	L	2	BCL	CMB-C2B-C3B	3.45	131.84	125.09
6	L	271	BPH	C3C-C4C-NC	3.47	111.40	107.93
6	M	5	BPH	C3D-CAD-CBD	3.65	112.75	107.60
5	L	4	BCL	CMB-C2B-C3B	3.76	132.43	125.09
6	M	5	BPH	CBA-CAA-C2A	3.82	124.52	113.73
5	L	2	BCL	C3D-CAD-CBD	3.85	113.04	107.60
7	L	272	U10	C20-C19-C21	3.85	121.30	115.41
7	M	303	U10	C7-C6-C5	3.90	123.15	118.56
6	M	5	BPH	C3C-C4C-NC	3.92	111.86	107.93
6	L	271	BPH	C3D-CAD-CBD	4.06	113.33	107.60
5	M	1	BCL	C3D-CAD-CBD	4.27	113.63	107.60
6	M	5	BPH	O2D-CGD-CBD	4.91	118.03	111.30
6	M	3	BPH	O2D-CGD-CBD	4.91	118.03	111.30
8	M	304	CRT	C38-C37-C36	5.40	133.23	113.86
6	M	3	BPH	C3C-C4C-NC	6.18	114.12	107.93
5	L	4	BCL	O2D-CGD-CBD	6.44	120.14	111.30
5	M	1	BCL	O2D-CGD-CBD	6.53	120.25	111.30
6	L	271	BPH	O2D-CGD-CBD	7.21	121.19	111.30

All (2) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
6	M	5	BPH	C8
6	M	5	BPH	C13

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	M	5	BPH	OBB-CAB-C3B-C4B
8	M	304	CRT	C32-C31-C30-C28

There are no ring outliers.

9 monomers are involved in 39 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	L	2	BCL	8	0
6	L	271	BPH	7	0
7	L	272	U10	5	0
5	L	4	BCL	6	0
5	M	1	BCL	8	0
6	M	3	BPH	6	0
7	M	303	U10	5	0
8	M	304	CRT	2	0
6	M	5	BPH	1	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.