Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 08:13 AM GMT

PDB ID	:	3DSY
Title	:	E(L212)Q mutant structure of photosynthetic reaction center from Rhodobacter sphaeroides
Authors	:	Pokkuluri, P.R.; Schiffer, M.
Deposited on	:	2008-07-14
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:

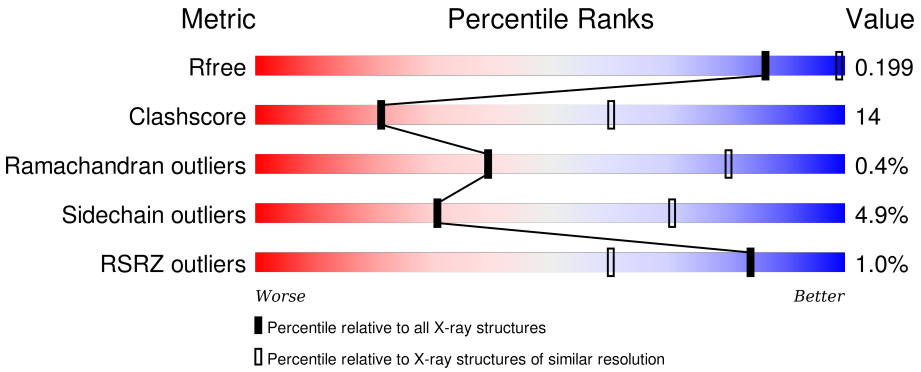
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	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))
R_{free}	91344	1578 (3.00-3.00)
Clashscore	102246	1912 (3.00-3.00)
Ramachandran outliers	100387	1853 (3.00-3.00)
Sidechain outliers	100360	1856 (3.00-3.00)
RSRZ outliers	91569	1592 (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.

Mol	Chain	Length	Quality of chain
1	L	281	69% 26%
2	M	314	% 65% 26%
3	H	260	2% 61% 27% 8%

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
10	LDA	H	703	-	-	-	X
10	LDA	L	709	-	-	-	X
5	BCL	L	501	X	-	-	-
5	BCL	M	501	X	-	-	X
6	BPH	M	503	X	-	-	-
7	U10	L	504	-	-	-	X
7	U10	M	504	-	-	-	X
8	SPN	M	600	-	-	-	X
9	CDL	M	800	-	-	-	X

2 Entry composition

There are 11 unique types of molecules in this entry. The entry contains 7287 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 Reaction center protein L chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	L	281	Total	C	N	O	S	0	0	0
			2232	1507	356	361	8			

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
L	212	GLN	GLU	ENGINEERED	UNP P0C0Y8

- Molecule 2 is a protein called Reaction center protein M chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	M	302	Total	C	N	O	S	0	0	0
			2408	1607	394	397	10			

There are 7 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
M	308	HIS	-	EXPRESSION TAG	UNP P0C0Y9
M	309	HIS	-	EXPRESSION TAG	UNP P0C0Y9
M	310	HIS	-	EXPRESSION TAG	UNP P0C0Y9
M	311	HIS	-	EXPRESSION TAG	UNP P0C0Y9
M	312	HIS	-	EXPRESSION TAG	UNP P0C0Y9
M	313	HIS	-	EXPRESSION TAG	UNP P0C0Y9
M	314	HIS	-	EXPRESSION TAG	UNP P0C0Y9

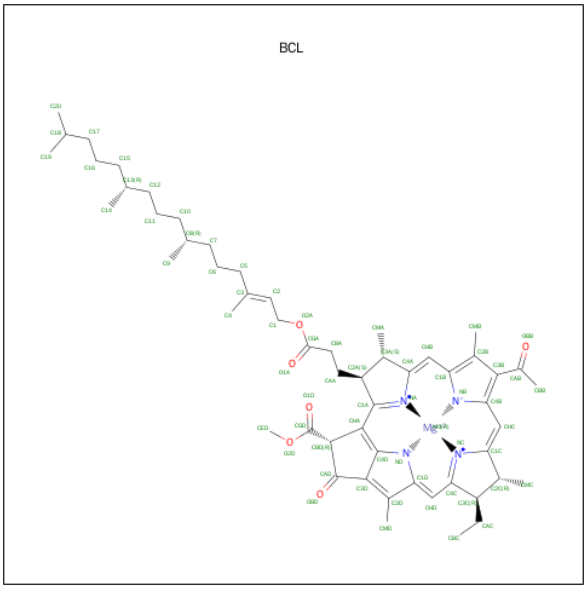
- Molecule 3 is a protein called Reaction center protein H chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	H	240	Total	C	N	O	S	0	0	0
			1829	1169	314	337	9			

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

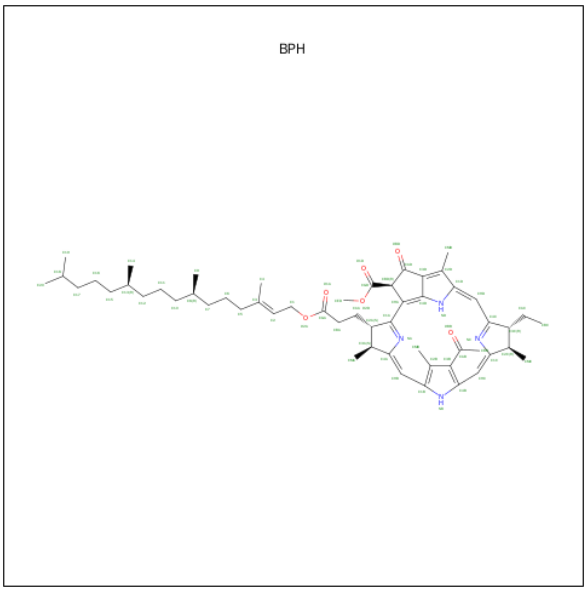
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	M	1	Total Fe 1 1	0	0

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



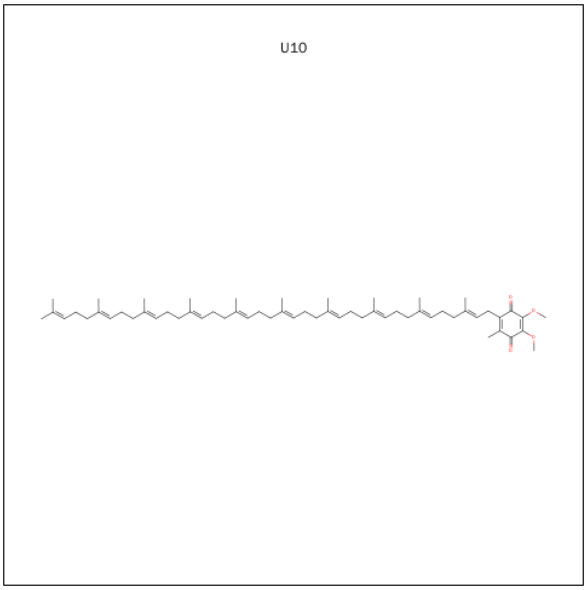
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	M	1	Total C Mg N O 66 55 1 4 6	0	0
5	L	1	Total C Mg N O 66 55 1 4 6	0	0
5	M	1	Total C Mg N O 66 55 1 4 6	0	0
5	L	1	Total C Mg N O 66 55 1 4 6	0	0

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



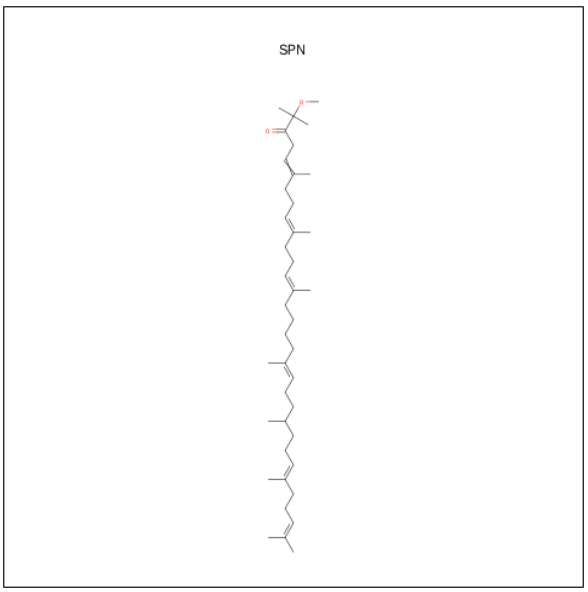
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
6	M	1	Total	C	N	O	10	0
			65	55	4	6		
6	L	1	Total	C	N	O	0	0
			65	55	4	6		

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



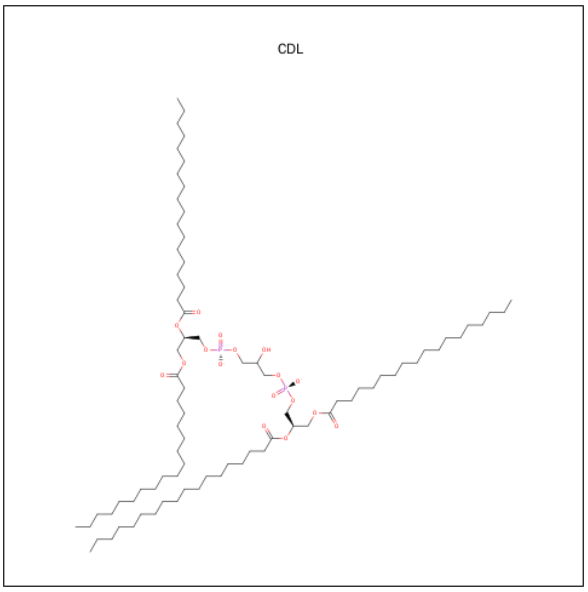
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	M	1	Total	C	O	0	0
			48	44	4		
7	L	1	Total	C	O	0	0
			48	44	4		

- Molecule 8 is SPEROIDENONE (three-letter code: SPN) (formula: $C_{41}H_{70}O_2$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	C	O		
8	M	1	43	41	2	0	0

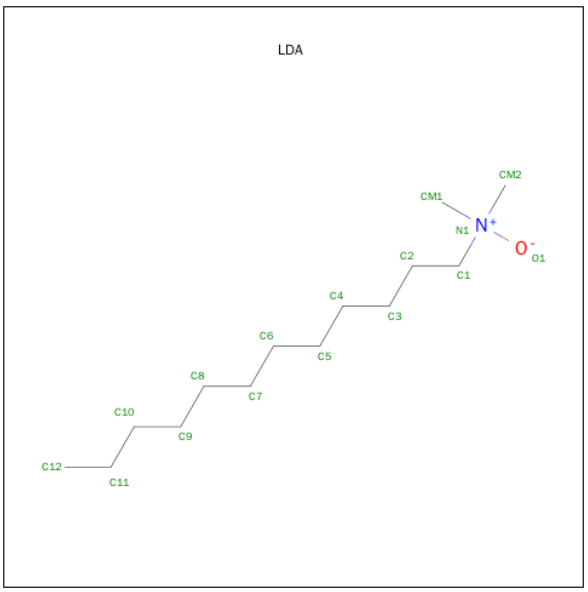
- Molecule 9 is CARDIOLIPIN (three-letter code: CDL) (formula: $C_{81}H_{156}O_{17}P_2$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	O	P		
9	M	1	81	62	17	2	0	0

- Molecule 10 is LAURYL DIMETHYLAMINE-N-OXIDE (three-letter code: LDA) (formula:

$C_{14}H_{31}NO$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
10	M	1	Total C N O 16 14 1 1	0	0
10	H	1	Total C N O 16 14 1 1	0	0
10	M	1	Total C N O 16 14 1 1	0	0
10	L	1	Total C N O 16 14 1 1	0	0

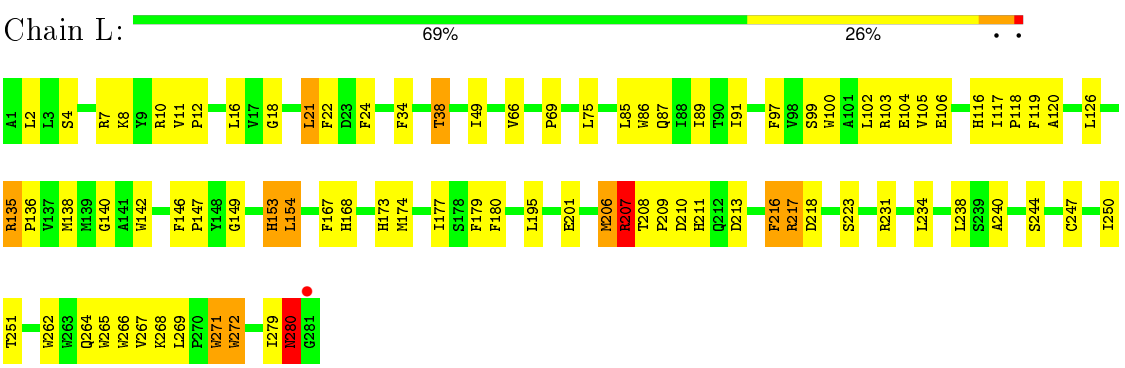
- Molecule 11 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
11	H	60	Total O 60 60	0	0
11	L	39	Total O 39 39	0	0
11	M	40	Total O 40 40	0	0

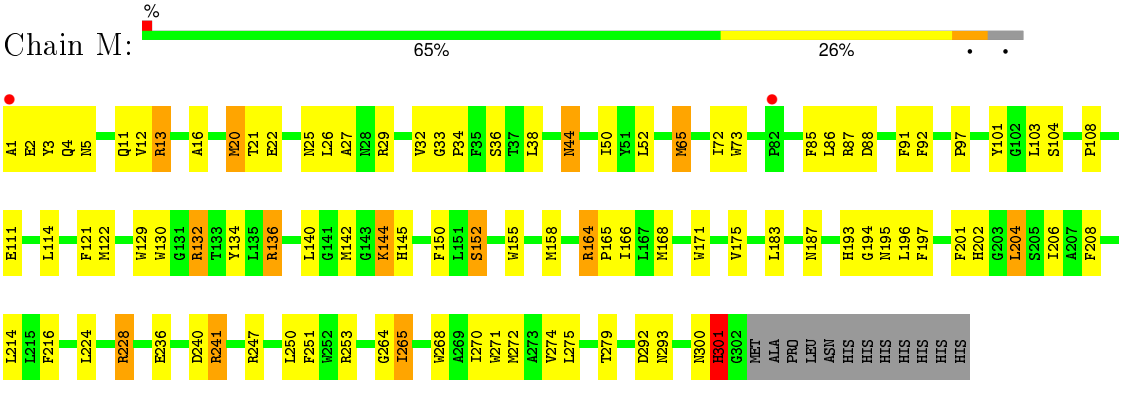
3 Residue-property plots (i)

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.

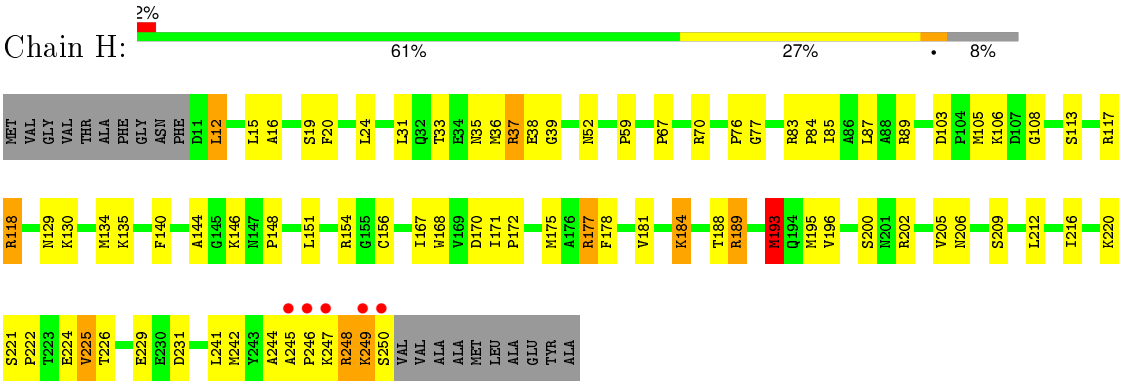
- Molecule 1: Reaction center protein L chain



- Molecule 2: Reaction center protein M chain



- Molecule 3: Reaction center protein H chain



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 31 2 1	Depositor
Cell constants a, b, c, α, β, γ	141.70Å 141.70Å 187.00Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	30.00 – 3.00 29.15 – 3.00	Depositor EDS
% Data completeness (in resolution range)	(Not available) (30.00-3.00) 94.9 (29.15-3.00)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	3.98 (at 3.00Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.191 , (Not available) 0.192 , 0.199	Depositor DCC
R_{free} test set	3058 reflections (7.88%)	DCC
Wilson B-factor (Å^2)	52.3	Xtriage
Anisotropy	0.108	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.30 , 68.6	EDS
Estimated twinning fraction	0.022 for -h,-k,l	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.33$	Xtriage
Outliers	0 of 43243 reflections	Xtriage
F_o,F_c correlation	0.92	EDS
Total number of atoms	7287	wwPDB-VP
Average B, all atoms (Å^2)	43.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.71% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: BCL, LDA, CDL, BPH, FE, SPN, 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	0.95	0/2320	1.08	13/3175 (0.4%)
2	M	1.05	2/2500 (0.1%)	1.13	18/3413 (0.5%)
3	H	0.93	2/1877 (0.1%)	1.24	21/2553 (0.8%)
All	All	0.98	4/6697 (0.1%)	1.15	52/9141 (0.6%)

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

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	H	76	PRO	C-N	-6.34	1.21	1.33
3	H	77	GLY	N-CA	5.73	1.54	1.46
2	M	247	ARG	CG-CD	-5.44	1.38	1.51
2	M	301	HIS	CA-C	-5.15	1.39	1.52

All (52) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	H	248	ARG	CD-NE-CZ	13.05	141.88	123.60
2	M	247	ARG	NE-CZ-NH2	11.49	126.04	120.30
1	L	103	ARG	NE-CZ-NH1	10.94	125.77	120.30
3	H	250	SER	CA-C-O	-8.26	102.76	120.10
1	L	207	ARG	NE-CZ-NH2	7.49	124.04	120.30
2	M	13	ARG	NE-CZ-NH2	7.33	123.97	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	H	202	ARG	NE-CZ-NH2	7.31	123.95	120.30
3	H	70	ARG	NE-CZ-NH2	7.29	123.95	120.30
3	H	154	ARG	NE-CZ-NH2	7.29	123.94	120.30
1	L	231	ARG	NE-CZ-NH2	7.28	123.94	120.30
3	H	37	ARG	NE-CZ-NH2	7.25	123.93	120.30
2	M	164	ARG	NE-CZ-NH2	7.24	123.92	120.30
3	H	117	ARG	NE-CZ-NH2	7.23	123.91	120.30
1	L	217	ARG	NE-CZ-NH2	7.14	123.87	120.30
3	H	189	ARG	NE-CZ-NH2	6.78	123.69	120.30
2	M	52	LEU	CB-CA-C	6.74	123.01	110.20
2	M	228	ARG	NE-CZ-NH2	6.71	123.66	120.30
3	H	248	ARG	NE-CZ-NH1	6.65	123.63	120.30
2	M	247	ARG	CD-NE-CZ	6.57	132.80	123.60
1	L	135	ARG	NE-CZ-NH2	6.56	123.58	120.30
2	M	136	ARG	NE-CZ-NH2	6.50	123.55	120.30
2	M	253	ARG	NE-CZ-NH2	6.49	123.54	120.30
2	M	132	ARG	NE-CZ-NH2	6.47	123.53	120.30
3	H	177	ARG	NE-CZ-NH2	6.44	123.52	120.30
1	L	103	ARG	NH1-CZ-NH2	-6.41	112.35	119.40
3	H	83	ARG	NE-CZ-NH2	6.38	123.49	120.30
1	L	280	ASN	O-C-N	-6.31	112.47	123.20
1	L	7	ARG	NE-CZ-NH2	6.28	123.44	120.30
2	M	241	ARG	NE-CZ-NH2	6.26	123.43	120.30
2	M	20	MET	CG-SD-CE	6.12	109.98	100.20
3	H	175	MET	CG-SD-CE	6.09	109.94	100.20
1	L	206	MET	CG-SD-CE	6.09	109.94	100.20
2	M	158	MET	CG-SD-CE	6.06	109.89	100.20
1	L	10	ARG	NE-CZ-NH2	6.06	123.33	120.30
3	H	36	MET	CG-SD-CE	6.04	109.86	100.20
3	H	89	ARG	NE-CZ-NH2	5.97	123.28	120.30
3	H	134	MET	CG-SD-CE	5.90	109.64	100.20
1	L	174	MET	CG-SD-CE	5.87	109.60	100.20
2	M	1	ALA	CB-CA-C	5.86	118.89	110.10
3	H	242	MET	CG-SD-CE	5.80	109.48	100.20
2	M	142	MET	CG-SD-CE	5.79	109.47	100.20
2	M	272	MET	CG-SD-CE	5.75	109.40	100.20
3	H	193	MET	CG-SD-CE	5.74	109.38	100.20
1	L	138	MET	CG-SD-CE	5.71	109.33	100.20
3	H	178	PHE	CB-CA-C	-5.69	99.02	110.40
2	M	122	MET	CG-SD-CE	5.65	109.24	100.20
3	H	105	MET	CG-SD-CE	5.64	109.22	100.20
2	M	65	MET	CG-SD-CE	5.62	109.19	100.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	H	195	MET	CG-SD-CE	5.54	109.06	100.20
3	H	118	ARG	NE-CZ-NH2	5.44	123.02	120.30
2	M	168	MET	CG-SD-CE	5.34	108.74	100.20
1	L	2	LEU	CB-CA-C	-5.07	100.56	110.20

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	L	280	ASN	Mainchain

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	L	2232	0	2189	74	0
2	M	2408	0	2321	77	0
3	H	1829	0	1836	46	0
4	M	1	0	0	0	0
5	L	132	0	148	15	0
5	M	132	0	148	17	0
6	L	65	0	76	2	0
6	M	65	0	76	1	0
7	L	48	0	63	6	0
7	M	48	0	63	6	0
8	M	43	0	69	1	0
9	M	81	0	106	1	0
10	H	16	0	31	4	0
10	L	16	0	31	4	0
10	M	32	0	62	4	0
11	H	60	0	0	2	0
11	L	39	0	0	1	0
11	M	40	0	0	1	0
All	All	7287	0	7219	203	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 (203) 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:33:THR:O	3:H:59:PRO:HG3	1.69	0.91
1:L:34:PHE:O	1:L:38:THR:HG23	1.71	0.89
7:M:504:U10:H202	10:H:703:LDA:H112	1.54	0.88
2:M:204:LEU:HB3	2:M:279:THR:HG21	1.56	0.85
3:H:146:LYS:NZ	3:H:200:SER:O	2.11	0.83
2:M:197:PHE:HZ	5:M:502:BCL:HBB2	1.47	0.80
5:L:502:BCL:HHC	5:L:502:BCL:OBB	1.81	0.79
1:L:179:PHE:CE1	7:L:504:U10:H18	2.21	0.76
1:L:208:THR:O	1:L:211:HIS:HB2	1.86	0.75
2:M:197:PHE:CZ	5:M:502:BCL:HBB2	2.22	0.75
5:M:502:BCL:HHC	5:M:502:BCL:CBB	2.19	0.72
2:M:270:ILE:HD13	9:M:800:CDL:H711	1.71	0.72
1:L:91:ILE:HG13	10:L:709:LDA:H91	1.71	0.72
2:M:21:THR:CG2	2:M:26:LEU:HD11	2.20	0.71
2:M:208:PHE:HE1	10:M:701:LDA:H91	1.55	0.70
2:M:152:SER:O	2:M:155:TRP:HB3	1.91	0.70
1:L:91:ILE:CG1	10:L:709:LDA:H91	2.22	0.70
2:M:21:THR:HG23	2:M:26:LEU:HD21	1.73	0.69
3:H:129:ASN:ND2	3:H:224:GLU:HG2	2.08	0.67
1:L:135:ARG:HB3	1:L:136:PRO:HD3	1.76	0.67
5:M:502:BCL:HHC	5:M:502:BCL:HBB3	1.77	0.67
3:H:171:ILE:HB	3:H:172:PRO:HD3	1.76	0.67
2:M:130:TRP:HD1	2:M:150:PHE:CD2	2.13	0.67
5:M:501:BCL:C11	5:M:502:BCL:H203	2.26	0.66
5:L:501:BCL:HBB2	5:L:501:BCL:HMB1	1.79	0.65
7:M:504:U10:H202	10:H:703:LDA:C11	2.27	0.64
1:L:208:THR:HB	1:L:209:PRO:HD2	1.80	0.64
1:L:38:THR:HG22	1:L:99:SER:HB3	1.79	0.63
1:L:216:PHE:CE2	7:L:504:U10:H4M2	2.34	0.63
1:L:22:PHE:HA	1:L:24:PHE:CE2	2.34	0.63
2:M:21:THR:HG23	2:M:26:LEU:HD11	1.80	0.63
2:M:13:ARG:O	3:H:140:PHE:HA	1.98	0.63
2:M:193:HIS:O	2:M:293:ASN:HA	1.98	0.63
5:M:501:BCL:H111	5:M:502:BCL:H203	1.81	0.62
2:M:134:TYR:CE2	2:M:144:LYS:HG2	2.36	0.61
1:L:69:PRO:HG2	1:L:142:TRP:HB2	1.83	0.61
5:L:501:BCL:H192	6:L:503:BPH:H7C2	1.83	0.60
3:H:241:LEU:O	3:H:248:ARG:NH2	2.34	0.60
3:H:37:ARG:HG2	3:H:37:ARG:HH11	1.67	0.60
5:M:501:BCL:HMB1	5:M:501:BCL:CBB	2.32	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:16:LEU:N	1:L:106:GLU:OE2	2.31	0.60
2:M:130:TRP:HD1	2:M:150:PHE:HD2	1.49	0.59
1:L:8:LYS:HA	3:H:87:LEU:CD1	2.33	0.59
1:L:244:SER:OG	5:L:502:BCL:HMA2	2.02	0.59
3:H:148:PRO:HA	3:H:151:LEU:HD12	1.84	0.59
2:M:194:GLY:O	2:M:195:ASN:HB3	2.03	0.58
3:H:196:VAL:HG12	3:H:205:VAL:HG22	1.85	0.58
2:M:208:PHE:CE1	10:M:701:LDA:H91	2.37	0.58
3:H:129:ASN:ND2	3:H:224:GLU:CG	2.66	0.58
1:L:8:LYS:HA	3:H:87:LEU:HD11	1.85	0.58
1:L:116:HIS:O	1:L:119:PHE:HB3	2.04	0.58
5:M:501:BCL:HMB1	5:M:501:BCL:HBB2	1.85	0.57
3:H:177:ARG:O	3:H:193:MET:HB2	2.03	0.57
1:L:173:HIS:CE1	1:L:177:ILE:HD11	2.40	0.57
1:L:180:PHE:CE2	1:L:240:ALA:HB1	2.39	0.56
1:L:264:GLN:HA	1:L:267:VAL:HG12	1.86	0.56
1:L:85:LEU:O	1:L:89:ILE:HG13	2.06	0.56
1:L:38:THR:HG22	1:L:99:SER:CB	2.35	0.56
2:M:21:THR:HG21	2:M:26:LEU:HD11	1.87	0.55
1:L:201:GLU:OE2	2:M:144:LYS:NZ	2.39	0.55
1:L:218:ASP:OD1	2:M:29:ARG:HD3	2.07	0.55
3:H:244:ALA:C	3:H:246:PRO:HD2	2.27	0.55
1:L:269:LEU:HB2	1:L:272:TRP:NE1	2.22	0.54
1:L:4:SER:OG	3:H:39:GLY:HA2	2.07	0.54
2:M:85:PHE:HD2	2:M:86:LEU:HD12	1.73	0.54
2:M:130:TRP:CD1	2:M:150:PHE:HD2	2.25	0.54
2:M:72:ILE:HG13	2:M:73:TRP:N	2.22	0.54
2:M:108:PRO:HG2	2:M:111:GLU:HB2	1.90	0.53
1:L:250:ILE:HD12	7:L:504:U10:H402	1.90	0.53
1:L:267:VAL:HG21	1:L:280:ASN:ND2	2.24	0.53
5:L:501:BCL:HMD1	2:M:206:ILE:HD13	1.91	0.53
5:L:502:BCL:H203	5:L:501:BCL:H102	1.91	0.52
10:M:701:LDA:H101	10:H:703:LDA:C12	2.39	0.52
3:H:20:PHE:HE2	3:H:24:LEU:HD22	1.74	0.52
1:L:234:LEU:O	1:L:238:LEU:HG	2.09	0.52
1:L:271:TRP:CD1	1:L:271:TRP:N	2.77	0.52
1:L:223:SER:O	2:M:44:ASN:HB2	2.10	0.52
1:L:142:TRP:CZ2	10:L:709:LDA:H51	2.44	0.52
2:M:20:MET:O	2:M:29:ARG:NH2	2.42	0.52
2:M:32:VAL:HG12	2:M:33:GLY:O	2.09	0.52
2:M:44:ASN:HB3	11:M:1048:HOH:O	2.10	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:M:25:ASN:OD1	2:M:27:ALA:HB3	2.10	0.52
3:H:184:LYS:HG3	3:H:184:LYS:O	2.10	0.52
2:M:187:ASN:HA	5:M:502:BCL:CBC	2.40	0.51
2:M:101:TYR:O	2:M:104:SER:HB2	2.10	0.51
6:L:503:BPH:ND	2:M:214:LEU:HD13	2.26	0.51
1:L:195:LEU:HB3	2:M:145:HIS:CD2	2.45	0.51
3:H:168:TRP:CZ3	3:H:225:VAL:HG22	2.44	0.51
3:H:226:THR:OG1	3:H:229:GLU:HG3	2.10	0.50
3:H:84:PRO:O	3:H:85:ILE:HD13	2.11	0.50
2:M:3:TYR:CZ	2:M:5:ASN:HA	2.47	0.50
1:L:213:ASP:O	1:L:217:ARG:HG3	2.11	0.50
2:M:175:VAL:HG11	8:M:600:SPN:H161	1.93	0.49
1:L:223:SER:OG	7:L:504:U10:H3M1	2.11	0.49
2:M:241:ARG:NH1	3:H:38:GLU:OE1	2.41	0.49
1:L:75:LEU:HD11	1:L:140:GLY:HA2	1.94	0.49
1:L:11:VAL:HB	1:L:12:PRO:HD2	1.94	0.49
3:H:129:ASN:HD22	3:H:224:GLU:HG2	1.75	0.49
1:L:135:ARG:HB3	1:L:136:PRO:CD	2.42	0.49
1:L:262:TRP:O	1:L:265:TRP:HD1	1.95	0.49
5:L:502:BCL:HAA2	5:L:501:BCL:HAC1	1.93	0.49
3:H:12:LEU:O	3:H:15:LEU:HB3	2.12	0.49
2:M:4:GLN:HA	2:M:4:GLN:HE21	1.78	0.49
1:L:168:HIS:HB3	2:M:183:LEU:HD13	1.95	0.49
2:M:88:ASP:HB2	2:M:92:PHE:CZ	2.48	0.48
1:L:207:ARG:NH1	2:M:140:LEU:O	2.38	0.48
2:M:97:PRO:HG2	2:M:171:TRP:HB2	1.95	0.48
3:H:84:PRO:C	3:H:85:ILE:HD13	2.34	0.48
2:M:101:TYR:O	2:M:104:SER:CB	2.62	0.48
5:L:502:BCL:CHC	5:L:502:BCL:OBB	2.55	0.48
1:L:104:GLU:HB3	1:L:118:PRO:HG3	1.96	0.48
3:H:20:PHE:CE2	3:H:24:LEU:HD22	2.48	0.47
1:L:87:GLN:NE2	1:L:142:TRP:CD1	2.82	0.47
2:M:164:ARG:HB3	2:M:165:PRO:HD3	1.95	0.47
1:L:168:HIS:CD2	5:M:501:BCL:CMD	2.98	0.47
10:M:701:LDA:H101	10:H:703:LDA:H121	1.97	0.47
2:M:130:TRP:CD1	2:M:150:PHE:CD2	3.00	0.47
1:L:49:ILE:HG12	1:L:89:ILE:HD13	1.97	0.46
1:L:279:ILE:HG21	2:M:91:PHE:HB3	1.97	0.46
3:H:170:ASP:HB2	3:H:177:ARG:HG3	1.97	0.46
1:L:102:LEU:O	1:L:105:VAL:HB	2.15	0.46
1:L:207:ARG:HG3	1:L:211:HIS:CG	2.51	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:34:PHE:HB2	11:L:1003:HOH:O	2.15	0.45
1:L:22:PHE:HA	1:L:24:PHE:HE2	1.80	0.45
2:M:16:ALA:HB1	2:M:32:VAL:HG11	1.98	0.45
1:L:177:ILE:HG23	5:L:502:BCL:HMB3	1.97	0.45
2:M:202:HIS:CE1	2:M:206:ILE:HD11	2.52	0.45
7:L:504:U10:H351	7:L:504:U10:H372	1.70	0.45
2:M:240:ASP:HB2	3:H:118:ARG:HH21	1.82	0.45
2:M:250:LEU:O	2:M:251:PHE:C	2.53	0.45
2:M:4:GLN:HA	2:M:4:GLN:NE2	2.31	0.45
2:M:268:TRP:CD1	7:M:504:U10:H111	2.52	0.45
2:M:201:PHE:HD1	2:M:279:THR:HG23	1.82	0.44
3:H:148:PRO:HD2	3:H:167:ILE:HD11	1.98	0.44
3:H:171:ILE:HB	3:H:172:PRO:CD	2.47	0.44
2:M:264:GLY:HA3	3:H:35:ASN:OD1	2.17	0.44
7:L:504:U10:H251	7:L:504:U10:H271	1.79	0.44
2:M:251:PHE:CD1	2:M:251:PHE:C	2.91	0.44
1:L:264:GLN:O	1:L:268:LYS:HB2	2.17	0.43
3:H:189:ARG:HD2	3:H:216:ILE:HB	1.99	0.43
5:L:502:BCL:HBB3	5:L:502:BCL:HMB1	2.00	0.43
2:M:25:ASN:OD1	2:M:25:ASN:C	2.57	0.43
2:M:236:GLU:HB3	11:H:1085:HOH:O	2.19	0.43
7:M:504:U10:H28	7:M:504:U10:H322	1.48	0.43
2:M:268:TRP:CE3	3:H:31:LEU:HD13	2.53	0.43
2:M:2:GLU:OE2	2:M:228:ARG:NH2	2.51	0.43
1:L:217:ARG:O	2:M:50:ILE:HA	2.18	0.43
5:M:502:BCL:HHC	5:M:502:BCL:HBB2	1.98	0.43
1:L:49:ILE:CG1	1:L:89:ILE:HD13	2.49	0.43
1:L:234:LEU:HD22	2:M:224:LEU:HD12	1.99	0.43
1:L:100:TRP:CH2	7:M:504:U10:H251	2.54	0.43
1:L:117:ILE:HB	1:L:118:PRO:HD3	2.00	0.43
3:H:37:ARG:HG2	3:H:37:ARG:NH1	2.32	0.43
1:L:265:TRP:CG	1:L:266:TRP:N	2.87	0.43
2:M:11:GLN:HB2	3:H:144:ALA:HB3	1.99	0.43
1:L:153:HIS:CE1	1:L:154:LEU:HD23	2.54	0.43
1:L:173:HIS:O	1:L:177:ILE:HG13	2.20	0.42
2:M:12:VAL:CG1	3:H:140:PHE:HD2	2.32	0.42
3:H:16:ALA:O	3:H:19:SER:HB2	2.20	0.42
2:M:129:TRP:CH2	2:M:132:ARG:NH1	2.88	0.42
1:L:85:LEU:HD23	1:L:85:LEU:HA	1.89	0.42
2:M:3:TYR:OH	2:M:5:ASN:HA	2.20	0.42
3:H:209:SER:OG	3:H:212:LEU:HD12	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:H:181:VAL:O	3:H:188:THR:HA	2.19	0.42
2:M:36:SER:OG	2:M:38:LEU:HB3	2.19	0.42
2:M:114:LEU:HD12	2:M:114:LEU:HA	1.84	0.42
2:M:300:ASN:O	2:M:301:HIS:HB2	2.20	0.42
1:L:167:PHE:HB3	5:L:502:BCL:HMC3	2.02	0.42
5:L:502:BCL:H141	5:L:502:BCL:H162	1.90	0.42
3:H:156:CYS:HB3	3:H:206:ASN:O	2.19	0.42
3:H:130:LYS:HD2	11:H:1118:HOH:O	2.19	0.42
1:L:168:HIS:NE2	5:M:501:BCL:HMD3	2.35	0.42
3:H:245:ALA:HB3	3:H:246:PRO:HD3	2.02	0.42
2:M:2:GLU:HG2	2:M:3:TYR:N	2.35	0.41
1:L:149:GLY:O	1:L:153:HIS:HB3	2.20	0.41
2:M:197:PHE:HA	2:M:197:PHE:HD1	1.72	0.41
1:L:97:PHE:CE1	5:L:502:BCL:H121	2.56	0.41
1:L:267:VAL:HG21	1:L:280:ASN:HD22	1.85	0.41
1:L:120:ALA:HB1	1:L:238:LEU:HD21	2.01	0.41
2:M:65:MET:HB3	2:M:121:PHE:CD2	2.56	0.41
2:M:265:ILE:HG12	7:M:504:U10:C2	2.51	0.41
2:M:134:TYR:CD2	2:M:144:LYS:HG2	2.55	0.41
3:H:247:LYS:O	3:H:249:LYS:NZ	2.53	0.41
3:H:103:ASP:HB3	3:H:106:LYS:HB2	2.02	0.41
2:M:271:TRP:O	2:M:275:LEU:HG	2.20	0.41
1:L:18:GLY:O	1:L:21:LEU:HB2	2.21	0.41
5:M:501:BCL:C4A	5:M:501:BCL:HBA1	2.50	0.41
5:L:501:BCL:H122	5:L:501:BCL:H161	1.80	0.41
3:H:148:PRO:O	3:H:151:LEU:HG	2.21	0.41
1:L:267:VAL:HG23	2:M:87:ARG:HG2	2.03	0.41
1:L:146:PHE:HA	1:L:147:PRO:HD3	1.93	0.41
1:L:206:MET:O	3:H:67:PRO:HG3	2.21	0.41
1:L:21:LEU:HD13	1:L:22:PHE:CE1	2.56	0.41
2:M:103:LEU:HD21	2:M:166:ILE:HA	2.03	0.41
5:M:502:BCL:H191	6:M:503:BPH:H8	2.03	0.40
2:M:270:ILE:O	2:M:274:VAL:HB	2.20	0.40
5:M:502:BCL:CBB	5:M:502:BCL:CHC	2.92	0.40
2:M:187:ASN:HA	5:M:502:BCL:HBC3	2.03	0.40
1:L:66:VAL:HG12	1:L:86:TRP:HB2	2.03	0.40
5:M:501:BCL:OBB	5:M:501:BCL:HHC	2.21	0.40
1:L:97:PHE:CZ	5:L:502:BCL:H121	2.57	0.40
1:L:91:ILE:HG12	10:L:709:LDA:H91	2.00	0.40
3:H:108:GLY:O	3:H:113:SER:HA	2.22	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	L	279/281 (99%)	265 (95%)	14 (5%)	0	100	100
2	M	300/314 (96%)	286 (95%)	11 (4%)	3 (1%)	19	61
3	H	238/260 (92%)	229 (96%)	9 (4%)	0	100	100
All	All	817/855 (96%)	780 (96%)	34 (4%)	3 (0%)	39	80

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	M	301	HIS
2	M	22	GLU
2	M	34	PRO

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	L	220/220 (100%)	208 (94%)	12 (6%)	27	65
2	M	236/247 (96%)	227 (96%)	9 (4%)	40	78
3	H	195/208 (94%)	184 (94%)	11 (6%)	26	65
All	All	651/675 (96%)	619 (95%)	32 (5%)	31	71

All (32) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	L	21	LEU
1	L	38	THR
1	L	126	LEU
1	L	153	HIS
1	L	154	LEU
1	L	207	ARG
1	L	210	ASP
1	L	216	PHE
1	L	247	CYS
1	L	251	THR
1	L	271	TRP
1	L	272	TRP
2	M	44	ASN
2	M	136	ARG
2	M	144	LYS
2	M	152	SER
2	M	196	LEU
2	M	204	LEU
2	M	216	PHE
2	M	265	ILE
2	M	292	ASP
3	H	12	LEU
3	H	52	ASN
3	H	135	LYS
3	H	184	LYS
3	H	193	MET
3	H	220	LYS
3	H	221	SER
3	H	222	PRO
3	H	225	VAL
3	H	231	ASP
3	H	249	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
1	L	280	ASN
2	M	4	GLN
2	M	188	ASN
3	H	129	ASN

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 15 ligands modelled in this entry, 1 is monoatomic - leaving 14 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	$\#\|Z\| > 2$
10	LDA	H	703	-	15,15,15	4.78	4 (26%)	16,17,17	0.83	0
5	BCL	L	501	1	53,74,74	1.20	4 (7%)	57,115,115	2.29	11 (19%)
5	BCL	L	502	1	53,74,74	1.36	7 (13%)	57,115,115	2.17	10 (17%)
6	BPH	L	503	-	64,70,70	1.31	9 (14%)	73,101,101	2.00	16 (21%)
7	U10	L	504	-	48,48,63	2.24	21 (43%)	58,61,79	1.05	4 (6%)
10	LDA	L	709	-	15,15,15	4.60	2 (13%)	16,17,17	0.58	0
5	BCL	M	501	2	53,74,74	1.29	7 (13%)	57,115,115	2.35	16 (28%)
5	BCL	M	502	2	53,74,74	0.96	3 (5%)	57,115,115	1.78	8 (14%)
6	BPH	M	503	-	64,70,70	1.32	7 (10%)	73,101,101	2.30	24 (32%)
7	U10	M	504	-	48,48,63	2.63	21 (43%)	58,61,79	1.39	10 (17%)
8	SPN	M	600	-	41,42,42	4.31	20 (48%)	41,52,52	3.02	18 (43%)
10	LDA	M	701	-	15,15,15	4.87	2 (13%)	16,17,17	0.51	0
10	LDA	M	704	-	15,15,15	3.75	1 (6%)	16,17,17	0.60	0
9	CDL	M	800	-	80,80,99	0.50	0	82,92,111	0.94	4 (4%)

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
10	LDA	H	703	-	-	0/13/13/13	0/0/0/0
5	BCL	L	501	1	1/1/21/25	0/37/137/137	0/0/9/9
5	BCL	L	502	1	-	0/37/137/137	0/0/9/9
6	BPH	L	503	-	-	0/54/105/105	0/1/6/6
7	U10	L	504	-	-	0/45/69/87	0/1/1/1
10	LDA	L	709	-	-	0/13/13/13	0/0/0/0
5	BCL	M	501	2	2/2/21/25	1/37/137/137	0/0/9/9
5	BCL	M	502	2	-	0/37/137/137	0/0/9/9
6	BPH	M	503	-	1/1/18/22	0/54/105/105	0/1/6/6
7	U10	M	504	-	-	0/45/69/87	0/1/1/1
8	SPN	M	600	-	-	0/50/51/51	0/0/0/0
10	LDA	M	701	-	-	0/13/13/13	0/0/0/0
10	LDA	M	704	-	-	0/13/13/13	0/0/0/0
9	CDL	M	800	-	-	0/91/91/110	0/0/0/0

All (108) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
10	M	701	LDA	O1-N1	-18.64	1.21	1.39
10	H	703	LDA	O1-N1	-17.69	1.22	1.39
10	L	709	LDA	O1-N1	-17.56	1.22	1.39
10	M	704	LDA	O1-N1	-14.44	1.25	1.39
7	M	504	U10	C27-C28	-8.54	1.26	1.50
8	M	600	SPN	C3-C4	-6.15	1.41	1.50
8	M	600	SPN	C17-C18	-5.51	1.39	1.51
8	M	600	SPN	C10-C9	-5.40	1.39	1.51
8	M	600	SPN	C14-C13	-5.05	1.40	1.51
5	L	502	BCL	O2D-CED	-4.89	1.33	1.45
8	M	600	SPN	C6-C5	-4.86	1.40	1.51
7	M	504	U10	C17-C18	-4.46	1.38	1.50
8	M	600	SPN	C20-C19	-4.08	1.39	1.50
7	M	504	U10	C37-C38	-3.82	1.39	1.50
5	L	502	BCL	C1-C2	-3.82	1.36	1.49
7	M	504	U10	C22-C23	-3.79	1.39	1.50
7	L	504	U10	C17-C18	-3.62	1.40	1.50
10	H	703	LDA	CM1-N1	-3.61	1.43	1.49
8	M	600	SPN	C11-C12	-3.59	1.40	1.50
8	M	600	SPN	C7-C8	-3.59	1.40	1.50
10	H	703	LDA	C1-N1	-3.25	1.45	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	L	504	U10	O4-C4M	-2.86	1.38	1.45
6	M	503	BPH	O2D-CED	-2.78	1.38	1.45
8	M	600	SPN	C21-C22	-2.62	1.39	1.52
5	L	501	BCL	CMB-C2B	-2.59	1.46	1.51
7	M	504	U10	O4-C4M	-2.42	1.39	1.45
10	H	703	LDA	CM2-N1	-2.36	1.45	1.49
6	L	503	BPH	O2D-CED	-2.35	1.39	1.45
7	L	504	U10	C7-C8	-2.33	1.47	1.50
5	M	502	BCL	O2D-CED	-2.27	1.39	1.45
7	M	504	U10	O3-C3M	-2.24	1.39	1.45
6	M	503	BPH	C2C-C3C	-2.22	1.47	1.54
5	M	501	BCL	C2C-C3C	-2.20	1.48	1.54
7	M	504	U10	C7-C8	-2.15	1.47	1.50
10	L	709	LDA	CM2-N1	-2.14	1.46	1.49
8	M	600	SPN	C16-C15	-2.13	1.39	1.51
10	M	701	LDA	CM2-N1	-2.12	1.46	1.49
5	L	502	BCL	CMC-C2C	-2.05	1.48	1.53
6	L	503	BPH	C4-C3	2.02	1.55	1.50
6	M	503	BPH	CAA-C2A	2.03	1.58	1.54
8	M	600	SPN	CM3-C5	2.03	1.55	1.50
5	L	502	BCL	O2D-CGD	2.04	1.38	1.33
7	L	504	U10	C25-C24	2.06	1.55	1.50
5	M	501	BCL	C4-C3	2.06	1.55	1.50
8	M	600	SPN	O1-C1	2.07	1.52	1.41
7	L	504	U10	C16-C14	2.08	1.56	1.51
5	M	502	BCL	O2A-CGA	2.08	1.39	1.33
6	L	503	BPH	C3D-C4D	2.14	1.44	1.41
7	M	504	U10	C28-C29	2.21	1.37	1.33
7	M	504	U10	O2-C2	2.23	1.28	1.23
5	M	501	BCL	CMA-C3A	2.25	1.58	1.53
7	L	504	U10	C35-C34	2.27	1.56	1.50
6	L	503	BPH	C4A-NA	2.29	1.40	1.34
5	L	502	BCL	C2-C3	2.31	1.37	1.33
6	L	503	BPH	CAA-C2A	2.34	1.58	1.54
7	L	504	U10	C15-C14	2.36	1.56	1.50
5	L	502	BCL	C4-C3	2.36	1.56	1.50
6	L	503	BPH	O1D-CGD	2.38	1.27	1.21
7	L	504	U10	C10-C9	2.43	1.56	1.50
5	L	501	BCL	O2A-CGA	2.43	1.40	1.33
6	M	503	BPH	C15-C13	2.45	1.65	1.52
5	M	501	BCL	CAA-C2A	2.45	1.59	1.54
7	M	504	U10	C15-C14	2.49	1.56	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	M	504	U10	C38-C39	2.56	1.40	1.32
7	L	504	U10	C21-C19	2.57	1.57	1.51
7	M	504	U10	C30-C29	2.59	1.57	1.50
7	L	504	U10	C31-C29	2.73	1.57	1.51
7	L	504	U10	C38-C39	2.77	1.40	1.32
5	M	501	BCL	C2-C3	2.85	1.38	1.33
8	M	600	SPN	C29-C30	2.89	1.41	1.32
6	M	503	BPH	C2-C3	2.90	1.38	1.33
8	M	600	SPN	O1-CMA	2.93	1.52	1.43
7	L	504	U10	C18-C19	2.93	1.38	1.33
7	M	504	U10	C18-C19	2.93	1.38	1.33
7	L	504	U10	C36-C34	2.96	1.58	1.51
7	M	504	U10	C13-C14	3.01	1.38	1.33
6	L	503	BPH	C2-C3	3.12	1.39	1.33
5	L	501	BCL	C2-C3	3.21	1.39	1.33
7	M	504	U10	C36-C34	3.21	1.58	1.51
5	M	502	BCL	C2-C3	3.31	1.39	1.33
7	M	504	U10	O4-C4	3.31	1.45	1.37
6	L	503	BPH	O2A-CGA	3.35	1.43	1.33
7	M	504	U10	C35-C34	3.39	1.58	1.50
7	M	504	U10	C23-C24	3.44	1.39	1.33
7	M	504	U10	C8-C9	3.48	1.39	1.33
7	L	504	U10	C7-C6	3.55	1.57	1.51
7	L	504	U10	C8-C9	3.62	1.40	1.33
5	M	501	BCL	O2A-CGA	3.63	1.44	1.33
7	L	504	U10	C13-C14	3.64	1.40	1.33
7	L	504	U10	O4-C4	3.64	1.46	1.37
6	M	503	BPH	O2D-CGD	3.67	1.42	1.33
6	L	503	BPH	O2D-CGD	3.70	1.42	1.33
6	M	503	BPH	O2A-CGA	3.75	1.44	1.33
7	M	504	U10	C33-C34	3.87	1.40	1.33
7	L	504	U10	C23-C24	3.87	1.40	1.33
5	L	502	BCL	O2A-CGA	4.04	1.45	1.33
8	M	600	SPN	C25-C26	4.11	1.41	1.33
7	L	504	U10	O3-C3	4.12	1.47	1.37
7	L	504	U10	C28-C29	4.14	1.41	1.33
7	L	504	U10	C33-C34	4.18	1.41	1.33
5	L	501	BCL	O2D-CGD	4.40	1.44	1.33
5	M	501	BCL	O2D-CGD	4.57	1.44	1.33
7	M	504	U10	O3-C3	6.72	1.54	1.37
8	M	600	SPN	C3-C2	7.36	1.60	1.52
8	M	600	SPN	C12-C13	9.99	1.52	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	M	600	SPN	C8-C9	10.30	1.53	1.33
8	M	600	SPN	C19-C18	10.74	1.54	1.33
8	M	600	SPN	C4-C5	10.87	1.54	1.33

All (121) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	L	501	BCL	O1D-CGD-CBD	-7.95	113.23	124.62
5	M	501	BCL	C4-C3-C5	-6.63	105.28	115.41
5	M	502	BCL	O1D-CGD-CBD	-5.48	116.77	124.62
8	M	600	SPN	C6-C5-C4	-5.46	110.70	121.05
8	M	600	SPN	C17-C18-C19	-5.18	111.23	121.05
6	L	503	BPH	O2A-CGA-O1A	-4.95	110.71	123.49
6	M	503	BPH	O1D-CGD-CBD	-4.69	117.91	124.62
5	M	501	BCL	OBD-CAD-CBD	-4.51	119.14	125.94
5	M	501	BCL	O2A-CGA-O1A	-4.51	111.86	123.49
8	M	600	SPN	C3-C4-C5	-4.49	119.09	126.70
8	M	600	SPN	C20-C19-C18	-4.46	118.07	127.76
6	L	503	BPH	O2D-CGD-O1D	-4.28	114.95	123.79
8	M	600	SPN	C7-C8-C9	-4.27	118.49	127.76
8	M	600	SPN	C11-C12-C13	-4.21	118.61	127.76
5	L	502	BCL	O1D-CGD-CBD	-4.19	118.62	124.62
5	L	501	BCL	OBB-CAB-CBB	-4.11	110.28	120.13
8	M	600	SPN	C10-C9-C8	-4.11	113.26	121.05
7	M	504	U10	C26-C27-C28	-3.99	101.24	111.69
8	M	600	SPN	C14-C13-C12	-3.90	113.66	121.05
5	M	501	BCL	CAA-C2A-C3A	-3.90	102.01	113.22
5	L	502	BCL	OBB-CAB-CBB	-3.84	110.92	120.13
6	M	503	BPH	O2D-CGD-O1D	-3.78	115.98	123.79
6	L	503	BPH	OBD-CAD-CBD	-3.55	120.58	125.94
6	L	503	BPH	O1D-CGD-CBD	-3.41	119.74	124.62
5	M	501	BCL	CMB-C2B-C1B	-3.28	122.94	128.36
6	M	503	BPH	CAA-C2A-C3A	-3.23	103.93	113.22
5	M	501	BCL	O1D-CGD-CBD	-3.08	120.20	124.62
6	L	503	BPH	CAA-C2A-C3A	-3.04	104.48	113.22
5	L	502	BCL	CBB-CAB-C3B	-3.03	111.34	120.33
5	L	502	BCL	OBD-CAD-CBD	-3.01	121.39	125.94
5	M	501	BCL	OBB-CAB-CBB	-3.01	112.91	120.13
5	M	501	BCL	O2D-CGD-O1D	-3.01	117.57	123.79
6	M	503	BPH	C11-C12-C13	-2.85	106.03	115.49
6	L	503	BPH	C4-C3-C5	-2.84	111.07	115.41
6	M	503	BPH	O2A-CGA-O1A	-2.81	116.25	123.49

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
6	L	503	BPH	CMA-C3A-C4A	-2.78	103.94	113.01
9	M	800	CDL	CB6-CB4-CB3	-2.76	105.62	112.07
5	L	501	BCL	CMB-C2B-C1B	-2.74	123.83	128.36
7	M	504	U10	C25-C24-C26	-2.74	111.22	115.41
6	M	503	BPH	CBB-CAB-C3B	-2.69	114.53	120.52
5	M	501	BCL	CMA-C3A-C2A	-2.67	102.53	114.35
5	M	502	BCL	OBD-CAD-CBD	-2.66	121.92	125.94
6	L	503	BPH	C3A-C4A-NA	-2.65	108.93	113.57
6	M	503	BPH	C5-C3-C2	-2.58	116.15	121.05
6	L	503	BPH	CAA-C2A-C1A	-2.54	106.17	112.86
6	M	503	BPH	CAA-C2A-C1A	-2.52	106.23	112.86
5	L	502	BCL	CMB-C2B-C1B	-2.44	124.33	128.36
5	L	501	BCL	O2A-CGA-O1A	-2.41	117.27	123.49
5	L	501	BCL	CAC-C3C-C4C	-2.38	107.31	112.58
7	M	504	U10	C20-C19-C21	-2.21	112.03	115.41
9	M	800	CDL	CA6-CA4-CA3	-2.21	106.91	112.07
6	M	503	BPH	OBD-CAD-CBD	-2.19	122.64	125.94
7	M	504	U10	C31-C29-C28	-2.15	116.98	121.05
6	M	503	BPH	C3A-C4A-NA	-2.14	109.82	113.57
6	M	503	BPH	C2A-C1A-NA	-2.14	109.34	112.08
9	M	800	CDL	OA8-CA7-OA9	-2.14	117.97	123.49
6	M	503	BPH	CMA-C3A-C4A	-2.14	106.05	113.01
5	M	502	BCL	CMB-C2B-C1B	-2.07	124.94	128.36
5	L	501	BCL	OBD-CAD-CBD	-2.06	122.83	125.94
7	M	504	U10	C10-C9-C11	-2.04	112.30	115.41
7	L	504	U10	C30-C29-C31	-2.02	112.32	115.41
8	M	600	SPN	CM5-C13-C12	-2.01	119.55	123.50
7	M	504	U10	C25-C24-C23	2.01	127.44	123.50
6	L	503	BPH	C2A-C3A-C4A	2.05	105.80	101.10
8	M	600	SPN	C11-C10-C9	2.06	119.43	112.71
6	L	503	BPH	C3A-C4A-CHB	2.07	125.68	121.84
7	M	504	U10	C22-C23-C24	2.07	132.27	127.76
6	M	503	BPH	CMD-C2D-C3D	2.10	129.19	125.09
7	L	504	U10	C4M-O4-C4	2.12	124.14	116.61
7	M	504	U10	C3M-O3-C3	2.15	124.26	116.61
6	M	503	BPH	C4-C3-C5	2.17	118.72	115.41
7	L	504	U10	C3M-O3-C3	2.18	124.35	116.61
8	M	600	SPN	C15-C16-C17	2.18	121.29	113.29
5	L	502	BCL	CED-O2D-CGD	2.22	121.20	115.99
6	M	503	BPH	C11-C10-C8	2.23	122.89	115.49
6	M	503	BPH	C14-C13-C12	2.25	119.74	111.08
5	M	501	BCL	C6-C5-C3	2.27	117.47	112.48

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	M	501	BCL	CMD-C2D-C3D	2.29	129.57	125.09
8	M	600	SPN	C7-C6-C5	2.30	120.20	112.71
6	M	503	BPH	C2C-C3C-C4C	2.40	105.57	101.50
7	M	504	U10	C7-C8-C9	2.44	130.83	126.70
5	L	501	BCL	CMD-C2D-C3D	2.50	129.98	125.09
6	L	503	BPH	CED-O2D-CGD	2.53	121.92	115.99
5	M	501	BCL	C2C-C3C-C4C	2.55	105.83	101.50
6	L	503	BPH	C4A-NA-C1A	2.59	110.53	108.21
8	M	600	SPN	CM3-C5-C6	2.64	119.44	115.41
6	L	503	BPH	CAC-C3C-C2C	2.75	121.04	114.13
7	L	504	U10	C7-C8-C9	2.78	131.40	126.70
5	M	502	BCL	CED-O2D-CGD	2.80	122.56	115.99
6	M	503	BPH	C17-C16-C15	2.87	127.22	112.99
5	L	501	BCL	O2A-CGA-CBA	2.89	120.72	111.90
5	M	502	BCL	C4A-NA-C1A	2.99	110.22	106.36
9	M	800	CDL	OB8-CB6-CB4	3.00	116.77	108.69
5	L	502	BCL	C4A-NA-C1A	3.14	110.42	106.36
5	L	501	BCL	C4A-NA-C1A	3.23	110.54	106.36
5	L	502	BCL	O2A-CGA-CBA	3.26	121.85	111.90
6	M	503	BPH	CBC-CAC-C3C	3.34	121.72	113.57
5	M	502	BCL	O2A-CGA-CBA	3.51	122.59	111.90
6	L	503	BPH	O2A-CGA-CBA	3.54	122.67	111.90
6	M	503	BPH	CED-O2D-CGD	3.62	124.48	115.99
7	M	504	U10	C27-C28-C29	3.80	136.03	127.76
5	M	502	BCL	OBB-CAB-C3B	3.92	126.20	120.00
8	M	600	SPN	CM7-C22-C21	4.06	126.67	111.08
8	M	600	SPN	C16-C17-C18	4.12	121.52	112.48
6	M	503	BPH	C4A-NA-C1A	4.12	111.89	108.21
8	M	600	SPN	CM4-C9-C10	4.17	121.77	115.41
5	M	501	BCL	C5-C3-C2	4.21	129.03	121.05
6	M	503	BPH	C6-C5-C3	4.23	121.76	112.48
6	M	503	BPH	C16-C15-C13	4.38	130.00	115.49
5	M	501	BCL	O2A-CGA-CBA	4.77	126.43	111.90
5	L	501	BCL	OBB-CAB-C3B	5.88	129.32	120.00
5	M	501	BCL	O2D-CGD-CBD	5.91	119.41	111.30
5	L	502	BCL	O2D-CGD-CBD	6.38	120.06	111.30
5	M	501	BCL	OBB-CAB-C3B	6.57	130.41	120.00
8	M	600	SPN	CM5-C13-C14	6.99	126.08	115.41
5	M	502	BCL	O2D-CGD-CBD	7.35	121.39	111.30
8	M	600	SPN	CM6-C18-C17	7.63	127.06	115.41
6	L	503	BPH	O2D-CGD-CBD	10.18	125.26	111.30
5	L	501	BCL	O2D-CGD-CBD	10.24	125.35	111.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	L	502	BCL	OBB-CAB-C3B	10.47	136.58	120.00
6	M	503	BPH	O2D-CGD-CBD	10.77	126.08	111.30

All (4) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
5	L	501	BCL	C13
6	M	503	BPH	C8
5	M	501	BCL	C8
5	M	501	BCL	C13

All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	M	501	BCL	C1-C2-C3-C4

There are no ring outliers.

13 monomers are involved in 55 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
10	H	703	LDA	4	0
5	L	501	BCL	6	0
5	L	502	BCL	11	0
6	L	503	BPH	2	0
7	L	504	U10	6	0
10	L	709	LDA	4	0
5	M	501	BCL	8	0
5	M	502	BCL	11	0
6	M	503	BPH	1	0
7	M	504	U10	6	0
8	M	600	SPN	1	0
10	M	701	LDA	4	0
9	M	800	CDL	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

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
1	L	281/281 (100%)	-0.77	1 (0%)	93	80	25, 36, 70, 88	0
2	M	302/314 (96%)	-0.70	2 (0%)	89	70	20, 42, 79, 95	0
3	H	240/260 (92%)	-0.56	5 (2%)	67	36	27, 40, 62, 102	0
All	All	823/855 (96%)	-0.68	8 (0%)	84	60	20, 39, 72, 102	0

All (8) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	H	250	SER	6.0
3	H	249	LYS	4.3
1	L	281	GLY	2.8
3	H	246	PRO	2.8
2	M	82	PRO	2.5
3	H	247	LYS	2.3
2	M	1	ALA	2.2
3	H	245	ALA	2.2

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

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

6.3 Carbohydrates

There are no carbohydrates in this entry.

6.4 Ligands

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron

density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
7	U10	L	504	48/63	0.68	0.58	18.12	85,90,93,94	0
9	CDL	M	800	81/100	0.86	0.50	5.63	41,64,78,79	81
10	LDA	L	709	16/16	0.73	0.52	4.60	92,96,99,99	0
5	BCL	M	501	66/66	0.95	0.20	3.21	24,34,99,100	0
10	LDA	H	703	16/16	0.88	0.25	2.74	62,63,68,68	0
8	SPN	M	600	43/43	0.86	0.26	2.54	42,55,71,74	0
7	U10	M	504	48/63	0.94	0.18	2.09	29,36,67,68	0
10	LDA	M	701	16/16	0.90	0.20	1.88	50,59,67,67	0
6	BPH	L	503	65/65	0.97	0.16	1.75	19,30,42,44	0
5	BCL	M	502	66/66	0.97	0.17	1.44	24,30,58,65	0
6	BPH	M	503	65/65	0.96	0.15	0.56	31,42,61,66	10
5	BCL	L	502	66/66	0.98	0.14	0.36	22,26,47,50	0
5	BCL	L	501	66/66	0.97	0.15	0.22	19,25,50,52	0
4	FE	M	500	1/1	0.99	0.05	-2.04	28,28,28,28	0
10	LDA	M	704	16/16	0.62	0.34	-	75,89,107,108	0

6.5 Other polymers (i)

There are no such residues in this entry.