



Full wwPDB X-ray Structure Validation Report

Oct 21, 2014 – 06:14 PM EDT

PDB ID : 2A06
Title : Bovine cytochrome bc1 complex with stigmatellin bound
Authors : Huang, L.S.; Cobessi, D.; Tung, E.Y.; Berry, E.A.
Deposited on : 2005-06-16
Resolution : 2.10 Å(reported)

This is a full wwPDB 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/ValidationPDFNotes.html>

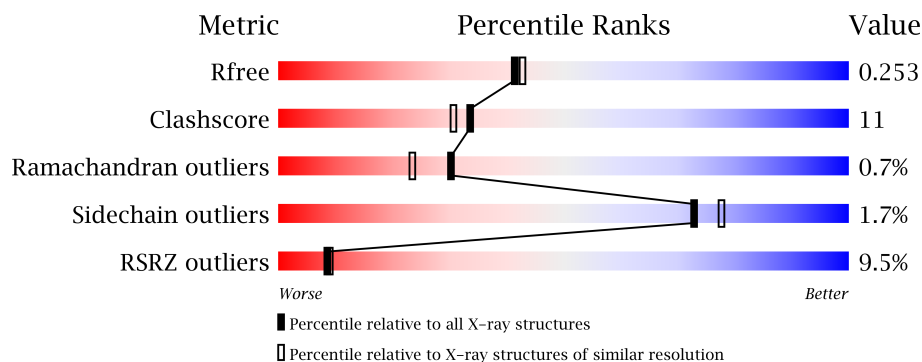
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.16 November 2013
Xtriage (Phenix) : dev-1439
EDS : stable24103
Percentile statistics : 21963
Refmac : 5.8.0049
CCP4 : 6.3.0 (Settle)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP) : stable24103

1 Overall quality at a glance

The reported resolution of this entry is 2.10 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	66092	3012 (2.10-2.10)
Clashscore	79885	3649 (2.10-2.10)
Ramachandran outliers	78287	3610 (2.10-2.10)
Sidechain outliers	78261	3611 (2.10-2.10)
RSRZ outliers	66119	3013 (2.10-2.10)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Mol	Chain	Length	Quality of chain
1	A	446	
1	N	446	
2	B	439	
2	O	439	
3	C	379	
3	P	379	
4	D	241	
4	Q	241	
5	E	196	
5	R	196	
6	F	110	
6	S	110	
7	G	81	
7	T	81	

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
8	H	78	
8	U	78	
9	I	78	
9	V	78	
10	J	62	
10	W	62	

The following table lists non-polymeric compounds that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Geometry	Electron density
11	BHG	C	2011	-	X
11	BHG	F	3012	-	X
11	BHG	F	4003	-	X
11	BHG	P	3011	-	X
11	BHG	S	2012	-	X
12	AZI	A	4002	-	X
12	AZI	C	2005	-	X
12	AZI	G	4001	-	X
12	AZI	P	3005	-	X
13	PO4	A	2010	-	X
13	PO4	B	3009	-	X
13	PO4	D	4011	-	X
13	PO4	R	4013	-	X
13	PO4	R	4014	-	X
20	PEE	B	4017	-	X
20	PEE	C	2007	-	X
20	PEE	D	2006	-	X
20	PEE	Q	3006	-	X
21	UNL	A	4032	-	X
21	UNL	A	4035	-	X
21	UNL	A	4038	-	X
21	UNL	A	4048	-	X
21	UNL	A	4075	-	X
21	UNL	A	4076	-	X
21	UNL	A	4087	-	X
21	UNL	A	4091	-	X
21	UNL	B	4025	-	X
21	UNL	B	4026	-	X
21	UNL	B	4030	-	X
21	UNL	B	4034	-	X
21	UNL	B	4039	-	X

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Geometry	Electron density
21	UNL	B	4051	-	X
21	UNL	B	4057	-	X
21	UNL	B	4079	-	X
21	UNL	B	4080	-	X
21	UNL	C	4018	-	X
21	UNL	C	4023	-	X
21	UNL	C	4045	-	X
21	UNL	C	4063	-	X
21	UNL	C	4068	-	X
21	UNL	C	4086	-	X
21	UNL	D	4027	-	X
21	UNL	D	4036	-	X
21	UNL	D	4054	-	X
21	UNL	D	4067	-	X
21	UNL	D	4083	-	X
21	UNL	E	4050	-	X
21	UNL	F	4028	-	X
21	UNL	G	4053	-	X
21	UNL	G	4064	-	X
21	UNL	I	4033	-	X
21	UNL	I	4072	-	X
21	UNL	N	4019	-	X
21	UNL	N	4022	-	X
21	UNL	N	4029	-	X
21	UNL	O	4031	-	X
21	UNL	O	4037	-	X
21	UNL	O	4041	-	X
21	UNL	O	4071	-	X
21	UNL	O	4084	-	X
21	UNL	P	4021	-	X
21	UNL	P	4040	-	X
21	UNL	P	4046	-	X
21	UNL	P	4058	-	X
21	UNL	P	4060	-	X
21	UNL	P	4074	-	X
21	UNL	P	4089	-	X
21	UNL	Q	4044	-	X
21	UNL	R	4069	-	X
21	UNL	T	4065	-	X
21	UNL	U	4049	-	X
21	UNL	U	4056	-	X
21	UNL	V	4078	-	X

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Geometry	Electron density
21	UNL	V	4090	-	X
22	GOL	C	2008	-	X
22	GOL	E	4006	-	X
22	GOL	E	4007	-	X
22	GOL	O	4005	-	X
22	GOL	P	3008	-	X
22	GOL	P	4009	-	X

2 Entry composition

There are 23 unique types of molecules in this entry. The entry contains 33890 atoms, of which 0 are hydrogen and 0 are deuterium.

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 Ubiquinol-cytochrome-c reductase complex core protein I, mitochondrial.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	443	Total	C	N	O	S	10	0	1
			3398	2118	602	658	20			
1	N	443	Total	C	N	O	S	10	0	1
			3398	2118	602	658	20			

- Molecule 2 is a protein called Ubiquinol-cytochrome-c reductase complex core protein 2, mitochondrial.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	424	Total	C	N	O	S	0	0	1
			3177	1996	562	612	7			
2	O	424	Total	C	N	O	S	0	0	0
			3180	1998	562	613	7			

- Molecule 3 is a protein called Cytochrome b, heme protein, mitochondrial.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	365	Total	C	N	O	S	0	0	0
			2897	1945	450	485	17			
3	P	370	Total	C	N	O	S	0	0	0
			2936	1973	455	490	18			

- Molecule 4 is a protein called Cytochrome c1, heme protein, mitochondrial.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	D	241	Total	C	N	O	S	0	0	0
			1919	1225	330	349	15			
4	Q	241	Total	C	N	O	S	0	0	0
			1919	1225	330	349	15			

- Molecule 5 is a protein called Ubiquinol-cytochrome c reductase iron-sulfur subunit, mitochondrial.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	E	196	Total	C	N	O	S	0	0	0
			1519	957	263	291	8			
5	R	196	Total	C	N	O	S	0	0	0
			1517	955	263	291	8			

- Molecule 6 is a protein called Ubiquinol-cytochrome c reductase complex 14 kDa protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	F	99	Total	C	N	O	S	0	0	0
			861	545	155	159	2			
6	S	99	Total	C	N	O	S	0	0	0
			861	545	155	159	2			

- Molecule 7 is a protein called Ubiquinol-cytochrome c reductase complex ubiquinone-binding protein QP-C.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
7	G	75	Total	C	N	O	S	0	0	2
			621	406	117	97	1			
7	T	76	Total	C	N	O	S	0	0	2
			626	409	118	98	1			

- Molecule 8 is a protein called Ubiquinol-cytochrome c reductase complex 11 kDa protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
8	H	66	Total	C	N	O	S	0	0	0
			539	327	98	109	5			
8	U	66	Total	C	N	O	S	0	0	0
			539	327	98	109	5			

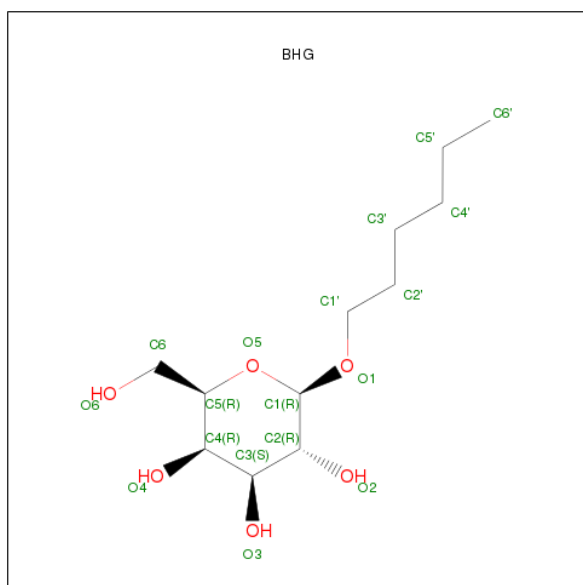
- Molecule 9 is a protein called Ubiquinol-cytochrome c reductase iron-sulfur subunit, mitochondrial.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
9	I	42	Total	C	N	O	S	0	0	0
			285	174	55	55	1			
9	V	42	Total	C	N	O	S	0	0	0
			285	174	55	55	1			

- Molecule 10 is a protein called Ubiquinol-cytochrome c reductase complex 7.2 kDa protein.

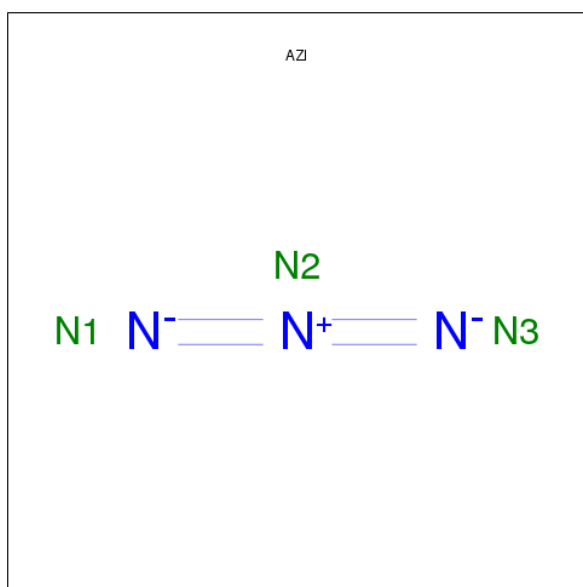
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
10	J	30	Total	C	N	O	0	0	1
			245	158	43	44			
10	W	62	Total	C	N	O	0	0	0
			507	333	88	86			

- Molecule 11 is SUGAR (2-HEXYLOXY-6-HYDROXYMETHYL-TETRAHYDRO-PYRAN-3,4,5-TRIOL) (three-letter code: BHG) (formula: C₁₂H₂₄O₆).



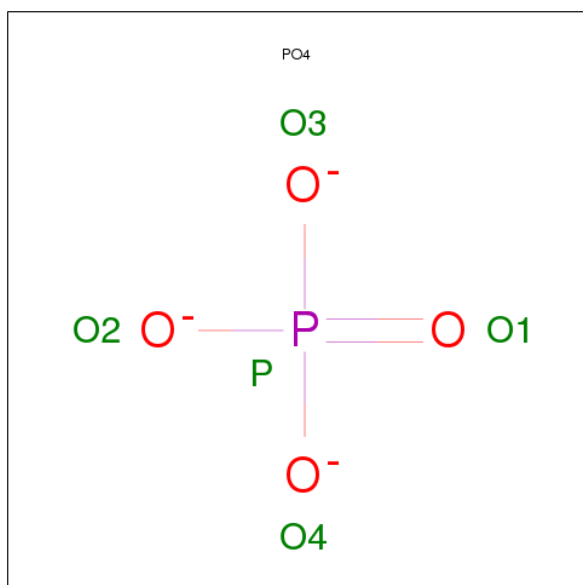
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
11	C	1	Total	C	O	0	0
			18	12	6		
11	S	1	Total	C	O	0	0
			18	12	6		
11	P	1	Total	C	O	0	0
			18	12	6		
11	F	1	Total	C	O	0	0
			18	12	6		
11	F	1	Total	C	O	0	0
			18	12	6		
11	A	1	Total	C	O	0	0
			18	12	6		

- Molecule 12 is AZIDE ION (three-letter code: AZI) (formula: N₃).



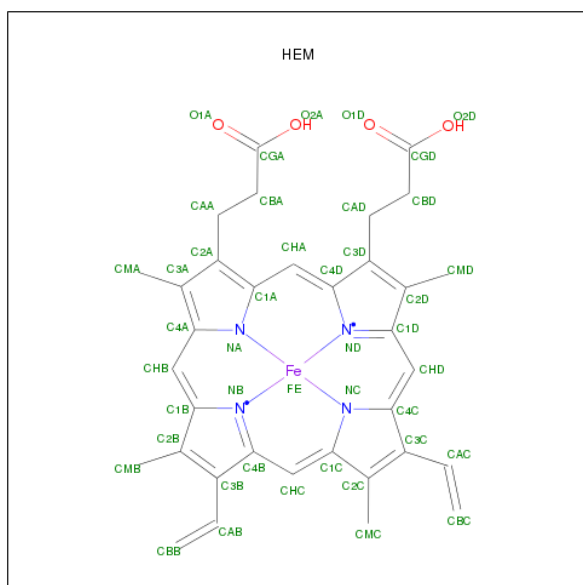
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
12	C	1	Total N 3 3	0	0
12	P	1	Total N 3 3	0	0
12	G	1	Total N 3 3	0	0
12	A	1	Total N 3 3	0	0

- Molecule 13 is PHOSPHATE ION (three-letter code: PO4) (formula: O₄P).



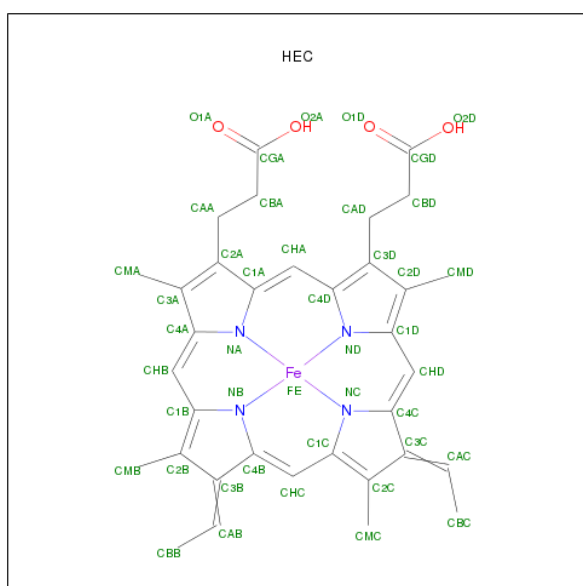
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
13	O	1	Total O P 5 4 1	0	0
13	A	1	Total O P 5 4 1	0	0
13	B	1	Total O P 5 4 1	0	0
13	P	1	Total O P 5 4 1	0	0
13	D	1	Total O P 5 4 1	0	0
13	D	1	Total O P 5 4 1	0	0
13	Q	1	Total O P 5 4 1	0	0
13	R	1	Total O P 5 4 1	0	0
13	R	1	Total O P 5 4 1	0	0
13	I	1	Total O P 5 4 1	0	0
13	T	1	Total O P 5 4 1	0	0

- Molecule 14 is PROTOPORPHYRIN IX CONTAINING FE (three-letter code: HEM) (formula: $C_{34}H_{32}FeN_4O_4$).



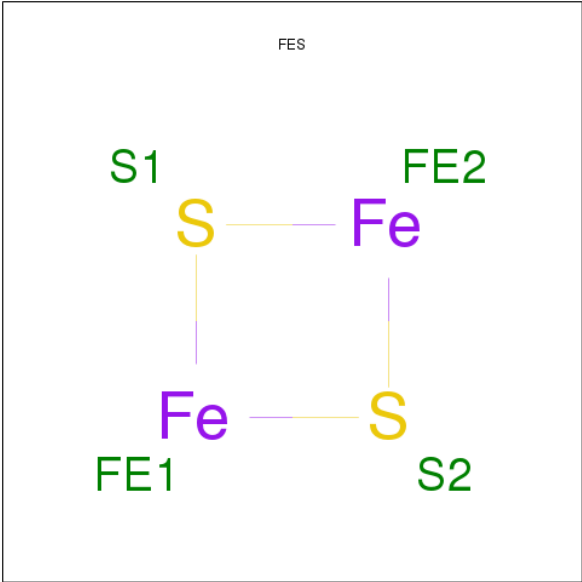
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
14	C	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
14	C	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
14	P	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
14	P	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		

- Molecule 15 is HEME C (three-letter code: HEC) (formula: $C_{34}H_{34}FeN_4O_4$).



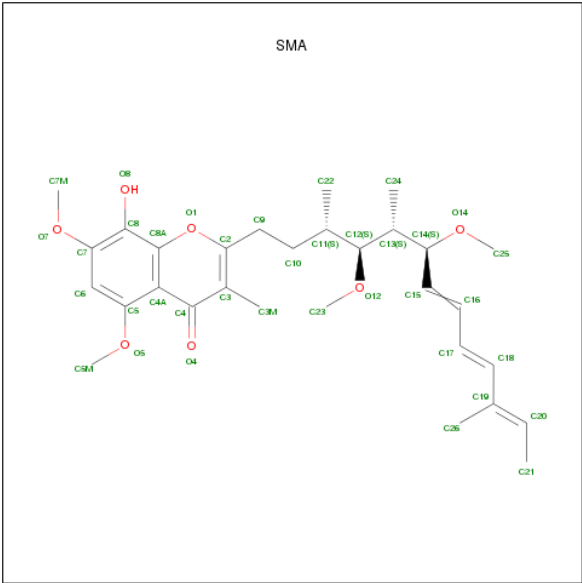
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
15	D	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
15	Q	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		

- Molecule 16 is FE2/S2 (INORGANIC) CLUSTER (three-letter code: FES) (formula: Fe_2S_2).



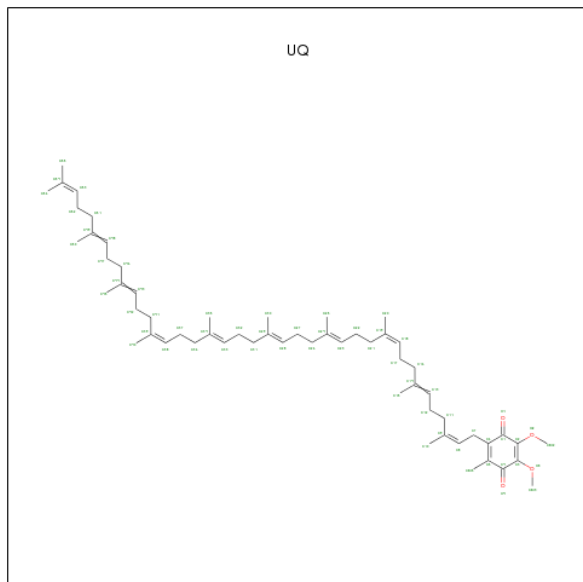
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
16	E	1	Total	Fe	S	0	0
			4	2	2		
16	R	1	Total	Fe	S	0	0
			4	2	2		

- Molecule 17 is STIGMATELLIN A (three-letter code: SMA) (formula: C₃₀H₄₂O₇).



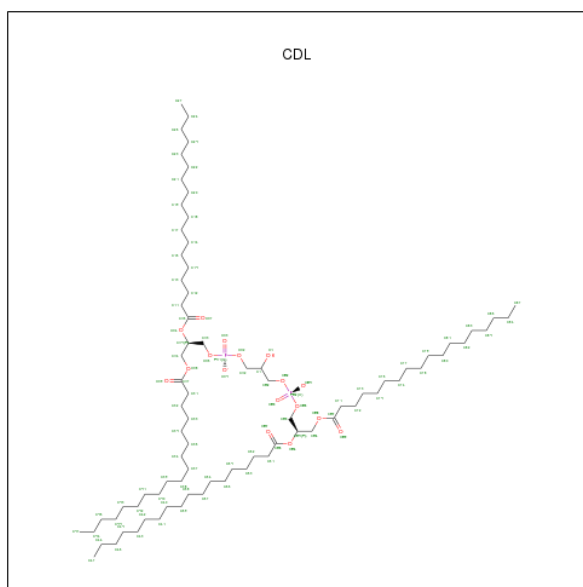
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
17	C	1	Total	C	O	0	0
			37	30	7		
17	P	1	Total	C	O	0	0
			37	30	7		

- Molecule 18 is COENZYME Q10, (2Z,6E,10Z,14E,18E,22E,26Z)-ISOMER (three-letter code: UQ) (formula: $C_{59}H_{90}O_4$).



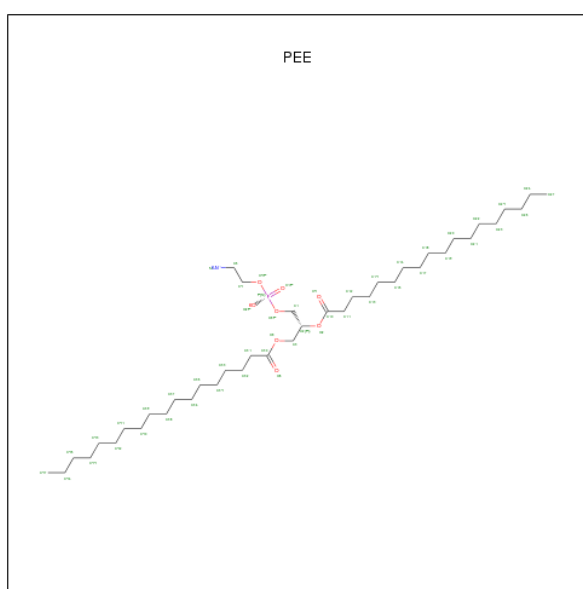
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
18	C	1	Total	C	O	0	0
			18	14	4		
18	P	1	Total	C	O	0	0
			18	14	4		

- Molecule 19 is CARDIOLIPIN (three-letter code: CDL) (formula: $C_{81}H_{156}O_{17}P_2$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
19	D	1	Total	C	O	P	0	0
			39	24	13	2		
19	C	1	Total	C	O	P	0	0
			44	25	17	2		
19	Q	1	Total	C	O	P	0	0
			39	24	13	2		
19	P	1	Total	C	O	P	0	0
			49	30	17	2		

- Molecule 20 is 1,2-DIOLEOYL-SN-GLYCERO-3-PHOSPHOETHANOLAMINE (three-letter code: PEE) (formula: $C_{41}H_{83}NO_8P$).

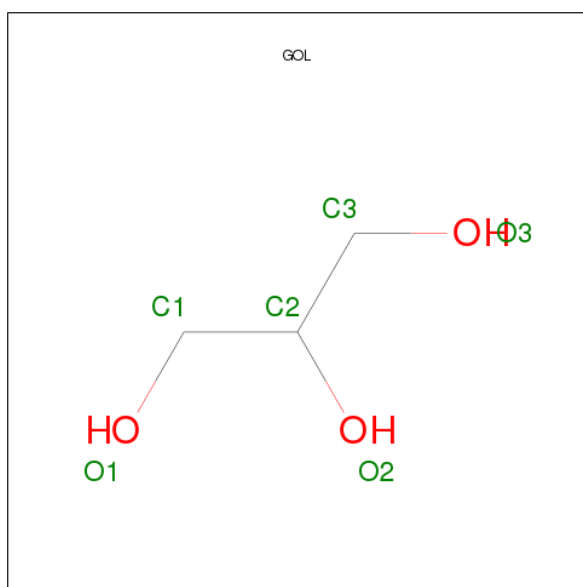


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	
20	D	1	Total 51	C 41	N 1	O 8	P 1	0	0	
20	C	1	Total 49	C 39	N 1	O 8	P 1	0	0	
20	Q	1	Total 51	C 41	N 1	O 8	P 1	0	0	
20	P	1	Total 49	C 39	N 1	O 8	P 1	0	0	
20	B	1	Total 8	C 6	O 2				0	0

- Molecule 21 is UNKNOWN LIGAND (three-letter code: UNL) (formula:).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
21	P	7	Total O 8 8	0	0
21	G	3	Total O 3 3	0	0
21	Q	1	Total O 1 1	0	0
21	D	7	Total O 7 7	0	0
21	E	2	Total O 2 2	0	0
21	B	11	Total O 11 11	0	0
21	I	2	Total O 2 2	0	0
21	C	6	Total O 7 7	0	0
21	V	4	Total O 4 4	0	0
21	W	1	Total O 1 1	0	0
21	A	10	Total O 10 10	0	0
21	T	2	Total O 2 2	0	0
21	N	4	Total O 5 5	0	0
21	U	2	Total O 2 2	0	0
21	O	8	Total O 9 9	0	0
21	R	2	Total O 2 2	0	0
21	S	1	Total O 1 1	0	0
21	F	1	Total O 1 1	0	0

- Molecule 22 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
22	C	1	Total	C	O	0	0
			6	3	3		
22	P	1	Total	C	O	0	0
			6	3	3		
22	O	1	Total	C	O	0	0
			6	3	3		
22	E	1	Total	C	O	0	0
			6	3	3		
22	E	1	Total	C	O	0	0
			5	3	2		
22	C	1	Total	C	O	0	0
			6	3	3		
22	P	1	Total	C	O	0	0
			6	3	3		

- Molecule 23 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
23	A	209	Total	O	0	0
			209	209		
23	B	170	Total	O	0	0
			170	170		
23	C	137	Total	O	0	0
			137	137		
23	D	133	Total	O	0	0
			133	133		
23	E	63	Total	O	0	0
			63	63		

Continued on next page...

Continued from previous page...

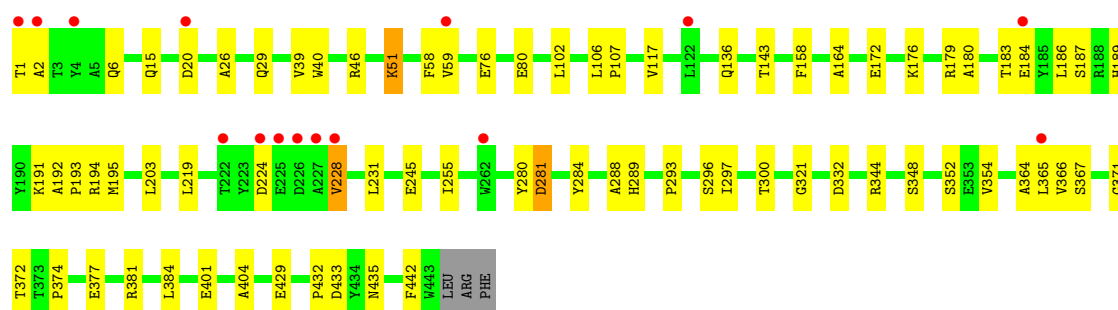
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
23	F	68	Total 68	O 68	0	0
23	G	31	Total 31	O 31	0	0
23	H	15	Total 15	O 15	0	0
23	I	18	Total 18	O 18	0	0
23	J	7	Total 7	O 7	0	0
23	N	145	Total 145	O 145	0	0
23	O	136	Total 136	O 136	0	0
23	P	135	Total 135	O 135	0	0
23	Q	126	Total 126	O 126	0	0
23	R	77	Total 77	O 77	0	0
23	S	81	Total 81	O 81	0	0
23	T	17	Total 17	O 17	0	0
23	U	16	Total 16	O 16	0	0
23	V	16	Total 16	O 16	0	0
23	W	12	Total 12	O 12	0	0

3 Residue-property plots

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.

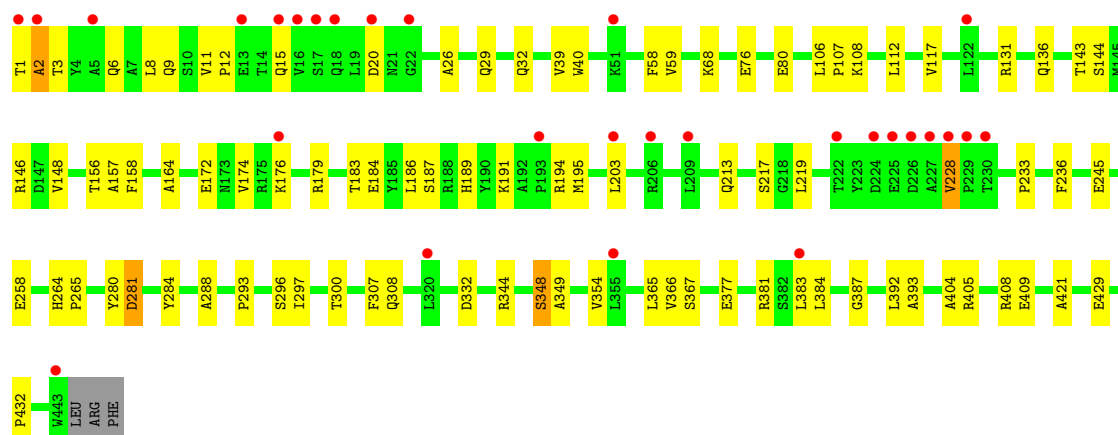
- Molecule 1: Ubiquinol-cytochrome-c reductase complex core protein I, mitochondrial

Chain A: 



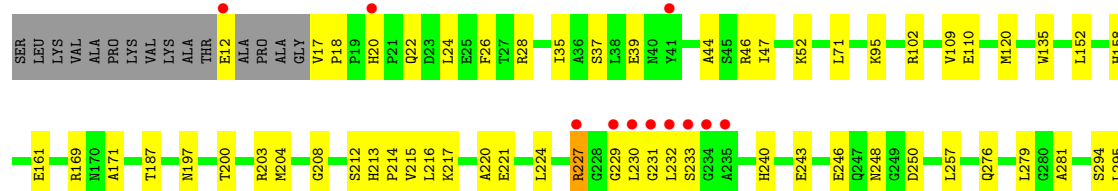
- Molecule 1: Ubiquinol-cytochrome-c reductase complex core protein I, mitochondrial

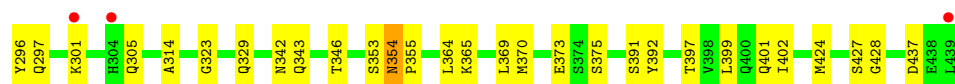
Chain N: 



- Molecule 2: Ubiquinol-cytochrome-c reductase complex core protein 2, mitochondrial

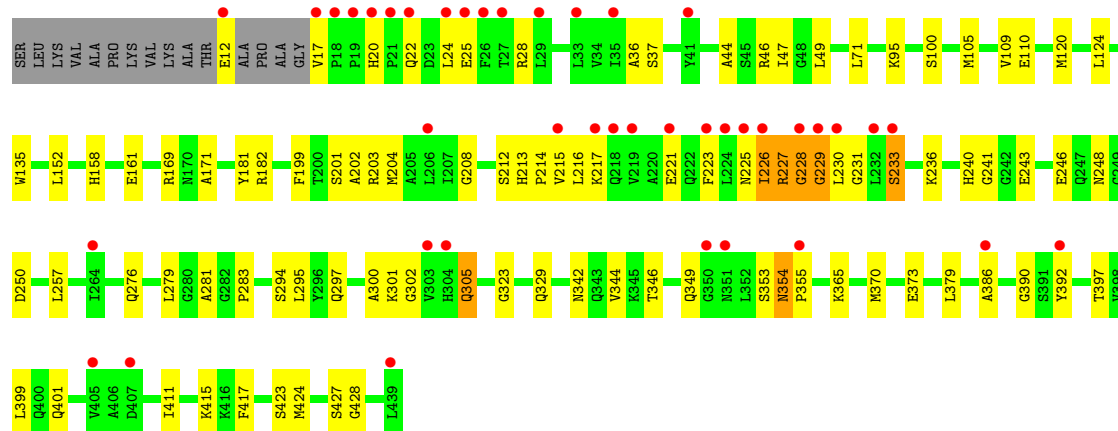
Chain B: 





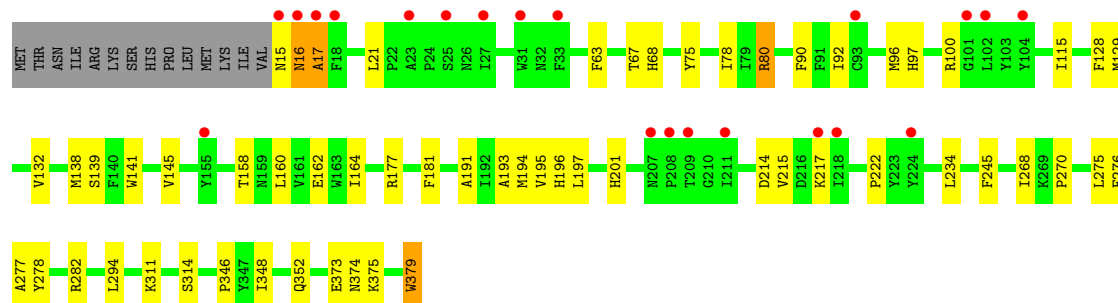
- Molecule 2: Ubiquinol-cytochrome-creductase complex core protein 2, mitochondrial

Chain O:



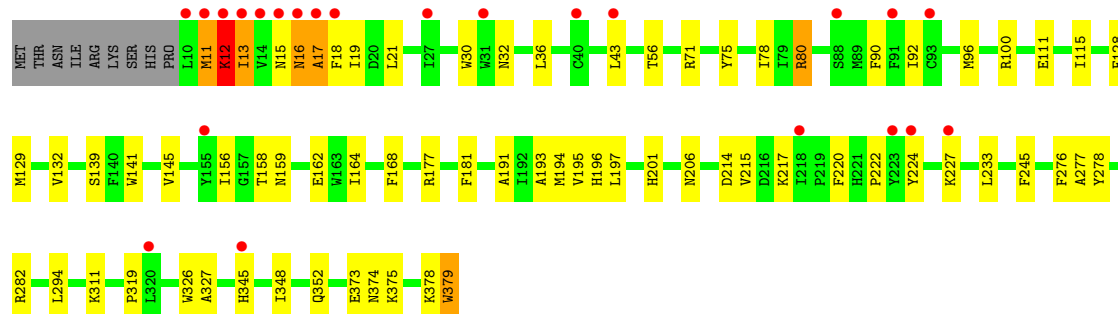
- Molecule 3: Cytochrome b, heme protein, mitochondrial

Chain C:



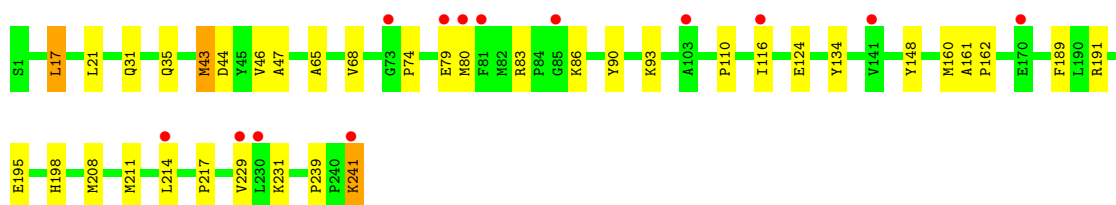
- Molecule 3: Cytochrome b, heme protein, mitochondrial

Chain P:



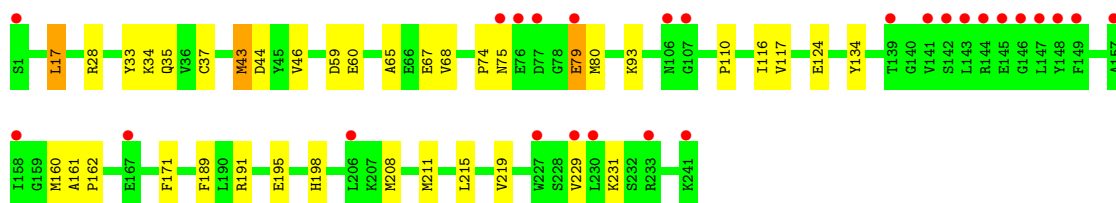
- Molecule 4: Cytochrome c1, heme protein, mitochondrial

Chain D:



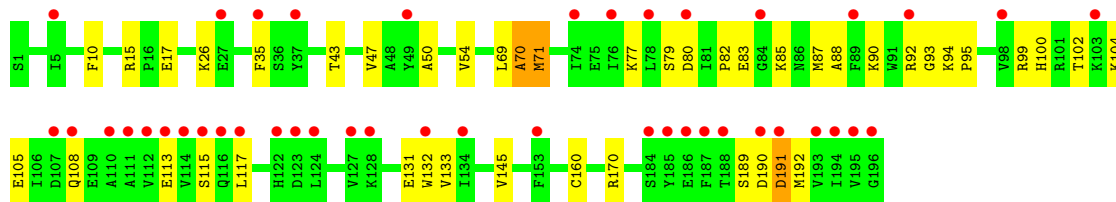
- Molecule 4: Cytochrome c1, heme protein, mitochondrial

Chain Q:



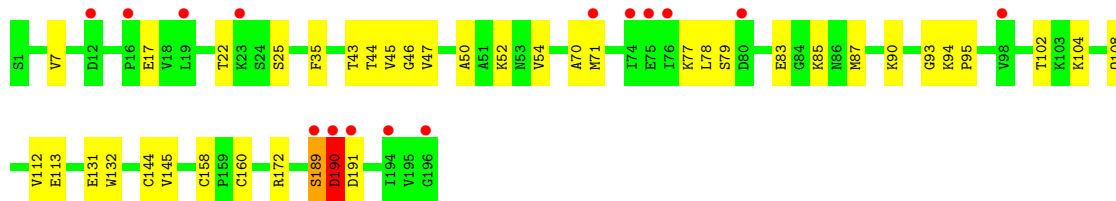
- Molecule 5: Ubiquinol-cytochrome c reductase iron-sulfur subunit, mitochondrial

Chain E:



- Molecule 5: Ubiquinol-cytochrome c reductase iron-sulfur subunit, mitochondrial

Chain R:



- Molecule 6: Ubiquinol-cytochrome c reductase complex 14 kDa protein

Chain F:



- Molecule 6: Ubiquinol-cytochrome c reductase complex 14 kDa protein

Chain S:



- Molecule 7: Ubiquinol-cytochrome c reductase complex ubiquinone-binding protein QP-C

- Molecule 7: Ubiquinol-cytochrome c reductase complex ubiquinone-binding protein QP-C

- Molecule 8: Ubiquinol-cytochrome c reductase complex 11 kDa protein

GLY	ASP	PRO	LYS	GLU	GLU	GLU	GLU	GLU	GLU	GLU	L13	V14	T18	T19	E22	Q23	E24	E25	Q26	L27	E28	K29	C30	V31	K32	A33	R34	E35	R36	L37	E38	D41	E42	R43	V44	S45	S46	R47	R48	Q49	T50	E51	E52	D53	H67	L78
-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----

- Molecule 8: Ubiquinol-cytochrome c reductase complex 11 kDa protein

GLY	ASP	PRO	LYS	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	L13	L14	D15	P16	L17	T18	T19	V20	R21	E22	Q23	Q24	C25	E26	Q26	L27	E28	V31	K32	A33	R34	E38	L39	C40	D41	E42	R43	R44	V45	S46	R47	S48	Q49	T50	E51	E56	H67
-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----

- Molecule 9: Ubiquinol-cytochrome c reductase iron-sulfur subunit, mitochondrial

Amino Acid	Percentage (%)
MET	100
LEU	100
SER	100
VAL	100
ALA	100
ALA	100
ARG	100
GLY	100
PRO	100
PHE	100
ALA	100
VAL	100
LEU	100
SER	100
THR	100
ARG	100
GLY	100
VAL	100
ALA	100
GLY	100
ALA	100
LEU	100
ARG	100
PRO	100
LEU	100
VAL	100
GLN	100
A32	100
A33	100
A36	100
I37	100
S38	100
E39	100
S40	100
P41	100
V42	100
LEU	100
ASP	100
LEU	100
LYS	100
ARG	100
S48	100
V49	100
L50	100
C51	100
R52	100
L55	100
Q58	100
A59	100
A60	100
G61	100
R62	100
MET	100

- Molecule 9: Ubiquinol-cytochrome c reductase iron-sulfur subunit, mitochondrial

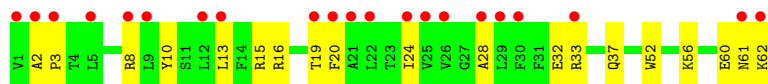
Figure 1: Schematic representation of the protein structure of the 120 kDa subunit of the 20S proteasome. The diagram shows a linear sequence of amino acids from MET to L64. Specific residues are highlighted: V68, N71, P73, and Y78 are in yellow boxes; A32, A33, A36, T37, S38, E39, S40, P41, V42, S48, V49, L50, C51, R52, L55, R56, G61, R62, P63, and L64 are in green boxes. Red dots above the sequence indicate the positions of the 20S proteasome subunits.

- Molecule 10: Ubiquinol-cytochrome c reductase complex 7.2 kDa protein

Sequence logo for the 10th position. The y-axis represents information content in bits, ranging from 0 to 0.4. The x-axis lists amino acids: VAL, ALA, PRO, THR, LEU, THR, ALA, ARG, LEU, TYR, SER, LEU, LEU, PHE, ARG, ARG, THR, SER, THR, PHE, ALA, LEU, THR, ILE, VAL, VAL, GLY, ALA, LEU, PHE, PHE, GLU, R33, Q37, K56, E60, N61, K62. The bars show the relative frequency of each amino acid at this position. Notable features include a high frequency of LEU and THR in the first half, and a high frequency of PHE and ARG in the second half. The R33, Q37, K56, E60, N61, and K62 positions show very low information content.

- Molecule 10: Ubiquinol-cytochrome c reductase complex 7.2 kDa protein

Chain W: 



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	128.25Å 168.80Å 230.82Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	37.87 – 2.10 37.87 – 2.00	Depositor EDS
% Data completeness (in resolution range)	95.3 (37.87-2.10) 91.8 (37.87-2.00)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.11	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.11 (at 2.00Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.222 , 0.258 0.221 , 0.253	Depositor DCC
R_{free} test set	15254 reflections (5.21%)	DCC
Wilson B-factor (Å ²)	38.4	Xtriage
Anisotropy	0.064	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.40 , 64.6	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning	$\langle L \rangle = 0.51$, $\langle L^2 \rangle = 0.35$	Xtriage
Outliers	0 of 308092 reflections	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	33890	wwPDB-VP
Average B, all atoms (Å ²)	48.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.20% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: AZI, GOL, CDL, UNL, PO4, UQ, BHG, FES, HEC, HEM, PEE, SMA

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.44	0/3467	0.67	0/4706
1	N	0.38	0/3467	0.64	0/4706
2	B	0.42	0/3235	0.65	0/4387
2	O	0.39	0/3239	0.65	1/4393 (0.0%)
3	C	0.48	0/2992	0.66	0/4097
3	P	0.44	0/3030	0.64	0/4145
4	D	0.44	0/1978	0.64	0/2684
4	Q	0.41	0/1978	0.62	0/2684
5	E	0.35	0/1553	0.70	3/2100 (0.1%)
5	R	0.41	0/1550	0.69	0/2094
6	F	0.45	0/878	0.66	0/1175
6	S	0.44	0/878	0.68	1/1175 (0.1%)
7	G	0.42	0/642	0.63	0/869
7	T	0.39	0/647	0.65	0/876
8	H	0.34	0/544	0.61	0/729
8	U	0.34	0/544	0.56	0/729
9	I	0.60	0/285	0.96	0/384
9	V	0.50	0/285	0.94	1/384 (0.3%)
10	J	0.38	0/252	0.56	0/333
10	W	0.36	0/520	0.59	0/699
All	All	0.42	0/31964	0.66	6/43349 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
5	E	0	1

There are no bond length outliers.

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	E	70	ALA	C-N-CA	-6.85	104.57	121.70
2	O	228	GLY	N-CA-C	-6.31	97.33	113.10
5	E	71	MET	C-N-CA	-6.26	106.05	121.70
6	S	33	ARG	NE-CZ-NH2	-6.11	117.24	120.30
9	V	62	ARG	NE-CZ-NH2	5.70	123.15	120.30
5	E	69	LEU	C-N-CA	-5.27	108.53	121.70

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
5	E	70	ALA	Peptide

5.2 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 hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3398	0	3295	68	0
1	N	3398	0	3295	64	0
2	B	3177	0	3152	88	0
2	O	3180	0	3156	87	0
3	C	2897	0	2943	47	0
3	P	2936	0	2994	74	0
4	D	1919	0	1868	38	0
4	Q	1919	0	1868	36	0
5	E	1519	0	1503	34	0
5	R	1517	0	1498	38	0
6	F	861	0	854	20	0
6	S	861	0	854	26	0
7	G	621	0	626	14	0
7	T	626	0	631	18	0
8	H	539	0	524	17	0
8	U	539	0	524	18	0
9	I	285	0	288	41	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
9	V	285	0	288	32	0
10	J	245	0	229	3	0
10	W	507	0	513	22	0
11	A	18	0	24	1	0
11	C	18	0	24	0	0
11	F	36	0	48	4	0
11	P	18	0	24	0	0
11	S	18	0	24	6	0
12	A	3	0	0	0	0
12	C	3	0	0	0	0
12	G	3	0	0	1	0
12	P	3	0	0	0	0
13	A	5	0	0	0	0
13	B	5	0	0	0	0
13	D	10	0	0	0	0
13	I	5	0	0	1	0
13	O	5	0	0	0	0
13	P	5	0	0	0	0
13	Q	5	0	0	1	0
13	R	10	0	0	0	0
13	T	5	0	0	0	0
14	C	86	0	60	5	0
14	P	86	0	60	3	0
15	D	43	0	30	4	0
15	Q	43	0	30	5	0
16	E	4	0	0	0	0
16	R	4	0	0	0	0
17	C	37	0	42	3	0
17	P	37	0	42	3	0
18	C	18	0	14	4	0
18	P	18	0	14	5	0
19	C	44	0	32	0	0
19	D	39	0	39	1	0
19	P	49	0	42	0	0
19	Q	39	0	39	0	0
20	B	8	0	8	1	0
20	C	49	0	72	0	0
20	D	51	0	82	2	0
20	P	49	0	72	3	0
20	Q	51	0	82	5	0
21	A	10	0	0	0	0
21	B	11	0	0	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
21	C	7	0	0	0	0
21	D	7	0	0	1	0
21	E	2	0	0	0	0
21	F	1	0	0	0	0
21	G	3	0	0	0	0
21	I	2	0	0	0	0
21	N	5	0	0	0	0
21	O	9	0	0	2	0
21	P	8	0	0	0	0
21	Q	1	0	0	0	0
21	R	2	0	0	0	0
21	S	1	0	0	0	0
21	T	2	0	0	0	0
21	U	2	0	0	0	0
21	V	4	0	0	0	0
21	W	1	0	0	0	0
22	C	12	0	16	0	0
22	E	11	0	13	0	0
22	O	6	0	8	0	0
22	P	12	0	16	2	0
23	A	209	0	0	4	0
23	B	170	0	0	2	0
23	C	137	0	0	6	0
23	D	133	0	0	0	0
23	E	63	0	0	0	0
23	F	68	0	0	4	0
23	G	31	0	0	2	0
23	H	15	0	0	0	0
23	I	18	0	0	4	0
23	J	7	0	0	0	0
23	N	145	0	0	3	0
23	O	136	0	0	6	0
23	P	135	0	0	8	0
23	Q	126	0	0	0	0
23	R	77	0	0	1	0
23	S	81	0	0	2	0
23	T	17	0	0	0	0
23	U	16	0	0	0	0
23	V	16	0	0	0	0
23	W	12	0	0	0	0
All	All	33890	0	31860	708	0

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including

hydrogens) of the entry. The overall clashscore for this entry is 11.

All (708) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:O:226:ILE:HG13	21:O:4043:UNL:O1	1.38	1.23
9:I:32:ALA:N	9:I:71:ASN:HB2	1.70	1.05
2:B:12:GLU:HG2	2:B:17:VAL:H	1.16	1.04
2:O:95:LYS:HB2	9:V:32:ALA:HB2	1.34	1.04
5:R:90:LYS:HE2	5:R:93:GLY:HA2	1.39	1.03
2:B:95:LYS:HD2	9:I:32:ALA:HB2	1.42	1.00
1:A:1:THR:HG21	2:B:212:SER:HB3	1.46	0.97
8:H:25:GLU:HB3	8:H:34:ARG:NH2	1.79	0.97
3:P:12:LYS:HE2	3:P:16:ASN:H	1.28	0.96
9:I:32:ALA:N	9:I:71:ASN:CB	2.31	0.92
2:B:12:GLU:HG2	2:B:17:VAL:N	1.86	0.90
8:U:25:GLU:HB3	8:U:34:ARG:NH2	1.87	0.89
2:B:95:LYS:HB2	9:I:32:ALA:HB2	1.55	0.86
4:Q:43:MET:HE3	4:Q:46:VAL:HG21	1.55	0.85
2:O:202:ALA:HB3	2:O:229:GLY:C	1.96	0.85
4:D:241:LYS:HA	4:D:241:LYS:NZ	1.92	0.85
2:B:397:THR:HG22	2:B:401:GLN:HE21	1.41	0.83
1:A:187:SER:O	1:A:191:LYS:HE2	1.79	0.82
10:W:16:ARG:HB2	10:W:19:THR:HG22	1.63	0.81
9:V:49:VAL:HG11	9:V:55:LEU:HD13	1.63	0.80
2:O:397:THR:HG22	2:O:401:GLN:HE21	1.46	0.80
3:P:21:LEU:HD21	18:P:3002:UQ:HM32	1.64	0.80
23:C:4219:HOH:O	3:P:56:THR:HG22	1.82	0.80
1:A:51:LYS:H	1:A:51:LYS:HE3	1.47	0.80
3:C:21:LEU:HD21	18:C:2002:UQ:HM32	1.64	0.80
1:A:29:GLN:HB3	2:B:12:GLU:O	1.81	0.79
23:A:4261:HOH:O	9:I:73:PRO:HG3	1.83	0.78
1:A:352:SER:HB3	6:S:110:LYS:HD2	1.65	0.78
2:B:95:LYS:HD2	9:I:32:ALA:CB	2.13	0.78
2:O:20:HIS:HB2	2:O:22:GLN:HG2	1.66	0.77
10:W:3:PRO:HB2	10:W:8:ARG:HD3	1.65	0.77
1:N:179:ARG:O	1:N:183:THR:HG23	1.85	0.77
4:D:116:ILE:HG12	15:D:501:HEC:HMA3	1.66	0.77
1:A:401:GLU:HG3	11:A:4004:BHG:H6'1	1.67	0.77
2:B:397:THR:HG22	2:B:401:GLN:NE2	1.99	0.77
20:B:4017:PEE:C15	9:I:77:ARG:HH22	1.98	0.76
2:B:20:HIS:HB2	2:B:22:GLN:HG2	1.66	0.75
9:I:49:VAL:HG11	9:I:55:LEU:HD13	1.68	0.75
6:F:58:ARG:HD3	23:F:4062:HOH:O	1.86	0.75
9:V:36:ALA:HB2	9:V:73:PRO:HD2	1.69	0.75

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Distance(Å)	Clash(Å)
4:Q:59:ASP:OD2	10:W:62:LYS:HB3	1.87	0.74
8:H:31:VAL:HA	8:H:34:ARG:NH1	2.02	0.74
9:I:62:ARG:O	9:I:78:TYR:HB3	1.87	0.74
2:O:161:GLU:OE1	9:V:64:LEU:HD12	1.88	0.74
2:O:95:LYS:HD2	2:O:110:GLU:OE2	1.88	0.74
3:P:129:MET:HE1	3:P:181:PHE:HD2	1.51	0.74
9:I:36:ALA:HB2	9:I:73:PRO:HD2	1.69	0.73
8:U:31:VAL:HA	8:U:34:ARG:NH1	2.03	0.73
4:D:241:LYS:HZ3	4:D:241:LYS:HA	1.50	0.73
3:P:43:LEU:HD21	20:Q:3006:PEE:H192	1.71	0.72
5:E:90:LYS:HE2	5:E:93:GLY:HA2	1.70	0.72
8:H:25:GLU:HB3	8:H:34:ARG:HH21	1.51	0.72
1:A:2:ALA:HB1	1:A:6:GLN:HB2	1.71	0.72
9:V:62:ARG:O	9:V:78:TYR:HB3	1.88	0.72
7:T:72:LYS:HG3	8:U:56:GLU:OE2	1.90	0.71
10:W:13:LEU:O	10:W:19:THR:HG23	1.91	0.71
8:U:25:GLU:HB3	8:U:34:ARG:HH21	1.55	0.71
10:W:33:ARG:O	10:W:37:GLN:HG3	1.91	0.70
7:G:63:THR:O	7:G:67:GLU:HG2	1.91	0.70
4:D:74:PRO:HD3	4:D:80:MET:HE1	1.73	0.70
2:O:397:THR:HG22	2:O:401:GLN:NE2	2.07	0.70
3:C:68:HIS:HD2	23:C:4195:HOH:O	1.74	0.69
4:D:43:MET:HE2	4:D:46:VAL:HG21	1.75	0.69
2:O:95:LYS:HE2	9:V:32:ALA:CB	2.22	0.69
5:R:44:THR:HG21	10:W:24:ILE:HD13	1.73	0.69
2:B:197:ASN:HB3	2:B:230:LEU:HG	1.74	0.69
5:R:70:ALA:N	5:R:71:MET:HE2	2.07	0.69
2:B:95:LYS:CD	9:I:32:ALA:HB2	2.21	0.68
4:D:110:PRO:HG3	15:D:501:HEC:HMD3	1.75	0.68
1:N:187:SER:O	1:N:191:LYS:HE2	1.93	0.68
4:Q:231:LYS:HD3	6:S:70:MET:HE3	1.75	0.68
7:T:63:THR:O	7:T:67:GLU:HG2	1.94	0.68
2:O:203:ARG:HH12	2:O:233:SER:HB3	1.58	0.68
2:O:49:LEU:HD11	2:O:204:MET:HE3	1.73	0.68
3:C:379:TRP:CZ3	6:F:33:ARG:HD3	2.28	0.67
10:J:33:ARG:O	10:J:37:GLN:HG3	1.94	0.67
8:U:28:GLU:HA	8:U:31:VAL:HG22	1.76	0.67
8:H:18:THR:O	8:H:22:GLU:HG3	1.94	0.67
4:Q:110:PRO:HG3	15:Q:501:HEC:HMD3	1.77	0.67
9:V:32:ALA:N	9:V:71:ASN:HB3	2.08	0.67
5:R:90:LYS:HE2	5:R:93:GLY:CA	2.22	0.67
3:P:12:LYS:HA	3:P:12:LYS:HE3	1.77	0.66

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Distance(Å)	Clash(Å)
3:C:129:MET:HE1	3:C:181:PHE:HD2	1.60	0.66
9:I:36:ALA:HB3	9:I:73:PRO:HG2	1.76	0.66
2:B:95:LYS:CB	9:I:32:ALA:HB2	2.25	0.66
9:I:32:ALA:N	9:I:71:ASN:HB3	2.11	0.66
5:E:87:MET:CE	5:E:88:ALA:H	2.09	0.65
1:A:293:PRO:O	1:A:297:ILE:HG12	1.97	0.65
1:A:344:ARG:HG2	1:A:344:ARG:HH11	1.61	0.65
9:V:32:ALA:N	9:V:71:ASN:CB	2.59	0.65
3:P:12:LYS:HE2	3:P:16:ASN:N	2.06	0.65
2:O:95:LYS:HE2	9:V:32:ALA:HB3	1.78	0.65
2:B:20:HIS:HB2	2:B:22:GLN:CG	2.27	0.65
2:O:203:ARG:HH12	2:O:233:SER:CA	2.09	0.65
2:B:200:THR:HG21	2:B:229:GLY:CA	2.26	0.65
14:P:501:HEM:HMC1	14:P:501:HEM:HBC2	1.79	0.65
1:A:179:ARG:O	1:A:183:THR:HG23	1.97	0.65
4:D:231:LYS:HD3	6:F:70:MET:HE3	1.78	0.64
1:A:372:THR:HA	23:A:4296:HOH:O	1.96	0.64
3:C:92:ILE:O	3:C:96:MET:HG2	1.96	0.64
5:E:83:GLU:HG2	5:E:100:HIS:CE1	2.33	0.64
4:Q:44:ASP:OD1	4:Q:93:LYS:HE2	1.97	0.64
5:E:85:LYS:NZ	5:E:87:MET:SD	2.69	0.64
5:E:79:SER:HB3	5:E:191:ASP:OD2	1.98	0.64
2:B:203:ARG:HH11	2:B:232:LEU:HA	1.63	0.64
8:U:18:THR:O	8:U:22:GLU:HG3	1.97	0.64
8:H:28:GLU:HA	8:H:31:VAL:HG22	1.80	0.63
2:B:35:ILE:HD11	2:B:220:ALA:CB	2.28	0.63
3:P:12:LYS:NZ	3:P:16:ASN:HD22	1.95	0.63
4:Q:74:PRO:HD3	4:Q:80:MET:HE1	1.80	0.63
2:B:35:ILE:HD11	2:B:220:ALA:HB3	1.80	0.63
1:N:59:VAL:HG11	1:N:186:LEU:HD21	1.80	0.63
1:N:293:PRO:O	1:N:297:ILE:HG12	1.99	0.63
2:O:250:ASP:HB3	23:O:4203:HOH:O	1.99	0.63
3:P:129:MET:CE	3:P:181:PHE:HD2	2.12	0.63
2:B:12:GLU:CG	2:B:17:VAL:H	2.03	0.62
6:S:108:ALA:C	6:S:110:LYS:H	2.00	0.62
2:O:158:HIS:HB3	23:O:4207:HOH:O	1.98	0.62
2:O:202:ALA:HB3	2:O:229:GLY:O	1.99	0.62
6:S:14:GLU:HG2	23:S:4108:HOH:O	1.98	0.62
1:A:15:GLN:HE21	2:B:12:GLU:HB2	1.64	0.62
1:N:344:ARG:HG2	1:N:344:ARG:HH11	1.63	0.62
23:A:4237:HOH:O	5:E:26:LYS:HE2	1.99	0.62
5:R:45:VAL:HG13	10:W:28:ALA:HA	1.82	0.62

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:O:95:LYS:CE	9:V:32:ALA:HB3	2.29	0.62
2:B:296:TYR:OH	9:I:52:ARG:HD3	2.00	0.62
8:H:25:GLU:HB3	8:H:34:ARG:HH22	1.63	0.62
1:A:136:GLN:NE2	9:I:51:CYS:HB2	2.15	0.62
2:B:354:ASN:N	2:B:355:PRO:HD2	2.15	0.61
2:B:24:LEU:HD13	2:B:392:TYR:CE2	2.35	0.61
1:A:143:THR:OG1	9:I:48:SER:HB3	2.00	0.61
5:E:160:CYS:HB3	17:P:3001:SMA:H4	1.82	0.61
2:B:200:THR:HG21	2:B:229:GLY:HA3	1.80	0.61
2:B:95:LYS:HB2	9:I:32:ALA:CB	2.29	0.61
2:B:95:LYS:HD3	2:B:110:GLU:OE2	2.01	0.61
1:A:117:VAL:HG11	1:A:195:MET:CE	2.30	0.61
1:A:366:VAL:HG21	2:B:44:ALA:HB2	1.82	0.61
1:N:366:VAL:HG21	2:O:44:ALA:HB2	1.82	0.61
5:R:17:GLU:OE2	5:R:17:GLU:N	2.28	0.61
2:B:37:SER:HB3	2:B:216:LEU:HD12	1.83	0.61
4:D:124:GLU:OE2	4:D:191:ARG:HD2	2.01	0.61
5:E:77:LYS:HD3	5:E:80:ASP:OD2	2.01	0.61
3:P:379:TRP:CZ3	6:S:33:ARG:HD3	2.36	0.61
2:O:28:ARG:HB2	2:O:28:ARG:NH1	2.16	0.61
2:B:276:GLN:HG2	2:B:281:ALA:HB2	1.82	0.60
3:P:92:ILE:O	3:P:96:MET:HG2	2.01	0.60
8:U:34:ARG:O	8:U:38:GLU:HG3	2.01	0.60
2:O:226:ILE:CG1	21:O:4043:UNL:O1	2.32	0.60
5:E:95:PRO:HG2	5:E:145:VAL:HG22	1.83	0.60
2:B:212:SER:OG	2:B:215:VAL:HG13	2.02	0.60
1:A:189:HIS:ND1	1:A:194:ARG:NH2	2.50	0.60
2:O:203:ARG:HH12	2:O:233:SER:CB	2.13	0.60
3:P:21:LEU:HD11	23:P:4171:HOH:O	2.01	0.60
4:D:44:ASP:OD1	4:D:93:LYS:HE2	2.01	0.60
2:O:24:LEU:HD23	2:O:392:TYR:CD2	2.37	0.60
10:W:10:TYR:OH	10:W:15:ARG:NH1	2.35	0.60
1:N:68:LYS:HA	1:N:68:LYS:HE3	1.83	0.60
2:O:226:ILE:HD11	23:O:4141:HOH:O	2.00	0.60
23:P:4186:HOH:O	6:S:20:TYR:HE1	1.84	0.60
9:V:36:ALA:CB	9:V:73:PRO:HD2	2.31	0.60
8:H:34:ARG:O	8:H:38:GLU:HG3	2.01	0.59
5:R:112:VAL:HG22	5:R:172:ARG:NH2	2.16	0.59
2:O:71:LEU:HD23	9:V:68:VAL:HG21	1.83	0.59
1:A:296:SER:O	1:A:300:THR:HG23	2.01	0.59
9:I:32:ALA:N	9:I:72:VAL:HG23	2.17	0.59
2:O:20:HIS:HB2	2:O:22:GLN:CG	2.32	0.59

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:O:279:LEU:HA	2:O:294:SER:HB3	1.84	0.59
2:B:161:GLU:OE1	9:I:64:LEU:HD12	2.02	0.59
1:N:195:MET:SD	1:N:219:LEU:HD21	2.43	0.59
9:V:32:ALA:N	9:V:72:VAL:HG23	2.18	0.59
5:R:112:VAL:CG2	5:R:172:ARG:NH2	2.66	0.59
2:B:169:ARG:HG3	2:B:240:HIS:HB2	1.83	0.59
2:O:28:ARG:HB2	2:O:28:ARG:HH11	1.67	0.59
8:U:28:GLU:O	8:U:31:VAL:HG22	2.03	0.59
1:A:288:ALA:HB2	1:A:300:THR:HG22	1.84	0.59
2:B:250:ASP:HB3	23:B:4230:HOH:O	2.02	0.59
5:E:71:MET:HE2	5:E:92:ARG:HD3	1.85	0.59
4:Q:60:GLU:HG3	10:W:62:LYS:NZ	2.18	0.58
4:Q:124:GLU:OE2	4:Q:191:ARG:HD2	2.03	0.58
8:H:28:GLU:O	8:H:31:VAL:HG22	2.03	0.58
5:E:145:VAL:HG23	3:P:141:TRP:CH2	2.38	0.58
5:R:79:SER:HB3	5:R:191:ASP:CG	2.23	0.58
1:N:189:HIS:ND1	1:N:194:ARG:NH2	2.49	0.58
3:C:141:TRP:CH2	5:R:145:VAL:HG23	2.39	0.58
5:E:17:GLU:N	5:E:17:GLU:OE2	2.28	0.58
1:N:1:THR:O	1:N:2:ALA:HB2	2.03	0.58
2:B:203:ARG:HH12	2:B:233:SER:H	1.50	0.58
2:O:365:LYS:HG2	2:O:399:LEU:HD22	1.85	0.58
2:B:35:ILE:HD13	2:B:217:LYS:HA	1.85	0.58
3:P:100:ARG:C	3:P:100:ARG:HD2	2.24	0.58
3:C:129:MET:CE	3:C:181:PHE:HD2	2.16	0.57
1:N:29:GLN:HG3	1:N:203:LEU:O	2.05	0.57
2:O:276:GLN:HG2	2:O:281:ALA:HB2	1.86	0.57
8:U:31:VAL:HA	8:U:34:ARG:HH12	1.68	0.57
5:E:191:ASP:O	5:E:192:MET:HG2	2.04	0.57
9:I:70:LEU:O	9:I:71:ASN:HB2	2.02	0.57
2:B:208:GLY:HA3	2:B:216:LEU:HD11	1.84	0.57
3:P:43:LEU:HD21	20:Q:3006:PEE:C19	2.34	0.57
9:V:36:ALA:HB3	9:V:73:PRO:HG2	1.85	0.57
2:O:365:LYS:HG2	2:O:399:LEU:CD2	2.35	0.57
1:A:15:GLN:NE2	2:B:12:GLU:HB2	2.19	0.57
2:B:365:LYS:HG2	2:B:399:LEU:CD2	2.35	0.57
2:O:297:GLN:O	2:O:301:LYS:HG3	2.05	0.57
4:D:43:MET:HE1	4:D:189:PHE:CZ	2.39	0.57
5:E:83:GLU:HG2	5:E:100:HIS:NE2	2.19	0.57
2:B:297:GLN:O	2:B:301:LYS:HG3	2.03	0.57
4:Q:75:ASN:HD21	4:Q:79:GLU:HG3	1.69	0.57
5:R:79:SER:HB3	5:R:191:ASP:OD2	2.05	0.57

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:117:VAL:HG11	1:A:195:MET:HE3	1.87	0.57
2:B:305:GLN:HB3	2:B:329:GLN:OE1	2.04	0.57
2:O:354:ASN:N	2:O:355:PRO:CD	2.68	0.57
2:O:427:SER:HB3	23:O:4207:HOH:O	2.04	0.57
1:A:172:GLU:OE2	1:A:176:LYS:HE3	2.05	0.56
2:O:236:LYS:H	2:O:236:LYS:HD2	1.70	0.56
6:S:49:ARG:HH22	11:S:2012:BHG:H4	1.70	0.56
1:N:189:HIS:HB3	1:N:194:ARG:HH21	1.71	0.56
2:B:365:LYS:HG2	2:B:399:LEU:HD22	1.87	0.56
2:O:212:SER:OG	2:O:215:VAL:HG13	2.05	0.56
5:E:94:LYS:HE3	3:P:168:PHE:O	2.05	0.56
6:S:100:GLU:HB3	11:S:2012:BHG:H62	1.88	0.56
17:C:2001:SMA:H4	5:R:160:CYS:HB3	1.87	0.56
9:I:70:LEU:HB2	23:I:1826:HOH:O	2.04	0.56
1:N:76:GLU:HG2	1:N:80:GLU:OE2	2.05	0.56
2:O:227:ARG:HA	23:O:4150:HOH:O	2.06	0.56
3:P:277:ALA:HB1	3:P:294:LEU:CD1	2.35	0.56
7:G:42:ARG:HG3	7:G:42:ARG:HH11	1.71	0.56
2:O:169:ARG:HG3	2:O:240:HIS:HB2	1.88	0.56
1:A:106:LEU:HB3	1:A:107:PRO:HD3	1.87	0.56
14:C:501:HEM:HBC2	14:C:501:HEM:HMC1	1.88	0.56
3:C:373:GLU:HB2	23:C:4111:HOH:O	2.06	0.55
9:I:62:ARG:HD3	13:I:4015:PO4:O3	2.07	0.55
4:Q:116:ILE:HG12	15:Q:501:HEC:HMA3	1.89	0.55
1:A:289:HIS:HE1	11:S:2012:BHG:H1'2	1.71	0.55
6:F:95:LYS:HB2	6:F:95:LYS:NZ	2.20	0.55
1:N:189:HIS:CB	1:N:194:ARG:HH21	2.19	0.55
6:S:49:ARG:NH2	11:S:2012:BHG:H4	2.21	0.55
10:W:16:ARG:HB2	10:W:19:THR:CG2	2.36	0.55
6:F:101:ARG:HG2	6:F:101:ARG:HH11	1.71	0.55
8:H:47:ARG:HD3	8:H:50:THR:HB	1.89	0.55
6:S:13:LEU:O	6:S:17:ARG:N	2.40	0.55
3:P:96:MET:HE2	3:P:96:MET:HA	1.89	0.55
4:D:241:LYS:HZ2	4:D:241:LYS:HA	1.70	0.55
5:E:104:LYS:O	5:E:108:GLN:HG3	2.07	0.55
5:E:82:PRO:O	5:E:100:HIS:HB3	2.07	0.55
3:C:15:ASN:O	3:C:16:ASN:C	2.46	0.55
7:T:34:ILE:HB	7:T:35:PRO:HD3	1.89	0.55
9:I:62:ARG:HB3	9:I:63:PRO:HD2	1.89	0.54
2:O:353:SER:HB3	2:O:355:PRO:HD2	1.89	0.54
5:R:25:SER:HA	23:R:4077:HOH:O	2.06	0.54
8:H:31:VAL:HA	8:H:34:ARG:HH12	1.69	0.54

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:76:GLU:HG2	1:A:80:GLU:OE2	2.08	0.54
2:B:46:ARG:HD2	2:B:375:SER:OG	2.07	0.54
3:C:277:ALA:HB1	3:C:294:LEU:CD1	2.38	0.54
1:A:189:HIS:CB	1:A:194:ARG:HH21	2.19	0.54
4:D:134:TYR:CG	4:D:162:PRO:HG3	2.42	0.54
4:D:43:MET:HE1	4:D:189:PHE:HZ	1.72	0.54
2:O:12:GLU:HG3	2:O:17:VAL:H	1.72	0.54
8:U:16:PRO:O	8:U:20:VAL:HG23	2.08	0.54
2:B:231:GLY:N	2:B:233:SER:OG	2.40	0.54
8:H:51:GLU:H	8:H:51:GLU:CD	2.10	0.54
4:Q:34:LYS:HE3	4:Q:67:GLU:OE1	2.07	0.54
1:A:189:HIS:HB3	1:A:194:ARG:HH21	1.72	0.54
1:N:296:SER:O	1:N:300:THR:HG23	2.07	0.54
3:P:156:ILE:HA	3:P:159:ASN:HD22	1.73	0.54
2:B:279:LEU:HB3	2:B:295:LEU:HG	1.90	0.54
5:E:87:MET:HE3	5:E:88:ALA:H	1.71	0.54
2:O:228:GLY:O	2:O:231:GLY:N	2.40	0.54
3:P:197:LEU:HD13	18:P:3002:UQ:HM53	1.89	0.54
5:E:50:ALA:O	5:E:54:VAL:HG23	2.08	0.54
1:N:381:ARG:HH11	1:N:381:ARG:HG2	1.73	0.53
2:O:225:ASN:HD21	2:O:227:ARG:NH2	2.06	0.53
1:A:39:VAL:HG11	1:A:195:MET:CE	2.37	0.53
7:G:34:ILE:HB	7:G:35:PRO:HD3	1.89	0.53
3:P:12:LYS:CA	3:P:12:LYS:HE3	2.39	0.53
1:N:354:VAL:HG21	1:N:404:ALA:HA	1.90	0.53
8:U:19:THR:O	8:U:23:GLN:HG3	2.07	0.53
1:A:51:LYS:N	1:A:51:LYS:HE3	2.21	0.53
2:B:203:ARG:NH1	2:B:233:SER:H	2.07	0.53
6:F:63:LYS:HE2	23:G:4088:HOH:O	2.08	0.53
2:O:225:ASN:HD21	2:O:227:ARG:CZ	2.22	0.53
5:R:104:LYS:O	5:R:108:GLN:HG3	2.09	0.53
6:S:12:TRP:O	6:S:15:GLY:N	2.41	0.53
3:P:145:VAL:HG21	17:P:3001:SMA:H6	1.91	0.53
3:C:375:LYS:O	6:F:17:ARG:NH1	2.42	0.53
2:B:279:LEU:HA	2:B:294:SER:HB3	1.91	0.53
3:P:201:HIS:NE2	18:P:3002:UQ:O4	2.31	0.53
7:T:29:TYR:O	7:T:33:GLY:HA3	2.09	0.53
1:A:429:GLU:OE2	7:G:7:LEU:HB2	2.09	0.52
1:N:106:LEU:HB3	1:N:107:PRO:HD3	1.92	0.52
2:O:279:LEU:HB3	2:O:295:LEU:HG	1.89	0.52
1:A:29:GLN:HG3	1:A:203:LEU:O	2.09	0.52
3:C:201:HIS:NE2	18:C:2002:UQ:O4	2.37	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Distance(Å)	Clash(Å)
14:C:502:HEM:HMC2	14:C:502:HEM:HBC2	1.92	0.52
2:O:225:ASN:ND2	2:O:227:ARG:CZ	2.72	0.52
1:N:117:VAL:HG11	1:N:195:MET:CE	2.40	0.52
15:Q:501:HEC:HBC3	15:Q:501:HEC:HMC1	1.91	0.52
3:C:138:MET:SD	3:C:268:ILE:HG13	2.49	0.52
1:N:2:ALA:HA	1:N:6:GLN:OE1	2.10	0.52
2:O:217:LYS:O	2:O:221:GLU:HG3	2.10	0.52
4:Q:75:ASN:OD1	4:Q:79:GLU:HG2	2.10	0.52
1:A:136:GLN:HB3	9:I:51:CYS:HB3	1.91	0.52
9:I:36:ALA:CB	9:I:73:PRO:HD2	2.37	0.52
3:P:311:LYS:HG2	3:P:374:ASN:CG	2.30	0.52
6:S:95:LYS:HB2	6:S:95:LYS:NZ	2.25	0.52
1:N:288:ALA:HB2	1:N:300:THR:HG22	1.92	0.52
3:C:100:ARG:C	3:C:100:ARG:HD2	2.29	0.52
1:N:228:VAL:O	1:N:228:VAL:HG13	2.11	0.52
9:V:36:ALA:HB3	9:V:73:PRO:CG	2.40	0.52
5:E:87:MET:HE2	5:E:88:ALA:H	1.75	0.51
1:N:146:ARG:HH21	1:N:308:GLN:HE22	1.57	0.51
1:A:281:ASP:OD2	9:I:73:PRO:HB3	2.10	0.51
1:N:172:GLU:OE2	1:N:176:LYS:HE3	2.09	0.51
1:N:408:ARG:HD2	23:N:4206:HOH:O	2.09	0.51
1:N:405:ARG:O	1:N:409:GLU:HG3	2.10	0.51
1:A:381:ARG:HG2	1:A:381:ARG:HH11	1.75	0.51
4:Q:231:LYS:HD3	6:S:70:MET:CE	2.40	0.51
7:T:32:LYS:C	7:T:35:PRO:HD2	2.31	0.51
9:V:32:ALA:N	9:V:71:ASN:HB2	2.25	0.51
1:N:39:VAL:HG11	1:N:195:MET:CE	2.40	0.51
3:P:158:THR:HB	23:P:4121:HOH:O	2.11	0.51
2:O:236:LYS:N	2:O:236:LYS:HD2	2.26	0.51
2:B:24:LEU:HD13	2:B:392:TYR:CD2	2.45	0.50
15:D:501:HEC:HMC1	15:D:501:HEC:HBC3	1.92	0.50
7:G:29:TYR:O	7:G:33:GLY:HA3	2.09	0.50
2:B:227:ARG:HD3	2:B:227:ARG:N	2.26	0.50
5:E:102:THR:OG1	5:E:105:GLU:HG3	2.11	0.50
4:D:21:LEU:HD21	4:D:191:ARG:HG2	1.94	0.50
2:B:71:LEU:HD23	9:I:68:VAL:HG21	1.91	0.50
1:N:40:TRP:CZ2	1:N:377:GLU:HA	2.47	0.50
2:B:248:ASN:OD1	2:B:428:GLY:HA2	2.11	0.50
1:A:180:ALA:O	1:A:184:GLU:HG3	2.11	0.50
5:R:50:ALA:O	5:R:54:VAL:HG23	2.11	0.50
5:E:190:ASP:O	5:E:192:MET:HG2	2.12	0.50
9:I:64:LEU:HD23	9:I:77:ARG:O	2.12	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Distance(Å)	Clash(Å)
4:Q:195:GLU:HG2	4:Q:198:HIS:HB2	1.94	0.50
1:N:429:GLU:OE2	7:T:7:LEU:HB2	2.12	0.50
1:N:136:GLN:NE2	9:V:51:CYS:HB2	2.27	0.50
3:C:245:PHE:CD1	4:D:17:LEU:HD13	2.47	0.50
10:J:56:LYS:HG2	10:J:60:GLU:CD	2.32	0.50
2:O:305:GLN:NE2	2:O:329:GLN:OE1	2.45	0.49
3:C:160:LEU:O	3:C:164:ILE:HG12	2.11	0.49
1:N:344:ARG:HG2	1:N:344:ARG:NH1	2.27	0.49
4:Q:208:MET:HA	20:Q:3006:PEE:H312	1.94	0.49
2:O:95:LYS:CE	9:V:32:ALA:CB	2.90	0.49
2:O:283:PRO:HB3	9:V:56:ARG:HG3	1.93	0.49
3:C:145:VAL:HG21	17:C:2001:SMA:H6	1.94	0.49
10:W:15:ARG:HG3	10:W:15:ARG:HH11	1.76	0.49
6:F:104:ARG:HH11	11:F:3012:BHG:H61	1.77	0.49
3:P:217:LYS:HG3	7:T:7:LEU:HD13	1.94	0.49
8:U:25:GLU:HB3	8:U:34:ARG:HH22	1.72	0.49
2:B:203:ARG:NH1	2:B:232:LEU:HA	2.28	0.49
3:C:197:LEU:HD13	18:C:2002:UQ:HM53	1.94	0.49
4:D:17:LEU:HD21	21:D:4083:UNL:O1	2.13	0.49
1:N:280:TYR:HA	1:N:284:TYR:CE2	2.47	0.49
1:N:383:LEU:O	1:N:387:GLY:HA2	2.12	0.49
2:O:95:LYS:O	2:O:109:VAL:HA	2.12	0.49
2:O:203:ARG:HH12	2:O:233:SER:HA	1.78	0.49
3:P:11:MET:HG2	3:P:12:LYS:N	2.27	0.49
7:G:32:LYS:C	7:G:35:PRO:HD2	2.33	0.49
3:P:164:ILE:O	3:P:177:ARG:HD2	2.13	0.49
2:O:47:ILE:HG21	2:O:120:MET:HE3	1.95	0.49
7:T:46:LEU:N	7:T:46:LEU:HD22	2.27	0.49
1:A:344:ARG:HG2	1:A:344:ARG:NH1	2.25	0.48
3:P:13:ILE:O	3:P:13:ILE:HG22	2.13	0.48
1:A:39:VAL:HG11	1:A:195:MET:HE2	1.93	0.48
1:A:354:VAL:HG21	1:A:404:ALA:HA	1.95	0.48
2:B:243:GLU:HA	2:B:424:MET:O	2.13	0.48
2:B:246:GLU:O	2:B:427:SER:HA	2.13	0.48
4:D:208:MET:HA	20:D:2006:PEE:H312	1.94	0.48
1:N:15:GLN:O	1:N:26:ALA:HA	2.13	0.48
8:U:39:LEU:O	8:U:42:GLU:HB3	2.13	0.48
2:O:95:LYS:HB2	9:V:32:ALA:CB	2.25	0.48
2:B:52:LYS:NZ	2:B:232:LEU:HD11	2.28	0.48
3:C:158:THR:O	3:C:162:GLU:HG3	2.13	0.48
3:C:68:HIS:CD2	23:C:4195:HOH:O	2.59	0.48
1:N:233:PRO:O	5:R:22:THR:HA	2.13	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Distance(Å)	Clash(Å)
3:P:129:MET:HE1	3:P:181:PHE:CD2	2.40	0.48
3:P:311:LYS:HG2	3:P:374:ASN:OD1	2.14	0.48
5:R:77:LYS:HE3	5:R:79:SER:OG	2.13	0.48
23:A:4251:HOH:O	9:I:39:GLU:CG	2.62	0.48
1:N:308:GLN:HB3	23:N:4088:HOH:O	2.13	0.48
2:O:199:PHE:O	2:O:226:ILE:HD13	2.14	0.48
2:B:47:ILE:HG13	2:B:120:MET:HE1	1.96	0.48
2:B:217:LYS:HE2	2:B:221:GLU:OE2	2.14	0.48
2:B:354:ASN:N	2:B:355:PRO:CD	2.76	0.48
5:E:131:GLU:HG2	5:E:132:TRP:CD1	2.47	0.48
2:O:201:SER:H	2:O:226:ILE:HG23	1.78	0.48
2:O:246:GLU:O	2:O:427:SER:HA	2.14	0.48
4:D:160:MET:HB2	15:D:501:HEC:C1D	2.44	0.48
7:G:50:PRO:HB2	7:G:51:PRO:HD3	1.96	0.48
2:O:202:ALA:HB3	2:O:230:LEU:N	2.28	0.48
4:Q:43:MET:HE2	4:Q:189:PHE:CZ	2.49	0.48
2:B:232:LEU:O	2:B:233:SER:HB3	2.13	0.48
6:F:49:ARG:NH2	11:F:3012:BHG:H1	2.28	0.48
2:B:437:ASP:OD2	2:O:240:HIS:CD2	2.67	0.48
9:I:36:ALA:HB3	9:I:73:PRO:CG	2.42	0.47
10:W:56:LYS:O	10:W:60:GLU:HG3	2.13	0.47
2:B:397:THR:CG2	2:B:401:GLN:HE21	2.18	0.47
1:N:158:PHE:O	1:N:164:ALA:HB2	2.14	0.47
2:O:124:LEU:HD13	2:O:223:PHE:CB	2.44	0.47
3:P:115:ILE:HD13	3:P:195:VAL:HG12	1.95	0.47
3:P:319:PRO:HD2	23:P:4186:HOH:O	2.13	0.47
4:Q:43:MET:HE2	4:Q:189:PHE:HZ	1.80	0.47
4:D:74:PRO:CD	4:D:80:MET:HE1	2.41	0.47
2:O:397:THR:CG2	2:O:401:GLN:HE21	2.23	0.47
5:R:144:CYS:HB2	5:R:158:CYS:SG	2.54	0.47
1:A:15:GLN:O	1:A:26:ALA:HA	2.14	0.47
1:A:40:TRP:CZ2	1:A:377:GLU:HA	2.50	0.47
5:E:77:LYS:HE3	5:E:79:SER:OG	2.15	0.47
6:F:34:ASP:O	6:F:58:ARG:NH2	2.47	0.47
2:B:47:ILE:HG21	2:B:120:MET:HE1	1.97	0.47
6:F:104:ARG:HH11	11:F:3012:BHG:C6	2.27	0.47
4:D:231:LYS:HD3	6:F:70:MET:CE	2.44	0.47
9:I:71:ASN:ND2	23:I:1406:HOH:O	2.47	0.47
9:I:78:TYR:HA	23:I:1201:HOH:O	2.14	0.47
3:P:214:ASP:CG	7:T:2:ARG:HH22	2.18	0.47
3:C:191:ALA:HA	3:C:194:MET:CE	2.45	0.47
3:C:96:MET:HA	3:C:96:MET:HE2	1.97	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Distance(Å)	Clash(Å)
3:P:327:ALA:HA	7:T:51:PRO:HB3	1.95	0.47
6:S:68:LEU:HD23	6:S:71:ARG:HH22	1.80	0.47
1:N:348:SER:O	1:N:349:ALA:C	2.54	0.47
10:W:2:ALA:HA	10:W:3:PRO:HD3	1.77	0.47
1:A:40:TRP:HB3	1:A:384:LEU:HD11	1.96	0.46
2:B:12:GLU:O	2:B:18:PRO:HD3	2.14	0.46
2:O:370:MET:O	2:O:373:GLU:HG2	2.15	0.46
5:R:189:SER:O	5:R:190:ASP:C	2.53	0.46
9:I:72:VAL:CG1	9:I:73:PRO:HD2	2.45	0.46
2:B:135:TRP:CE2	6:S:49:ARG:HD3	2.50	0.46
4:D:211:MET:HG3	20:D:2006:PEE:H311	1.97	0.46
5:R:131:GLU:HG2	5:R:132:TRP:CD1	2.50	0.46
10:W:20:PHE:CE1	10:W:24:ILE:HD11	2.49	0.46
4:D:47:ALA:HA	4:D:90:TYR:HA	1.96	0.46
8:H:19:THR:O	8:H:23:GLN:HG3	2.15	0.46
1:N:264:HIS:HA	1:N:265:PRO:HD3	1.83	0.46
1:N:3:THR:OG1	1:N:6:GLN:HG3	2.15	0.46
6:S:101:ARG:HG2	6:S:101:ARG:HH11	1.80	0.46
5:E:99:ARG:HB3	5:E:133:VAL:CG1	2.46	0.46
3:P:12:LYS:HA	3:P:12:LYS:CE	2.43	0.46
5:R:93:GLY:O	5:R:94:LYS:HG3	2.14	0.46
2:O:213:HIS:N	2:O:214:PRO:CD	2.79	0.46
2:O:344:VAL:HG11	2:O:417:PHE:CD2	2.50	0.46
4:Q:74:PRO:HB3	4:Q:80:MET:CE	2.45	0.46
5:R:83:GLU:HG2	5:R:102:THR:HG22	1.98	0.46
2:B:102:ARG:HH22	2:B:161:GLU:CD	2.19	0.46
2:B:370:MET:O	2:B:373:GLU:HG2	2.16	0.46
3:C:215:VAL:HG13	23:C:4154:HOH:O	2.15	0.46
3:C:75:TYR:O	3:C:78:ILE:HG22	2.15	0.46
4:D:83:ARG:CZ	4:D:86:LYS:HE2	2.45	0.46
1:N:281:ASP:OD2	9:V:73:PRO:HB3	2.15	0.46
3:P:373:GLU:HB2	23:P:4170:HOH:O	2.16	0.46
6:S:13:LEU:HD22	23:S:4129:HOH:O	2.15	0.46
3:P:375:LYS:O	6:S:17:ARG:NH1	2.49	0.46
2:B:342:ASN:O	2:B:346:THR:HG23	2.15	0.46
2:B:354:ASN:H	2:B:355:PRO:HD2	1.81	0.46
6:S:108:ALA:C	6:S:110:LYS:N	2.68	0.46
10:W:3:PRO:CB	10:W:8:ARG:HD3	2.41	0.46
6:F:49:ARG:HD3	2:O:135:TRP:CE2	2.51	0.46
2:O:25:GLU:O	2:O:36:ALA:HA	2.15	0.46
8:U:28:GLU:CA	8:U:31:VAL:HG22	2.44	0.46
6:F:71:ARG:HD3	23:F:4076:HOH:O	2.15	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Distance(Å)	Clash(Å)
3:C:214:ASP:CG	7:G:2:ARG:HH22	2.19	0.46
1:N:156:THR:HA	5:R:7:VAL:HG21	1.98	0.46
3:P:278:TYR:CZ	3:P:282:ARG:HD3	2.50	0.46
4:Q:134:TYR:CG	4:Q:162:PRO:HG3	2.51	0.46
4:Q:74:PRO:CD	4:Q:80:MET:HE1	2.46	0.46
23:O:4201:HOH:O	9:V:32:ALA:HB1	2.16	0.46
9:V:50:LEU:O	9:V:51:CYS:HB3	2.16	0.46
3:C:115:ILE:HD13	3:C:195:VAL:HG12	1.98	0.45
14:C:502:HEM:HBA1	18:C:2002:UQ:O2	2.16	0.45
1:N:29:GLN:HB3	2:O:12:GLU:O	2.16	0.45
1:A:228:VAL:O	1:A:228:VAL:HG13	2.16	0.45
7:G:2:ARG:HA	23:G:4101:HOH:O	2.16	0.45
2:O:181:TYR:CE1	2:O:182:ARG:HG2	2.51	0.45
3:P:15:ASN:O	3:P:17:ALA:N	2.49	0.45
8:U:28:GLU:HA	8:U:31:VAL:CG2	2.44	0.45
10:W:3:PRO:HB2	10:W:8:ARG:CD	2.43	0.45
7:T:28:HIS:ND1	7:T:32:LYS:HD2	2.31	0.45
3:C:276:PHE:CG	3:C:277:ALA:N	2.84	0.45
6:S:109:LYS:O	6:S:110:LYS:HG2	2.16	0.45
4:D:148:TYR:CZ	4:D:161:ALA:HB2	2.52	0.45
2:O:386:ALA:O	2:O:390:GLY:HA2	2.17	0.45
5:R:190:ASP:HB2	5:R:191:ASP:H	1.42	0.45
3:P:158:THR:O	3:P:162:GLU:HG3	2.16	0.45
2:B:217:LYS:O	2:B:221:GLU:HG3	2.17	0.45
1:A:158:PHE:O	1:A:164:ALA:HB2	2.17	0.45
2:B:95:LYS:O	2:B:109:VAL:HA	2.17	0.45
3:C:80:ARG:C	3:C:80:ARG:HD3	2.37	0.45
3:C:164:ILE:O	3:C:177:ARG:HD2	2.16	0.45
1:A:39:VAL:CG1	1:A:195:MET:HE2	2.47	0.45
6:F:101:ARG:HG2	6:F:101:ARG:NH1	2.32	0.45
9:I:61:GLY:C	9:I:62:ARG:HG3	2.37	0.45
1:N:213:GLN:O	1:N:217:SER:OG	2.27	0.45
2:O:342:ASN:O	2:O:346:THR:HG23	2.16	0.45
5:R:44:THR:HG22	10:W:24:ILE:HG21	1.97	0.45
1:N:117:VAL:HG11	1:N:195:MET:HE1	1.99	0.44
2:O:100:SER:OG	2:O:105:MET:HG2	2.17	0.44
3:P:13:ILE:HA	3:P:17:ALA:HB2	1.99	0.44
1:A:288:ALA:CB	1:A:300:THR:HG22	2.46	0.44
2:O:227:ARG:HD2	2:O:227:ARG:N	2.32	0.44
3:P:348:ILE:O	3:P:352:GLN:HG3	2.17	0.44
3:P:75:TYR:O	3:P:78:ILE:HG22	2.17	0.44
8:U:42:GLU:HG2	8:U:43:ARG:N	2.32	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Distance(Å)	Clash(Å)
4:D:74:PRO:HB3	4:D:80:MET:CE	2.47	0.44
3:P:129:MET:HE1	17:P:3001:SMA:H26	1.98	0.44
3:P:220:PHE:HE1	18:P:3002:UQ:HM23	1.82	0.44
4:Q:160:MET:HB2	15:Q:501:HEC:C1D	2.47	0.44
5:R:112:VAL:HG22	5:R:172:ARG:HH22	1.82	0.44
4:Q:60:GLU:HG3	10:W:62:LYS:HZ3	1.81	0.44
3:C:270:PRO:HG2	3:C:278:TYR:CG	2.52	0.44
1:A:102:LEU:CD2	2:B:369:LEU:HD12	2.47	0.44
3:C:348:ILE:O	3:C:352:GLN:HG3	2.17	0.44
4:D:195:GLU:HG2	4:D:198:HIS:HB2	2.00	0.44
10:J:56:LYS:O	10:J:60:GLU:HG3	2.17	0.44
2:O:248:ASN:OD1	2:O:428:GLY:HA2	2.17	0.44
3:P:11:MET:HE3	3:P:12:LYS:HB2	1.99	0.44
5:R:102:THR:OG1	5:R:104:LYS:HG2	2.18	0.44
10:W:52:TRP:O	10:W:56:LYS:HB2	2.17	0.44
4:D:74:PRO:HA	4:D:79:GLU:O	2.18	0.44
6:F:95:LYS:NZ	6:F:95:LYS:CB	2.80	0.44
1:N:39:VAL:HG11	1:N:195:MET:HE2	1.98	0.44
14:P:502:HEM:HBA1	18:P:3002:UQ:O2	2.18	0.44
1:A:371:GLY:O	1:A:374:PRO:HD2	2.18	0.44
3:C:191:ALA:HA	3:C:194:MET:HE3	2.00	0.44
4:D:214:LEU:O	4:D:217:PRO:HG2	2.17	0.44
9:V:32:ALA:N	9:V:72:VAL:CG2	2.80	0.44
2:B:46:ARG:O	2:B:47:ILE:HD13	2.17	0.44
3:C:132:VAL:HA	3:C:139:SER:HB3	1.98	0.44
2:O:217:LYS:HE2	2:O:221:GLU:OE2	2.18	0.44
5:R:112:VAL:HG21	5:R:172:ARG:NH2	2.32	0.44
5:R:43:THR:O	5:R:47:VAL:HG23	2.17	0.44
9:V:72:VAL:HG13	9:V:73:PRO:HD2	2.00	0.44
9:V:72:VAL:CG1	9:V:73:PRO:HD2	2.47	0.44
5:E:83:GLU:HG2	5:E:100:HIS:CD2	2.53	0.43
4:D:43:MET:CE	4:D:189:PHE:CZ	3.01	0.43
9:I:50:LEU:O	9:I:51:CYS:HB3	2.18	0.43
2:O:215:VAL:CG2	2:O:216:LEU:N	2.80	0.43
6:S:34:ASP:O	6:S:58:ARG:NH2	2.50	0.43
1:A:195:MET:SD	1:A:219:LEU:HD21	2.58	0.43
5:E:99:ARG:HB3	5:E:133:VAL:HG12	2.01	0.43
1:N:1:THR:O	1:N:2:ALA:CB	2.66	0.43
3:P:100:ARG:O	3:P:100:ARG:HD2	2.18	0.43
3:P:282:ARG:NH2	23:P:4173:HOH:O	2.51	0.43
3:P:43:LEU:HD21	20:Q:3006:PEE:H181	2.00	0.43
9:V:64:LEU:HD23	9:V:78:TYR:C	2.38	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:289:HIS:HE1	11:S:2012:BHG:C1'	2.32	0.43
2:B:28:ARG:CG	2:B:28:ARG:HH11	2.32	0.43
2:O:46:ARG:HG2	2:O:379:LEU:HD22	2.00	0.43
4:Q:195:GLU:O	4:Q:195:GLU:HG2	2.19	0.43
1:A:352:SER:OG	6:S:110:LYS:HB2	2.18	0.43
1:A:433:ASP:OD2	1:A:435:ASN:HB2	2.19	0.43
2:B:52:LYS:HZ3	2:B:232:LEU:HD11	1.82	0.43
3:C:197:LEU:HD23	3:C:197:LEU:HA	1.66	0.43
8:H:25:GLU:CB	8:H:34:ARG:NH2	2.67	0.43
3:P:378:LYS:HE3	6:S:17:ARG:NE	2.34	0.43
4:Q:211:MET:HG3	20:Q:3006:PEE:H311	2.00	0.43
2:B:46:ARG:HG2	2:B:110:GLU:HG2	2.00	0.43
1:A:364:ALA:HB2	9:I:33:ALA:HB1	2.01	0.43
2:O:46:ARG:O	2:O:47:ILE:HD13	2.19	0.43
3:P:227:LYS:HE3	22:P:4009:GOL:O1	2.18	0.43
3:P:80:ARG:C	3:P:80:ARG:HD3	2.39	0.43
2:B:187:THR:HB	23:B:4154:HOH:O	2.18	0.43
1:N:236:PHE:CG	1:N:258:GLU:HB2	2.54	0.43
7:T:30:PHE:O	7:T:34:ILE:HG12	2.18	0.43
4:D:124:GLU:OE2	4:D:191:ARG:CD	2.67	0.43
4:D:195:GLU:HG2	4:D:195:GLU:O	2.19	0.43
5:E:191:ASP:CG	5:E:191:ASP:O	2.56	0.43
3:P:191:ALA:HA	3:P:194:MET:CE	2.48	0.43
9:V:62:ARG:HB3	9:V:63:PRO:HD2	2.01	0.43
2:O:203:ARG:HD2	2:O:230:LEU:O	2.19	0.43
4:Q:229:VAL:CG2	7:T:20:PRO:HD3	2.48	0.43
3:C:100:ARG:CZ	14:C:502:HEM:HBD1	2.49	0.43
4:D:239:PRO:O	4:D:241:LYS:HE2	2.19	0.43
9:I:64:LEU:HD23	9:I:78:TYR:C	2.39	0.43
8:U:43:ARG:HD2	8:U:47:ARG:HH21	1.83	0.43
2:B:213:HIS:N	2:B:214:PRO:CD	2.81	0.42
5:E:113:GLU:HG3	5:E:115:SER:OG	2.19	0.42
5:R:17:GLU:H	5:R:17:GLU:CD	2.17	0.42
1:A:192:ALA:HB3	1:A:193:PRO:HD3	1.99	0.42
1:A:59:VAL:HG11	1:A:186:LEU:HD21	2.00	0.42
3:C:97:HIS:CD2	14:C:502:HEM:NC	2.86	0.42
7:G:30:PHE:O	7:G:34:ILE:HG12	2.19	0.42
4:Q:65:ALA:O	4:Q:68:VAL:HG22	2.18	0.42
3:C:193:ALA:O	3:C:196:HIS:HB3	2.19	0.42
3:C:270:PRO:HD2	3:C:275:LEU:HD23	2.01	0.42
4:D:31:GLN:O	4:D:35:GLN:HG2	2.19	0.42
6:F:39:GLU:HG3	23:F:4047:HOH:O	2.19	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:N:157:ALA:HB2	1:N:421:ALA:CB	2.49	0.42
1:N:40:TRP:HB3	1:N:384:LEU:HD11	2.00	0.42
1:N:8:LEU:HD22	1:N:392:LEU:HB3	2.01	0.42
3:P:193:ALA:O	3:P:196:HIS:HB3	2.19	0.42
1:A:352:SER:CB	6:S:110:LYS:HB2	2.50	0.42
3:P:378:LYS:HE3	6:S:17:ARG:CD	2.49	0.42
1:N:8:LEU:O	1:N:11:VAL:HG23	2.19	0.42
1:A:195:MET:HE2	1:A:195:MET:HB3	1.91	0.42
5:E:10:PHE:HB3	7:G:18:LEU:HD11	2.02	0.42
5:E:43:THR:O	5:E:47:VAL:HG23	2.20	0.42
3:P:276:PHE:CG	3:P:277:ALA:N	2.87	0.42
4:Q:43:MET:CE	4:Q:189:PHE:CZ	3.02	0.42
1:A:289:HIS:CE1	11:S:2012:BHG:H1'2	2.52	0.42
2:O:95:LYS:HE2	9:V:32:ALA:N	2.35	0.42
3:C:217:LYS:HG3	7:G:7:LEU:HD13	2.02	0.42
7:G:28:HIS:ND1	7:G:32:LYS:HD2	2.34	0.42
2:B:314:ALA:HA	9:I:63:PRO:HD3	2.02	0.42
5:R:112:VAL:HG21	5:R:172:ARG:HH21	1.84	0.42
5:E:117:LEU:HD13	5:E:170:ARG:HD2	2.01	0.42
5:E:15:ARG:NH2	12:G:4001:AZI:N1	2.68	0.42
5:R:85:LYS:NZ	5:R:87:MET:SD	2.72	0.42
1:N:284:TYR:HE1	9:V:73:PRO:HG3	1.84	0.42
10:W:16:ARG:O	10:W:19:THR:HG22	2.20	0.42
2:B:294:SER:OG	2:B:343:GLN:NE2	2.53	0.42
3:C:314:SER:O	23:C:4170:HOH:O	2.21	0.42
4:D:231:LYS:HA	4:D:231:LYS:HD3	1.89	0.42
1:N:131:ARG:NH1	1:N:174:VAL:O	2.51	0.42
2:O:241:GLY:HA2	2:O:423:SER:OG	2.20	0.42
2:B:353:SER:HB3	2:B:355:PRO:HG2	2.01	0.42
4:D:116:ILE:HA	4:D:116:ILE:HD12	1.86	0.42
2:O:152:LEU:HD13	2:O:158:HIS:CE1	2.55	0.42
3:P:12:LYS:HE2	3:P:16:ASN:HB2	2.02	0.42
3:P:345:HIS:HE1	7:T:65:GLU:OE2	2.02	0.42
5:R:78:LEU:HB2	5:R:191:ASP:HB2	2.02	0.42
1:A:281:ASP:C	1:A:281:ASP:OD1	2.59	0.42
2:B:204:MET:HE1	2:B:224:LEU:HD22	2.01	0.42
3:C:234:LEU:HD12	19:D:2003:CDL:H712	2.01	0.42
3:C:311:LYS:HG2	3:C:374:ASN:CG	2.41	0.42
6:F:102:LYS:HD3	6:F:102:LYS:HA	1.83	0.42
8:H:28:GLU:CA	8:H:31:VAL:HG22	2.47	0.42
3:P:18:PHE:CD2	3:P:19:ILE:HD13	2.55	0.42
3:P:215:VAL:HG13	23:P:4193:HOH:O	2.18	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Distance(Å)	Clash(Å)
3:P:233:LEU:HD11	4:Q:219:VAL:HG21	2.01	0.42
1:A:1:THR:CG2	2:B:212:SER:HB3	2.34	0.41
2:B:364:LEU:HG	2:B:402:ILE:HD13	2.00	0.41
3:P:224:TYR:HB3	22:P:4009:GOL:H31	2.02	0.41
3:P:326:TRP:NE1	7:T:48:VAL:HG22	2.35	0.41
1:N:143:THR:OG1	9:V:48:SER:HB3	2.20	0.41
6:S:77:LYS:HA	6:S:80:TRP:CE2	2.55	0.41
1:A:117:VAL:HG11	1:A:195:MET:HE1	2.01	0.41
3:C:15:ASN:O	3:C:17:ALA:N	2.53	0.41
9:I:52:ARG:NH1	23:I:859:HOH:O	2.54	0.41
1:N:11:VAL:HA	1:N:12:PRO:HD3	1.92	0.41
1:N:146:ARG:NH2	1:N:308:GLN:HE22	2.17	0.41
2:O:257:LEU:O	2:O:323:GLY:HA3	2.21	0.41
1:A:280:TYR:HA	1:A:284:TYR:CE2	2.55	0.41
3:C:277:ALA:HB1	3:C:294:LEU:HD12	2.02	0.41
3:C:278:TYR:CZ	3:C:282:ARG:HD3	2.56	0.41
5:E:189:SER:C	5:E:190:ASP:OD1	2.59	0.41
6:F:99:ARG:NH2	23:F:4055:HOH:O	2.53	0.41
4:D:229:VAL:CG2	7:G:20:PRO:HD3	2.50	0.41
8:H:31:VAL:HA	8:H:34:ARG:HH11	1.84	0.41
1:N:39:VAL:CG1	1:N:195:MET:HE2	2.51	0.41
3:P:30:TRP:CZ3	20:P:3007:PEE:H151	2.55	0.41
3:P:96:MET:HE2	20:P:3007:PEE:H181	2.03	0.41
4:Q:215:LEU:HD21	5:R:46:GLY:HA3	2.02	0.41
5:R:70:ALA:C	5:R:71:MET:HE2	2.40	0.41
23:N:4088:HOH:O	9:V:39:GLU:CG	2.69	0.41
2:B:28:ARG:HG2	2:B:28:ARG:HH11	1.86	0.41
6:F:19:TRP:CD2	11:F:4003:BHG:H1'2	2.56	0.41
1:N:108:LYS:O	1:N:112:LEU:HG	2.21	0.41
2:O:411:ILE:O	2:O:415:LYS:HG3	2.20	0.41
5:R:95:PRO:HG2	5:R:145:VAL:HG22	2.02	0.41
5:R:44:THR:CG2	10:W:24:ILE:HG21	2.51	0.41
1:A:1:THR:HG22	2:B:39:GLU:OE1	2.20	0.41
2:B:46:ARG:HD2	2:B:375:SER:CB	2.50	0.41
3:C:129:MET:HE1	17:C:2001:SMA:H26	2.02	0.41
4:Q:28:ARG:HB3	4:Q:171:PHE:CE1	2.55	0.41
15:Q:501:HEC:HMB1	15:Q:501:HEC:HBB3	2.02	0.41
8:U:31:VAL:HG23	8:U:32:LYS:N	2.35	0.41
1:A:46:ARG:HG2	1:A:231:LEU:HD22	2.03	0.41
2:B:152:LEU:HD13	2:B:158:HIS:CE1	2.55	0.41
2:O:236:LYS:CD	2:O:236:LYS:H	2.32	0.41
5:R:52:LYS:NZ	10:W:32:GLU:OE2	2.48	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:B:257:LEU:O	2:B:323:GLY:HA3	2.21	0.41
2:B:26:PHE:CZ	2:B:391:SER:HA	2.56	0.41
1:N:332:ASP:OD1	1:N:432:PRO:HG3	2.21	0.41
4:Q:117:VAL:O	13:Q:4012:PO4:O2	2.38	0.41
1:A:332:ASP:OD1	1:A:432:PRO:HG3	2.21	0.41
3:P:206:ASN:HB3	14:P:502:HEM:O2D	2.20	0.41
1:A:366:VAL:HG23	1:A:367:SER:N	2.35	0.40
2:O:37:SER:HA	2:O:208:GLY:O	2.21	0.40
2:O:243:GLU:HA	2:O:424:MET:O	2.22	0.40
3:P:245:PHE:CD1	4:Q:17:LEU:HD13	2.56	0.40
4:D:74:PRO:CA	4:D:80:MET:HE2	2.51	0.40
3:P:326:TRP:CH2	20:P:3007:PEE:H322	2.57	0.40
3:P:32:ASN:O	3:P:36:LEU:HG	2.22	0.40
1:A:255:ILE:O	1:A:321:GLY:HA3	2.22	0.40
1:A:442:PHE:C	1:A:442:PHE:CD1	2.95	0.40
3:C:63:PHE:O	3:C:67:THR:HG23	2.22	0.40
4:D:65:ALA:O	4:D:68:VAL:HG22	2.21	0.40
9:I:72:VAL:HG13	9:I:73:PRO:HD2	2.03	0.40
1:N:9:GLN:HE22	1:N:393:ALA:HB1	1.87	0.40
3:P:197:LEU:HA	3:P:197:LEU:HD23	1.73	0.40
3:P:71:ARG:HD3	23:P:4196:HOH:O	2.22	0.40
7:T:50:PRO:HB2	7:T:51:PRO:HD3	2.02	0.40
7:T:72:LYS:HE2	7:T:72:LYS:HB2	1.97	0.40
1:A:2:ALA:HB1	1:A:6:GLN:CB	2.48	0.40
1:N:144:SER:O	1:N:148:VAL:HG23	2.20	0.40
1:N:307:PHE:CD1	1:N:307:PHE:C	2.94	0.40
1:N:366:VAL:HG23	1:N:367:SER:N	2.37	0.40
2:O:120:MET:HB2	2:O:120:MET:HE2	1.92	0.40
2:O:300:ALA:C	2:O:302:GLY:H	2.25	0.40
4:Q:33:TYR:CD1	4:Q:37:CYS:HB2	2.56	0.40
4:Q:79:GLU:HG2	4:Q:79:GLU:H	1.62	0.40
8:H:28:GLU:HA	8:H:31:VAL:CG2	2.48	0.40
8:H:31:VAL:HG23	8:H:32:LYS:N	2.36	0.40
3:P:111:GLU:CD	3:P:111:GLU:H	2.25	0.40
3:P:132:VAL:HA	3:P:139:SER:HB3	2.03	0.40
4:Q:116:ILE:HD12	4:Q:116:ILE:HA	1.90	0.40
4:Q:161:ALA:O	4:Q:162:PRO:C	2.60	0.40
7:T:38:LEU:O	7:T:42:ARG:HG3	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	A	441/446 (99%)	427 (97%)	12 (3%)	2 (0%)	38	33
1	N	441/446 (99%)	425 (96%)	14 (3%)	2 (0%)	38	33
2	B	418/439 (95%)	406 (97%)	11 (3%)	1 (0%)	56	57
2	O	420/439 (96%)	404 (96%)	11 (3%)	5 (1%)	19	11
3	C	363/379 (96%)	353 (97%)	8 (2%)	2 (1%)	33	28
3	P	366/379 (97%)	353 (96%)	8 (2%)	5 (1%)	16	9
4	D	239/241 (99%)	234 (98%)	5 (2%)	0	100	100
4	Q	239/241 (99%)	235 (98%)	4 (2%)	0	100	100
5	E	194/196 (99%)	179 (92%)	14 (7%)	1 (0%)	38	33
5	R	193/196 (98%)	183 (95%)	8 (4%)	2 (1%)	22	14
6	F	97/110 (88%)	97 (100%)	0	0	100	100
6	S	97/110 (88%)	95 (98%)	2 (2%)	0	100	100
7	G	73/81 (90%)	70 (96%)	3 (4%)	0	100	100
7	T	74/81 (91%)	71 (96%)	2 (3%)	1 (1%)	16	9
8	H	64/78 (82%)	63 (98%)	1 (2%)	0	100	100
8	U	64/78 (82%)	61 (95%)	3 (5%)	0	100	100
9	I	38/78 (49%)	35 (92%)	1 (3%)	2 (5%)	3	0
9	V	38/78 (49%)	36 (95%)	1 (3%)	1 (3%)	8	2
10	J	28/62 (45%)	26 (93%)	1 (4%)	1 (4%)	5	1
10	W	60/62 (97%)	58 (97%)	1 (2%)	1 (2%)	14	6
All	All	3947/4220 (94%)	3811 (97%)	110 (3%)	26 (1%)	30	23

All (26) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
9	I	41	PRO

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
10	J	61	ASN
1	N	2	ALA
2	O	226	ILE
2	O	233	SER
3	P	11	MET
3	P	16	ASN
3	P	17	ALA
9	V	41	PRO
10	W	61	ASN
1	A	224	ASP
2	B	171	ALA
3	C	17	ALA
5	E	191	ASP
2	O	171	ALA
3	P	12	LYS
5	R	190	ASP
7	T	72	LYS
3	C	16	ASN
9	I	71	ASN
2	O	227	ARG
5	R	189	SER
2	O	229	GLY
1	A	228	VAL
3	P	13	ILE
1	N	228	VAL

5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution. The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	363/370 (98%)	356 (98%)	7 (2%)	69	73
1	N	363/370 (98%)	355 (98%)	8 (2%)	64	68
2	B	332/343 (97%)	330 (99%)	2 (1%)	92	95
2	O	332/343 (97%)	329 (99%)	3 (1%)	87	91
3	C	313/327 (96%)	307 (98%)	6 (2%)	69	73
3	P	317/327 (97%)	311 (98%)	6 (2%)	69	73

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
4	D	206/206 (100%)	203 (98%)	3 (2%)	76	81
4	Q	206/206 (100%)	202 (98%)	4 (2%)	69	73
5	E	168/168 (100%)	167 (99%)	1 (1%)	92	95
5	R	168/168 (100%)	165 (98%)	3 (2%)	71	75
6	F	90/98 (92%)	89 (99%)	1 (1%)	84	88
6	S	90/98 (92%)	88 (98%)	2 (2%)	64	68
7	G	66/71 (93%)	64 (97%)	2 (3%)	53	55
7	T	66/71 (93%)	63 (96%)	3 (4%)	38	35
8	H	63/74 (85%)	61 (97%)	2 (3%)	51	52
8	U	63/74 (85%)	63 (100%)	0	100	100
9	I	28/60 (47%)	27 (96%)	1 (4%)	47	46
9	V	28/60 (47%)	26 (93%)	2 (7%)	21	16
10	J	23/52 (44%)	23 (100%)	0	100	100
10	W	51/52 (98%)	51 (100%)	0	100	100
All	All	3336/3538 (94%)	3280 (98%)	56 (2%)	73	78

All (56) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	20	ASP
1	A	51	LYS
1	A	58	PHE
1	A	245	GLU
1	A	281	ASP
1	A	348	SER
1	A	365	LEU
2	B	227	ARG
2	B	354	ASN
3	C	80	ARG
3	C	90	PHE
3	C	128	PHE
3	C	222	PRO
3	C	346	PRO
3	C	379	TRP
4	D	17	LEU
4	D	43	MET
4	D	241	LYS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
5	E	35	PHE
6	F	33	ARG
7	G	45	ILE
7	G	73	ASN
8	H	48	SER
8	H	51	GLU
9	I	42	VAL
1	N	20	ASP
1	N	32	GLN
1	N	58	PHE
1	N	184	GLU
1	N	245	GLU
1	N	281	ASP
1	N	348	SER
1	N	365	LEU
2	O	305	GLN
2	O	349	GLN
2	O	354	ASN
3	P	12	LYS
3	P	80	ARG
3	P	90	PHE
3	P	128	PHE
3	P	222	PRO
3	P	379	TRP
4	Q	17	LEU
4	Q	35	GLN
4	Q	43	MET
4	Q	79	GLU
5	R	35	PHE
5	R	113	GLU
5	R	190	ASP
6	S	13	LEU
6	S	33	ARG
7	T	45	ILE
7	T	72	LYS
7	T	73	ASN
9	V	42	VAL
9	V	62	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (41) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	15	GLN
1	A	119	ASN
1	A	136	GLN
1	A	213	GLN
1	A	271	GLN
1	A	289	HIS
1	A	308	GLN
2	B	104	ASN
2	B	240	HIS
2	B	305	GLN
2	B	343	GLN
2	B	401	GLN
2	B	412	ASN
2	B	432	HIS
3	C	54	HIS
3	C	159	ASN
3	C	345	HIS
5	E	57	GLN
7	G	73	ASN
1	N	9	GLN
1	N	32	GLN
1	N	119	ASN
1	N	136	GLN
1	N	213	GLN
1	N	271	GLN
1	N	301	ASN
1	N	308	GLN
2	O	104	ASN
2	O	154	ASN
2	O	240	HIS
2	O	305	GLN
2	O	401	GLN
2	O	412	ASN
2	O	432	HIS
3	P	16	ASN
3	P	159	ASN
3	P	345	HIS
4	Q	35	GLN
5	R	57	GLN
5	R	116	GLN
8	U	49	GLN

5.3.3 RNA ⓘ

There are no RNA chains 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 123 ligands modelled in this entry, 74 are unknown - leaving 49 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$
13	PO4	A	2010	-	4,4,4	0.82	0	6,6,6	0.82	0
12	AZI	A	4002	-	2,2,2	1.19	0	0,1,1	0.00	-
11	BHG	A	4004	-	18,18,18	1.31	3 (16%)	23,23,23	0.61	0
13	PO4	B	3009	-	4,4,4	0.81	0	6,6,6	0.82	0
20	PEE	B	4017	-	5,7,50	4.41	2 (40%)	4,7,55	0.43	0
17	SMA	C	2001	-	38,38,38	1.88	6 (15%)	50,52,52	1.74	7 (14%)
18	UQ	C	2002	-	17,18,63	2.89	11 (64%)	21,24,79	0.66	0
19	CDL	C	2004	-	41,43,99	1.16	1 (2%)	50,55,111	1.56	6 (12%)
12	AZI	C	2005	-	2,2,2	0.97	0	0,1,1	0.00	-
20	PEE	C	2007	-	48,48,50	1.08	4 (8%)	53,53,55	0.87	5 (9%)
22	GOL	C	2008	-	5,5,5	1.20	0	5,5,5	0.74	0
11	BHG	C	2011	-	18,18,18	1.77	5 (27%)	23,23,23	0.72	0
22	GOL	C	4008	-	5,5,5	1.14	0	5,5,5	0.62	0
14	HEM	C	501	3	42,50,50	3.24	14 (33%)	27,82,82	1.62	4 (14%)
14	HEM	C	502	3	42,50,50	2.66	13 (30%)	27,82,82	1.67	6 (22%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
19	CDL	D	2003	-	38,38,99	1.17	2 (5%)	47,47,111	1.29	6 (12%)
20	PEE	D	2006	-	50,50,50	1.20	6 (12%)	55,55,55	0.92	5 (9%)
13	PO4	D	4010	-	4,4,4	0.81	0	6,6,6	0.82	0
13	PO4	D	4011	-	4,4,4	0.78	0	6,6,6	0.83	0
15	HEC	D	501	4	50,50,50	3.27	9 (18%)	56,82,82	1.96	7 (12%)
22	GOL	E	4006	-	5,5,5	1.22	0	5,5,5	0.71	0
22	GOL	E	4007	-	3,4,5	2.56	1 (33%)	2,4,5	1.73	1 (50%)
16	FES	E	501	5	0,4,4	0.00	-	0,4,4	0.00	-
11	BHG	F	3012	-	18,18,18	1.82	5 (27%)	23,23,23	0.75	0
11	BHG	F	4003	-	18,18,18	1.78	4 (22%)	23,23,23	0.72	0
12	AZI	G	4001	-	2,2,2	1.45	0	0,1,1	0.00	-
13	PO4	I	4015	-	4,4,4	0.80	0	6,6,6	0.83	0
13	PO4	O	2009	-	4,4,4	0.82	0	6,6,6	0.82	0
22	GOL	O	4005	-	5,5,5	1.20	0	5,5,5	0.70	0
17	SMA	P	3001	-	38,38,38	1.84	6 (15%)	50,52,52	1.62	7 (14%)
18	UQ	P	3002	-	17,18,63	2.65	10 (58%)	21,24,79	0.56	0
19	CDL	P	3004	-	46,48,99	1.13	3 (6%)	56,60,111	1.40	6 (10%)
12	AZI	P	3005	-	2,2,2	1.27	0	0,1,1	0.00	-
20	PEE	P	3007	-	48,48,50	1.11	4 (8%)	53,53,55	0.86	4 (7%)
22	GOL	P	3008	-	5,5,5	1.15	0	5,5,5	0.60	0
13	PO4	P	3010	-	4,4,4	0.78	0	6,6,6	0.82	0
11	BHG	P	3011	-	18,18,18	1.76	4 (22%)	23,23,23	0.76	1 (4%)
22	GOL	P	4009	-	5,5,5	1.00	0	5,5,5	0.60	0
14	HEM	P	501	3	42,50,50	2.84	12 (28%)	27,82,82	1.77	5 (18%)
14	HEM	P	502	3	42,50,50	2.91	10 (23%)	27,82,82	1.42	5 (18%)
19	CDL	Q	3003	-	38,38,99	1.22	3 (7%)	47,47,111	1.26	6 (12%)
20	PEE	Q	3006	-	50,50,50	1.18	6 (12%)	55,55,55	0.90	6 (10%)
13	PO4	Q	4012	-	4,4,4	0.89	0	6,6,6	0.82	0
15	HEC	Q	501	4	50,50,50	3.04	8 (16%)	56,82,82	2.28	17 (30%)
13	PO4	R	4013	-	4,4,4	0.86	0	6,6,6	0.82	0
13	PO4	R	4014	-	4,4,4	0.83	0	6,6,6	0.82	0
16	FES	R	501	5	0,4,4	0.00	-	0,4,4	0.00	-
11	BHG	S	2012	-	18,18,18	1.81	4 (22%)	23,23,23	0.72	0
13	PO4	T	4016	-	4,4,4	0.78	0	6,6,6	0.82	0

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
13	PO4	A	2010	-	-	0/0/0/0	0/0/0/0
12	AZI	A	4002	-	-	0/0/0/0	0/0/0/0
11	BHG	A	4004	-	1/1/5/5	0/9/29/29	0/1/1/1
13	PO4	B	3009	-	-	0/0/0/0	0/0/0/0
20	PEE	B	4017	-	-	0/3/5/54	0/0/0/0
17	SMA	C	2001	-	-	0/33/34/34	0/2/2/2
18	UQ	C	2002	-	-	0/7/33/87	0/1/1/1
19	CDL	C	2004	-	1/1/9/9	1/52/52/110	0/0/0/0
12	AZI	C	2005	-	-	0/0/0/0	0/0/0/0
20	PEE	C	2007	-	-	0/52/52/54	0/0/0/0
22	GOL	C	2008	-	-	0/4/4/4	0/0/0/0
11	BHG	C	2011	-	1/1/5/5	0/9/29/29	0/1/1/1
22	GOL	C	4008	-	-	0/4/4/4	0/0/0/0
14	HEM	C	501	3	-	0/14/114/114	0/0/8/8
14	HEM	C	502	3	-	0/14/114/114	0/0/8/8
19	CDL	D	2003	-	-	0/43/43/110	0/0/0/0
20	PEE	D	2006	-	-	0/54/54/54	0/0/0/0
13	PO4	D	4010	-	-	0/0/0/0	0/0/0/0
13	PO4	D	4011	-	-	0/0/0/0	0/0/0/0
15	HEC	D	501	4	-	0/10/54/54	0/0/8/8
22	GOL	E	4006	-	-	0/4/4/4	0/0/0/0
22	GOL	E	4007	-	-	0/2/2/4	0/0/0/0
16	FES	E	501	5	-	0/0/4/4	0/1/1/1
11	BHG	F	3012	-	1/1/5/5	0/9/29/29	0/1/1/1
11	BHG	F	4003	-	1/1/5/5	0/9/29/29	0/1/1/1
12	AZI	G	4001	-	-	0/0/0/0	0/0/0/0
13	PO4	I	4015	-	-	0/0/0/0	0/0/0/0
13	PO4	O	2009	-	-	0/0/0/0	0/0/0/0
22	GOL	O	4005	-	-	0/4/4/4	0/0/0/0
17	SMA	P	3001	-	-	0/33/34/34	0/2/2/2
18	UQ	P	3002	-	-	0/7/33/87	0/1/1/1
19	CDL	P	3004	-	1/1/9/9	1/57/57/110	0/0/0/0
12	AZI	P	3005	-	-	0/0/0/0	0/0/0/0
20	PEE	P	3007	-	-	0/52/52/54	0/0/0/0
22	GOL	P	3008	-	-	0/4/4/4	0/0/0/0
13	PO4	P	3010	-	-	0/0/0/0	0/0/0/0
11	BHG	P	3011	-	1/1/5/5	0/9/29/29	0/1/1/1
22	GOL	P	4009	-	-	0/4/4/4	0/0/0/0
14	HEM	P	501	3	-	0/14/114/114	0/0/8/8
14	HEM	P	502	3	-	0/14/114/114	0/0/8/8
19	CDL	Q	3003	-	-	0/43/43/110	0/0/0/0
20	PEE	Q	3006	-	-	0/54/54/54	0/0/0/0
13	PO4	Q	4012	-	-	0/0/0/0	0/0/0/0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
15	HEC	Q	501	4	-	0/10/54/54	0/0/8/8
13	PO4	R	4013	-	-	0/0/0/0	0/0/0/0
13	PO4	R	4014	-	-	0/0/0/0	0/0/0/0
16	FES	R	501	5	-	0/0/4/4	0/1/1/1
11	BHG	S	2012	-	1/1/5/5	0/9/29/29	0/1/1/1
13	PO4	T	4016	-	-	0/0/0/0	0/0/0/0

All (156) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	D	501	HEC	C3B-CAB	15.07	1.55	1.34
15	Q	501	HEC	C3B-CAB	13.46	1.52	1.34
15	D	501	HEC	C3C-CAC	13.38	1.52	1.34
15	Q	501	HEC	C3C-CAC	12.66	1.51	1.34
14	C	501	HEM	C3C-C2C	-12.51	1.35	1.45
14	P	501	HEM	C3C-C2C	-11.99	1.36	1.45
14	P	502	HEM	C3C-C2C	-11.80	1.36	1.45
20	B	4017	PEE	C11-C10	9.22	1.55	1.49
14	C	502	HEM	C3C-C2C	-8.74	1.38	1.45
14	C	501	HEM	C3B-C2B	-8.03	1.37	1.45
17	C	2001	SMA	C4-C4A	6.90	1.50	1.41
18	C	2002	UQ	C11-C9	6.82	1.54	1.46
14	C	502	HEM	C3B-C2B	-6.60	1.39	1.45
15	D	501	HEC	C3B-C2B	-6.59	1.34	1.40
18	P	3002	UQ	C11-C9	6.51	1.54	1.46
14	P	502	HEM	C3B-C2B	-6.46	1.39	1.45
14	P	502	HEM	CMB-C2B	6.39	1.55	1.45
17	P	3001	SMA	C4-C4A	6.29	1.50	1.41
14	C	501	HEM	CMC-C2C	5.90	1.55	1.45
14	P	501	HEM	CMC-C2C	5.87	1.55	1.45
14	C	501	HEM	CMD-C2D	5.64	1.54	1.45
14	P	502	HEM	CMC-C2C	5.54	1.54	1.45
15	Q	501	HEC	C3B-C2B	-5.35	1.35	1.40
14	C	502	HEM	CMD-C2D	5.35	1.54	1.45
14	P	501	HEM	C3B-C2B	-5.28	1.40	1.45
14	C	502	HEM	CMC-C2C	5.19	1.54	1.45
17	C	2001	SMA	C20-C19	5.19	1.36	1.33
14	C	502	HEM	CMB-C2B	5.14	1.53	1.45
15	D	501	HEC	C3C-C2C	-5.14	1.35	1.40
14	C	501	HEM	C3C-C4C	-5.13	1.41	1.45
14	C	501	HEM	CMB-C2B	5.01	1.53	1.45
14	P	502	HEM	CMD-C2D	4.75	1.53	1.45

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
17	P	3001	SMA	C20-C19	4.74	1.36	1.33
14	P	501	HEM	CMB-C2B	4.74	1.53	1.45
11	S	2012	BHG	O1-C1	4.55	1.48	1.40
11	F	3012	BHG	O1-C1	4.53	1.48	1.40
11	P	3011	BHG	O1-C1	4.52	1.48	1.40
11	C	2011	BHG	O1-C1	4.47	1.48	1.40
11	F	4003	BHG	O1-C1	4.44	1.48	1.40
14	P	501	HEM	CMD-C2D	4.33	1.52	1.45
17	P	3001	SMA	O1-C2	4.27	1.40	1.35
14	P	501	HEM	CBC-CAC	4.13	1.52	1.29
22	E	4007	GOL	C1-C2	4.07	1.56	1.50
18	C	2002	UQ	C7-C6	4.03	1.59	1.51
14	C	501	HEM	CBB-CAB	4.02	1.51	1.29
15	Q	501	HEC	C4A-NA	3.99	1.42	1.36
14	P	502	HEM	CBC-CAC	3.95	1.51	1.29
15	Q	501	HEC	C3C-C2C	-3.77	1.36	1.40
17	C	2001	SMA	O1-C2	3.76	1.39	1.35
14	P	502	HEM	CBB-CAB	3.66	1.49	1.29
17	C	2001	SMA	C4-C3	3.65	1.51	1.41
19	Q	3003	CDL	PA1-OA5	3.57	1.57	1.51
14	C	501	HEM	C3D-C2D	-3.56	1.34	1.43
11	F	3012	BHG	O5-C1	3.52	1.50	1.41
11	S	2012	BHG	O5-C1	3.49	1.50	1.41
18	C	2002	UQ	C6-C1	3.49	1.56	1.46
18	P	3002	UQ	C6-C1	3.48	1.56	1.46
14	C	502	HEM	CBB-CAB	3.46	1.48	1.29
18	P	3002	UQ	C7-C6	3.40	1.57	1.51
11	F	4003	BHG	O5-C1	3.38	1.50	1.41
20	B	4017	PEE	C15-C14	-3.36	1.53	1.55
14	P	501	HEM	CBB-CAB	3.35	1.48	1.29
19	D	2003	CDL	PA1-OA5	3.34	1.57	1.51
14	C	501	HEM	CBC-CAC	3.33	1.48	1.29
14	C	501	HEM	CMA-C3A	3.32	1.58	1.51
14	C	501	HEM	C4C-NC	3.28	1.41	1.33
14	C	502	HEM	CBC-CAC	3.27	1.47	1.29
11	C	2011	BHG	O5-C1	3.21	1.50	1.41
18	C	2002	UQ	C2-C1	3.19	1.58	1.48
14	P	502	HEM	C1D-ND	3.15	1.41	1.33
15	Q	501	HEC	C1C-NC	3.14	1.41	1.36
17	P	3001	SMA	C4-C3	3.11	1.50	1.41
14	P	501	HEM	C3C-C4C	3.11	1.47	1.45
18	C	2002	UQ	O2-C2	3.10	1.45	1.37

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	P	501	HEM	C4A-C3A	3.10	1.48	1.43
11	P	3011	BHG	O5-C1	3.03	1.49	1.41
14	C	502	HEM	C4C-NC	2.98	1.41	1.33
14	C	502	HEM	C3D-C2D	-2.96	1.35	1.43
14	P	502	HEM	C1C-NC	2.96	1.41	1.33
14	C	502	HEM	C1D-ND	2.94	1.41	1.33
20	P	3007	PEE	O3-C30	2.93	1.42	1.33
18	P	3002	UQ	O2-C2	2.91	1.44	1.37
20	P	3007	PEE	C22-C21	-2.90	1.34	1.51
20	Q	3006	PEE	O3-C30	2.88	1.42	1.33
18	C	2002	UQ	C6-C5	2.86	1.41	1.35
17	P	3001	SMA	C7-C8	2.84	1.44	1.40
20	C	2007	PEE	C22-C21	-2.83	1.34	1.51
18	P	3002	UQ	C2-C1	2.82	1.57	1.48
20	Q	3006	PEE	C19-C18	-2.82	1.34	1.51
20	C	2007	PEE	C19-C18	-2.79	1.34	1.51
11	A	4004	BHG	O1-C1	2.80	1.45	1.40
20	D	2006	PEE	P-O1P	2.79	1.61	1.51
20	D	2006	PEE	C19-C18	-2.79	1.34	1.51
14	P	501	HEM	C4D-ND	2.79	1.40	1.33
20	D	2006	PEE	C22-C21	-2.76	1.34	1.51
20	P	3007	PEE	C19-C18	-2.76	1.34	1.51
11	A	4004	BHG	C4-C5	2.74	1.59	1.53
18	C	2002	UQ	O3-C3	2.74	1.44	1.37
20	D	2006	PEE	O3-C30	2.73	1.41	1.33
18	P	3002	UQ	CM5-C5	2.74	1.56	1.50
20	Q	3006	PEE	C22-C21	-2.73	1.35	1.51
15	Q	501	HEC	C4C-NC	2.72	1.40	1.36
14	C	502	HEM	C1C-NC	2.70	1.40	1.33
18	C	2002	UQ	C12-C11	2.67	1.56	1.55
18	C	2002	UQ	CM5-C5	2.65	1.56	1.50
20	D	2006	PEE	O2-C10	2.63	1.42	1.34
18	P	3002	UQ	O3-C3	2.57	1.43	1.37
18	P	3002	UQ	C6-C5	2.57	1.41	1.35
20	Q	3006	PEE	O2-C10	2.55	1.42	1.34
15	Q	501	HEC	C1B-NB	2.53	1.40	1.36
11	C	2011	BHG	C4-C5	2.52	1.58	1.53
20	Q	3006	PEE	P-O1P	2.52	1.60	1.51
15	D	501	HEC	FE-NC	2.45	2.02	1.92
11	A	4004	BHG	O5-C1	2.44	1.48	1.41
20	C	2007	PEE	P-O1P	2.40	1.60	1.51
11	P	3011	BHG	C4-C5	2.39	1.58	1.53

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	F	4003	BHG	C4-C5	2.37	1.58	1.53
15	D	501	HEC	C1C-NC	2.35	1.40	1.36
18	P	3002	UQ	C3-C4	2.35	1.55	1.48
15	D	501	HEC	FE-NB	2.35	2.02	1.92
15	D	501	HEC	C3C-C4C	2.35	1.48	1.42
11	S	2012	BHG	C4-C5	2.35	1.58	1.53
11	F	3012	BHG	O5-C5	2.34	1.50	1.44
20	Q	3006	PEE	C3-C2	2.32	1.57	1.50
18	C	2002	UQ	C5-C4	2.32	1.56	1.46
14	C	502	HEM	C1B-C2B	-2.30	1.43	1.45
20	C	2007	PEE	O3-C30	2.29	1.40	1.33
19	C	2004	CDL	OA8-CA6	-2.25	1.40	1.45
20	P	3007	PEE	P-O1P	2.23	1.59	1.51
11	S	2012	BHG	O5-C5	2.23	1.49	1.44
14	C	501	HEM	C1C-NC	2.21	1.39	1.33
15	D	501	HEC	C3B-C4B	2.21	1.47	1.42
14	C	501	HEM	FE-ND	2.21	2.04	1.95
17	P	3001	SMA	C6-C7	2.21	1.42	1.38
14	C	502	HEM	FE-NB	2.21	2.03	1.95
19	P	3004	CDL	OA8-CA6	-2.20	1.40	1.45
18	C	2002	UQ	C3-C4	2.20	1.55	1.48
11	F	3012	BHG	C4-C5	2.18	1.57	1.53
14	P	501	HEM	C1D-ND	2.17	1.39	1.33
19	Q	3003	CDL	O1-C1	2.17	1.50	1.43
14	C	501	HEM	C1A-NA	2.16	1.40	1.36
19	D	2003	CDL	O1-C1	2.16	1.50	1.43
19	P	3004	CDL	O1-C1	2.14	1.50	1.43
18	P	3002	UQ	C5-C4	2.14	1.55	1.46
11	F	3012	BHG	C1-C2	2.14	1.58	1.52
19	Q	3003	CDL	OB8-CB6	-2.12	1.40	1.45
11	P	3011	BHG	C1-C2	2.12	1.58	1.52
11	F	4003	BHG	O5-C5	2.09	1.49	1.44
14	P	502	HEM	C4D-ND	2.09	1.39	1.33
14	P	501	HEM	C3D-C2D	-2.09	1.38	1.43
11	C	2011	BHG	C1-C2	2.08	1.58	1.52
20	D	2006	PEE	C3-C2	2.08	1.56	1.50
11	C	2011	BHG	O5-C5	2.06	1.49	1.44
19	P	3004	CDL	CA3-CA4	2.02	1.56	1.50
17	C	2001	SMA	C6-C7	2.01	1.42	1.38
17	C	2001	SMA	C7-C8	2.00	1.43	1.40

All (104) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
15	Q	501	HEC	CBB-CAB-C3B	-8.16	109.52	127.36
15	D	501	HEC	CBC-CAC-C3C	-8.06	109.75	127.36
17	C	2001	SMA	C9-C2-C3	7.63	129.63	120.42
15	D	501	HEC	CBB-CAB-C3B	-7.16	111.72	127.36
15	Q	501	HEC	CBC-CAC-C3C	-7.04	111.97	127.36
17	P	3001	SMA	C9-C2-C3	6.38	128.12	120.42
15	Q	501	HEC	C2C-C1C-NC	5.39	113.10	109.50
15	D	501	HEC	C2B-C1B-NB	5.02	112.85	109.50
17	C	2001	SMA	C3-C4-C4A	-4.83	114.85	121.30
17	P	3001	SMA	C3-C4-C4A	-4.72	115.01	121.30
14	P	501	HEM	C3A-C4A-NA	4.64	112.60	109.50
15	Q	501	HEC	C2B-C1B-NB	4.54	112.53	109.50
19	D	2003	CDL	OB4-PB2-OB3	-4.53	105.17	118.70
14	C	501	HEM	C3A-C4A-NA	4.51	112.51	109.50
19	Q	3003	CDL	OB4-PB2-OB3	-4.48	105.33	118.70
19	C	2004	CDL	OA4-PA1-OA3	-4.40	105.56	118.70
19	C	2004	CDL	OB4-PB2-OB3	-4.39	105.60	118.70
14	P	501	HEM	C4A-C3A-C2A	-4.26	104.03	107.00
19	P	3004	CDL	OA4-PA1-OA3	-4.24	106.04	118.70
19	P	3004	CDL	OB4-PB2-OB3	-4.20	106.16	118.70
19	C	2004	CDL	CA4-OA6-CA5	-4.17	109.98	117.68
14	C	502	HEM	CBD-CAD-C3D	-3.90	106.04	114.51
17	P	3001	SMA	C9-C10-C11	-3.85	109.07	114.60
19	P	3004	CDL	CA6-OA8-CA7	-3.77	109.98	116.47
14	P	502	HEM	CBD-CAD-C3D	-3.74	106.39	114.51
17	C	2001	SMA	C9-C10-C11	-3.66	109.35	114.60
14	C	501	HEM	C4A-C3A-C2A	-3.65	104.46	107.00
19	P	3004	CDL	CA4-OA6-CA5	-3.55	111.14	117.68
17	C	2001	SMA	O1-C2-C9	-3.51	107.13	112.08
19	C	2004	CDL	CB4-OB6-CB5	-3.46	109.72	117.86
14	P	502	HEM	C4A-NA-C1A	-3.44	103.64	107.93
14	C	502	HEM	C4A-NA-C1A	-3.44	103.65	107.93
15	D	501	HEC	C2C-C1C-NC	3.37	111.75	109.50
14	C	501	HEM	C4A-NA-C1A	-3.33	103.78	107.93
15	Q	501	HEC	C4D-ND-C1D	-3.32	103.92	107.12
15	Q	501	HEC	CBD-CAD-C3D	-3.24	107.23	112.63
14	P	501	HEM	C4A-NA-C1A	-3.19	103.96	107.93
19	D	2003	CDL	OA4-PA1-OA3	-3.18	105.37	112.74
19	C	2004	CDL	CA6-OA8-CA7	-3.16	111.03	116.47
14	P	501	HEM	CMA-C3A-C2A	3.01	130.62	124.94
19	Q	3003	CDL	OA4-PA1-OA3	-2.98	105.83	112.74
14	C	502	HEM	CBA-CAA-C2A	-2.98	107.66	112.63
19	P	3004	CDL	CB4-OB6-CB5	-2.95	110.93	117.86

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	C	502	HEM	C3A-C4A-NA	2.91	111.44	109.50
19	D	2003	CDL	CB6-CB4-CB3	-2.90	105.20	111.86
19	Q	3003	CDL	CB4-OB6-CB5	-2.87	111.12	117.86
14	C	501	HEM	CBA-CAA-C2A	-2.84	107.90	112.63
15	Q	501	HEC	C4C-NC-C1C	-2.84	102.70	106.77
20	P	3007	PEE	C20-C19-C18	2.77	129.27	114.56
19	D	2003	CDL	CB4-OB6-CB5	-2.73	111.43	117.86
20	C	2007	PEE	C20-C19-C18	2.73	129.07	114.56
15	Q	501	HEC	C2D-C1D-ND	2.69	111.29	109.50
19	Q	3003	CDL	CB6-CB4-CB3	-2.68	105.69	111.86
20	Q	3006	PEE	C20-C19-C18	2.66	128.72	114.56
20	D	2006	PEE	C20-C19-C18	2.64	128.60	114.56
15	Q	501	HEC	C4B-NB-C1B	-2.64	102.99	106.77
20	D	2006	PEE	O4P-C4-C5	2.63	113.62	109.37
20	C	2007	PEE	O4P-C4-C5	2.58	113.54	109.37
19	C	2004	CDL	CA6-CA4-CA3	-2.55	106.01	111.86
15	Q	501	HEC	C4B-CHC-C1C	-2.53	121.68	126.92
17	P	3001	SMA	O1-C2-C3	2.53	123.26	120.32
17	C	2001	SMA	O1-C2-C3	2.49	123.22	120.32
15	Q	501	HEC	C4A-C3A-C2A	-2.47	103.95	106.69
17	P	3001	SMA	O1-C2-C9	-2.46	108.62	112.08
15	D	501	HEC	CBD-CAD-C3D	-2.44	108.56	112.63
20	D	2006	PEE	C19-C18-C17	2.43	127.48	114.56
20	C	2007	PEE	C19-C18-C17	2.42	127.41	114.56
20	P	3007	PEE	C19-C18-C17	2.40	127.32	114.56
14	P	502	HEM	CBA-CAA-C2A	2.39	116.61	112.63
20	Q	3006	PEE	C22-C21-C20	2.37	127.14	114.56
20	D	2006	PEE	C22-C21-C20	2.36	127.12	114.56
15	Q	501	HEC	C3A-C4A-NA	2.36	112.61	109.32
20	Q	3006	PEE	C19-C18-C17	2.35	127.05	114.56
20	Q	3006	PEE	O4P-C4-C5	2.35	113.16	109.37
15	Q	501	HEC	CMA-C3A-C4A	2.35	130.80	126.16
17	C	2001	SMA	C10-C9-C2	2.34	119.21	113.35
15	Q	501	HEC	C2B-C1B-CHB	-2.33	121.59	126.00
20	C	2007	PEE	C22-C21-C20	2.29	126.74	114.56
20	P	3007	PEE	C22-C21-C20	2.29	126.72	114.56
20	C	2007	PEE	C23-C22-C21	2.28	126.68	114.56
14	C	502	HEM	C1A-C2A-C3A	-2.28	104.56	106.92
22	E	4007	GOL	O1-C1-C2	2.27	114.59	110.50
15	Q	501	HEC	C3D-C4D-ND	2.24	112.85	109.73
20	P	3007	PEE	C23-C22-C21	2.24	126.47	114.56
15	Q	501	HEC	C1A-C2A-C3A	2.21	108.49	106.70

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
15	D	501	HEC	C4D-ND-C1D	-2.19	105.01	107.12
17	P	3001	SMA	C10-C9-C2	2.18	118.81	113.35
15	D	501	HEC	C4B-NB-C1B	-2.17	103.66	106.77
20	D	2006	PEE	C23-C22-C21	2.16	126.06	114.56
11	P	3011	BHG	O1-C1-C2	2.16	110.92	108.15
20	Q	3006	PEE	C23-C22-C21	2.16	126.02	114.56
14	P	502	HEM	CMC-C2C-C3C	2.14	129.32	124.26
14	C	502	HEM	CMC-C2C-C3C	2.13	129.29	124.26
19	D	2003	CDL	OA4-PA1-OA2	2.12	112.33	105.91
17	P	3001	SMA	C3M-C3-C4	-2.11	117.52	121.04
14	P	502	HEM	C3A-C4A-NA	2.10	110.90	109.50
19	D	2003	CDL	OA2-PA1-OA3	2.09	111.57	105.95
19	P	3004	CDL	CB6-CB4-CB3	-2.08	107.09	111.86
19	Q	3003	CDL	OA2-PA1-OA3	2.07	111.52	105.95
20	Q	3006	PEE	O4P-P-O3P	2.06	110.56	104.68
17	C	2001	SMA	O8-C8-C8A	2.06	123.52	119.82
14	P	501	HEM	CMA-C3A-C4A	-2.05	125.32	128.46
15	Q	501	HEC	C2C-C1C-CHC	-2.04	122.13	126.00
19	Q	3003	CDL	OA4-PA1-OA2	2.04	112.07	105.91

All (8) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
19	C	2004	CDL	CA4
11	C	2011	BHG	C4
11	P	3011	BHG	C4
11	F	3012	BHG	C4
19	P	3004	CDL	CA4
11	S	2012	BHG	C4
11	F	4003	BHG	C4
11	A	4004	BHG	C4

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
19	C	2004	CDL	CA6-OA8-CA7-C31
19	P	3004	CDL	CA6-OA8-CA7-C31

There are no ring outliers.

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, 95th 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	A	442/446 (99%)	0.17	15 (3%) 43 47	24, 37, 59, 111	1 (0%)
1	N	442/446 (99%)	0.51	29 (6%) 18 20	31, 50, 77, 132	1 (0%)
2	B	424/439 (96%)	0.29	14 (3%) 44 49	28, 41, 66, 102	0
2	O	424/439 (96%)	0.59	41 (9%) 8 9	31, 48, 87, 185	0
3	C	365/379 (96%)	0.42	21 (5%) 22 25	24, 34, 48, 108	0
3	P	370/379 (97%)	0.56	23 (6%) 20 22	28, 37, 52, 218	0
4	D	241/241 (100%)	0.41	13 (5%) 25 27	29, 39, 61, 78	0
4	Q	241/241 (100%)	0.65	26 (10%) 6 7	31, 45, 67, 87	0
5	E	196/196 (100%)	1.13	43 (21%) 1 1	32, 57, 105, 117	0
5	R	196/196 (100%)	0.41	15 (7%) 13 15	27, 46, 71, 99	0
6	F	99/110 (90%)	0.50	13 (13%) 4 5	24, 39, 71, 83	0
6	S	99/110 (90%)	0.29	4 (4%) 36 41	28, 40, 67, 88	0
7	G	75/81 (92%)	0.88	11 (14%) 3 3	26, 49, 77, 86	0
7	T	76/81 (93%)	1.65	20 (26%) 1 1	32, 55, 98, 114	0
8	H	66/78 (84%)	1.19	19 (28%) 1 1	40, 56, 73, 78	0
8	U	66/78 (84%)	1.13	14 (21%) 1 1	44, 63, 94, 104	0
9	I	42/78 (53%)	2.18	19 (45%) 1 1	33, 62, 90, 93	0
9	V	42/78 (53%)	2.10	16 (38%) 1 1	36, 78, 94, 100	0
10	J	30/62 (48%)	1.07	4 (13%) 4 4	40, 52, 80, 109	0
10	W	62/62 (100%)	2.29	21 (33%) 1 1	41, 64, 92, 123	0
All	All	3998/4220 (94%)	0.59	381 (9%) 8 9	24, 43, 80, 218	2 (0%)

All (381) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	P	13	ILE	23.4
10	W	1	VAL	21.5
7	T	1	GLY	13.5
7	T	76	ALA	12.4
9	I	50	LEU	12.1
10	W	2	ALA	11.1
10	W	62	LYS	10.9
2	O	12	GLU	10.7
2	O	19	PRO	10.5
5	E	112	VAL	9.8
9	V	50	LEU	9.6
1	A	2	ALA	9.5
9	I	49	VAL	9.3
1	A	225	GLU	8.5
10	W	12	LEU	8.1
10	J	62	LYS	8.0
3	P	18	PHE	8.0
3	P	11	MET	7.9
2	B	231	GLY	7.9
2	B	233	SER	7.8
4	Q	241	LYS	7.7
1	N	222	THR	7.7
1	N	1	THR	7.5
3	P	16	ASN	7.1
1	A	222	THR	6.8
3	P	12	LYS	6.8
3	C	17	ALA	6.7
8	U	50	THR	6.5
3	P	17	ALA	6.4
10	W	13	LEU	6.4
2	B	230	LEU	6.3
3	C	18	PHE	6.2
7	G	30	PHE	6.2
1	A	227	ALA	6.1
6	F	13	LEU	6.1
10	W	5	LEU	6.1
7	T	30	PHE	5.8
3	P	14	VAL	5.8
9	V	49	VAL	5.8
5	E	114	VAL	5.7
2	O	218	GLN	5.6
7	T	34	ILE	5.6
2	B	232	LEU	5.6

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	226	ASP	5.5
2	O	20	HIS	5.5
2	O	228	GLY	5.5
5	E	117	LEU	5.5
10	J	61	ASN	5.4
5	E	115	SER	5.4
4	Q	76	GLU	5.3
9	I	78	TYR	5.3
1	A	1	THR	5.3
9	V	38	SER	5.2
1	N	2	ALA	5.1
8	U	47	ARG	5.1
9	I	48	SER	5.1
7	T	73	ASN	5.0
5	R	189	SER	5.0
9	V	37	THR	5.0
2	B	20	HIS	4.9
3	P	10	LEU	4.8
5	E	196	GLY	4.8
10	W	61	ASN	4.8
10	W	3	PRO	4.8
4	Q	146	GLY	4.7
7	T	32	LYS	4.7
5	E	111	ALA	4.7
5	R	76	ILE	4.6
10	W	30	PHE	4.6
8	H	34	ARG	4.6
8	U	48	SER	4.6
1	N	227	ALA	4.5
5	E	116	GLN	4.5
5	E	127	VAL	4.5
5	E	124	LEU	4.5
4	Q	139	THR	4.5
5	E	194	ILE	4.4
5	E	128	LYS	4.4
2	B	235	ALA	4.4
8	U	44	VAL	4.4
7	T	61	TRP	4.4
8	U	49	GLN	4.4
5	E	35	PHE	4.3
9	I	42	VAL	4.3
5	R	191	ASP	4.3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
4	Q	145	GLU	4.3
2	O	230	LEU	4.3
7	T	31	SER	4.2
4	Q	158	ILE	4.2
10	W	25	VAL	4.2
5	E	113	GLU	4.2
1	A	4	TYR	4.1
1	A	224	ASP	4.1
4	Q	143	LEU	4.1
4	Q	147	LEU	4.1
9	V	61	GLY	4.1
10	W	9	LEU	4.1
5	E	195	VAL	4.1
2	O	392	TYR	4.0
5	R	74	ILE	4.0
2	O	221	GLU	4.0
5	E	108	GLN	4.0
2	B	12	GLU	4.0
10	W	8	ARG	3.9
2	B	41	TYR	3.9
3	C	218	ILE	3.9
7	G	42	ARG	3.9
3	C	155	TYR	3.9
1	N	15	GLN	3.9
2	O	232	LEU	3.8
7	T	2	ARG	3.8
9	V	42	VAL	3.8
3	C	16	ASN	3.8
7	T	75	ALA	3.8
6	S	12	TRP	3.7
3	C	27	ILE	3.7
5	R	75	GLU	3.7
7	T	29	TYR	3.6
2	O	224	LEU	3.6
6	F	110	LYS	3.6
5	E	188	THR	3.6
2	O	223	PHE	3.6
8	U	13	LEU	3.6
9	V	41	PRO	3.6
5	E	122	HIS	3.6
2	B	229	GLY	3.5
4	D	241	LYS	3.5

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	N	206	ARG	3.5
4	Q	144	ARG	3.5
8	U	45	SER	3.5
2	O	18	PRO	3.5
2	B	304	HIS	3.5
2	O	217	LYS	3.5
4	Q	227	TRP	3.5
5	E	89	PHE	3.4
5	E	187	PHE	3.4
3	C	23	ALA	3.4
7	G	29	TYR	3.4
9	I	51	CYS	3.4
3	C	15	ASN	3.4
2	B	439	LEU	3.4
5	E	134	ILE	3.4
7	G	34	ILE	3.4
2	O	264	ILE	3.4
10	W	29	LEU	3.4
6	S	70	MET	3.3
7	T	42	ARG	3.3
1	N	225	GLU	3.3
5	R	23	LYS	3.3
9	V	36	ALA	3.3
1	N	230	THR	3.3
4	D	141	VAL	3.2
1	N	228	VAL	3.2
1	N	226	ASP	3.2
5	E	80	ASP	3.2
8	H	42	GLU	3.2
4	Q	157	ALA	3.2
7	T	28	HIS	3.2
8	U	51	GLU	3.2
8	H	49	GLN	3.2
8	H	31	VAL	3.2
4	Q	1	SER	3.1
3	C	31	TRP	3.1
8	H	37	LEU	3.1
10	W	19	THR	3.1
5	R	190	ASP	3.1
5	E	193	VAL	3.1
7	T	74	PRO	3.1
5	R	194	ILE	3.1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	262	TRP	3.1
2	O	41	TYR	3.1
5	E	76	ILE	3.1
9	V	48	SER	3.1
5	R	19	LEU	3.0
5	R	16	PRO	3.0
4	Q	77	ASP	3.0
10	W	20	PHE	3.0
1	N	193	PRO	3.0
3	P	223	TYR	3.0
9	I	60	ALA	3.0
5	E	184	SER	3.0
4	Q	79	GLU	3.0
1	N	209	LEU	3.0
5	E	110	ALA	3.0
1	N	229	PRO	3.0
9	V	63	PRO	3.0
9	I	71	ASN	3.0
1	N	13	GLU	3.0
4	D	229	VAL	3.0
2	O	304	HIS	3.0
7	T	38	LEU	3.0
5	E	132	TRP	2.9
5	R	12	ASP	2.9
8	H	41	ASP	2.9
2	O	17	VAL	2.9
4	Q	229	VAL	2.9
8	U	67	HIS	2.9
2	O	35	ILE	2.9
2	O	233	SER	2.9
4	Q	142	SER	2.9
4	Q	141	VAL	2.9
5	R	71	MET	2.9
5	E	185	TYR	2.9
2	O	215	VAL	2.9
9	V	78	TYR	2.9
5	E	107	ASP	2.9
5	E	74	ILE	2.9
5	E	49	TYR	2.9
4	D	85	GLY	2.8
8	H	44	VAL	2.8
4	Q	148	TYR	2.8

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
5	E	5	ILE	2.8
5	E	27	GLU	2.8
2	O	439	LEU	2.8
5	E	186	GLU	2.8
4	Q	149	PHE	2.8
8	H	53	ASP	2.8
1	A	228	VAL	2.8
2	O	219	VAL	2.8
2	O	405	VAL	2.8
7	T	64	GLN	2.8
10	W	26	VAL	2.8
2	B	234	GLY	2.8
8	H	51	GLU	2.8
8	U	14	VAL	2.7
1	A	20	ASP	2.7
4	Q	206	LEU	2.7
3	P	27	ILE	2.7
10	W	22	LEU	2.7
1	N	51	LYS	2.7
9	I	62	ARG	2.7
2	O	229	GLY	2.7
3	P	218	ILE	2.7
9	V	33	ALA	2.7
8	H	29	LYS	2.7
9	V	52	ARG	2.7
2	O	303	VAL	2.7
1	N	443	TRP	2.7
9	V	32	ALA	2.7
10	J	60	GLU	2.7
4	D	214	LEU	2.7
9	I	52	ARG	2.7
2	O	25	GLU	2.7
4	D	81	PHE	2.7
4	D	230	LEU	2.7
2	O	226	ILE	2.6
3	P	155	TYR	2.6
4	D	79	GLU	2.6
9	I	73	PRO	2.6
3	C	25	SER	2.6
10	W	24	ILE	2.6
1	N	22	GLY	2.6
3	C	224	TYR	2.6

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
2	O	21	PRO	2.6
1	A	365	LEU	2.6
5	E	190	ASP	2.6
5	R	80	ASP	2.6
7	G	60	THR	2.6
4	Q	106	ASN	2.6
8	H	35	GLU	2.6
1	N	16	VAL	2.6
7	G	64	GLN	2.6
6	F	12	TRP	2.5
3	P	224	TYR	2.5
8	H	14	VAL	2.5
3	P	345	HIS	2.5
9	V	40	SER	2.5
2	O	26	PHE	2.5
3	C	209	THR	2.5
2	O	355	PRO	2.5
5	E	84	GLY	2.5
3	P	88	SER	2.5
6	F	108	ALA	2.5
4	D	170	GLU	2.5
5	E	153	PHE	2.5
1	N	122	LEU	2.5
2	O	22	GLN	2.5
7	G	56	TYR	2.5
2	O	33	LEU	2.5
4	Q	230	LEU	2.5
9	I	63	PRO	2.5
2	O	206	LEU	2.4
3	P	320	LEU	2.4
2	O	407	ASP	2.4
3	P	227	LYS	2.4
9	I	64	LEU	2.4
9	I	58	GLN	2.4
5	E	98	VAL	2.4
4	D	116	ILE	2.4
5	R	98	VAL	2.4
6	F	22	ASN	2.4
1	N	17	SER	2.4
3	P	15	ASN	2.4
3	C	104	TYR	2.4
8	H	67	HIS	2.4

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
8	H	48	SER	2.4
3	P	31	TRP	2.4
10	W	28	ALA	2.4
2	O	350	GLY	2.4
4	Q	75	ASN	2.4
1	N	320	LEU	2.3
9	I	70	LEU	2.3
1	N	224	ASP	2.3
4	Q	167	GLU	2.3
1	N	18	GLN	2.3
1	A	122	LEU	2.3
10	W	33	ARG	2.3
2	O	386	ALA	2.3
5	E	191	ASP	2.3
2	O	351	ASN	2.3
2	O	27	THR	2.3
9	I	37	THR	2.3
4	D	80	MET	2.3
6	F	19	TRP	2.3
2	O	29	LEU	2.3
7	T	60	THR	2.3
9	V	51	CYS	2.3
6	F	16	ILE	2.3
9	I	55	LEU	2.3
8	U	41	ASP	2.3
5	R	196	GLY	2.2
7	G	38	LEU	2.2
6	S	69	SER	2.2
7	T	37	VAL	2.2
1	N	176	LYS	2.2
1	N	203	LEU	2.2
8	H	46	SER	2.2
2	O	225	ASN	2.2
3	P	93	CYS	2.2
2	O	24	LEU	2.2
3	C	211	ILE	2.2
5	E	37	TYR	2.2
3	C	93	CYS	2.2
3	P	43	LEU	2.2
8	U	39	LEU	2.2
7	T	17	SER	2.2
8	H	36	ARG	2.1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
3	C	217	LYS	2.1
10	W	21	ALA	2.1
8	U	26	GLN	2.1
7	G	58	VAL	2.1
5	E	103	LYS	2.1
6	S	15	GLY	2.1
1	A	184	GLU	2.1
8	U	42	GLU	2.1
3	P	40	CYS	2.1
1	N	20	ASP	2.1
5	E	78	LEU	2.1
2	B	227	ARG	2.1
4	D	73	GLY	2.1
8	H	22	GLU	2.1
1	A	59	VAL	2.1
7	G	61	TRP	2.1
6	F	70	MET	2.1
1	N	5	ALA	2.1
6	F	14	GLU	2.1
6	F	106	GLU	2.1
8	H	45	SER	2.1
5	E	123	ASP	2.1
3	C	33	PHE	2.1
3	P	91	PHE	2.1
9	I	61	GLY	2.1
3	C	207	ASN	2.1
4	Q	107	GLY	2.1
4	D	103	ALA	2.1
6	F	66	LEU	2.1
2	B	301	LYS	2.1
7	T	35	PRO	2.1
6	F	107	TRP	2.1
1	N	355	LEU	2.0
8	H	27	LEU	2.0
5	E	92	ARG	2.0
6	F	109	LYS	2.0
3	C	102	LEU	2.0
4	Q	233	ARG	2.0
9	I	41	PRO	2.0
10	J	37	GLN	2.0
7	G	26	PHE	2.0
1	N	383	LEU	2.0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
3	C	208	PRO	2.0
3	C	101	GLY	2.0

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, 95th 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	RSR	LLDF	B-factors(Å ²)	Q<0.9
13	PO4	R	4014	5/5	0.32	451.00	173,174,174,174	0
21	UNL	B	4039	1/-	0.36	259.00	73,73,73,73	0
21	UNL	D	4083	1/-	0.54	142.33	82,82,82,82	0
21	UNL	P	4046	1/-	0.48	123.00	65,65,65,65	0
21	UNL	N	4029	1/-	1.34	117.47	94,94,94,94	0
21	UNL	C	4068	1/-	0.56	77.00	72,72,72,72	0
21	UNL	N	4022	1/-	0.38	69.50	81,81,81,81	0
21	UNL	R	4069	1/-	0.42	49.18	62,62,62,62	0
21	UNL	B	4025	1/-	1.73	45.59	93,93,93,93	0
21	UNL	B	4026	1/-	1.25	43.74	92,92,92,92	0
21	UNL	I	4072	1/-	2.04	38.33	93,93,93,93	0
11	BHG	F	3012	18/18	0.92	33.87	159,162,164,164	0
21	UNL	A	4075	1/-	0.88	33.18	64,64,64,64	0
21	UNL	V	4078	1/-	1.51	32.00	94,94,94,94	0
21	UNL	A	4087	1/-	0.34	30.78	60,60,60,60	0
21	UNL	C	4023	1/-	0.53	29.94	55,55,55,55	0
21	UNL	A	4035	1/-	0.96	29.77	69,69,69,69	0
21	UNL	A	4076	1/-	0.48	28.66	68,68,68,68	0
21	UNL	A	4091	1/-	0.72	27.86	72,72,72,72	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(Å ²)	Q<0.9
21	UNL	C	4045	1/-	0.41	27.59	71,71,71,71	0
21	UNL	B	4080	1/-	0.66	25.60	67,67,67,67	0
21	UNL	Q	4044	1/-	1.27	25.49	88,88,88,88	0
21	UNL	B	4057	1/-	0.85	24.81	57,57,57,57	0
21	UNL	C	4063	1/-	0.98	22.67	74,74,74,74	0
21	UNL	B	4030	1/-	0.41	21.83	70,70,70,70	0
21	UNL	N	4019	2/-	0.27	20.35	76,76,76,76	0
21	UNL	I	4033	1/-	0.86	19.47	69,69,69,69	0
21	UNL	O	4084	1/-	0.61	19.28	67,67,67,67	0
21	UNL	F	4028	1/-	0.59	19.13	82,82,82,82	0
21	UNL	A	4032	1/-	0.71	18.59	65,65,65,65	0
21	UNL	B	4079	1/-	0.42	18.09	66,66,66,66	0
21	UNL	U	4056	1/-	1.00	17.02	101,101,101,101	0
21	UNL	G	4064	1/-	0.49	16.73	56,56,56,56	0
11	BHG	F	4003	18/18	0.65	16.38	176,180,181,181	0
21	UNL	C	4018	2/-	0.32	15.93	74,74,74,76	0
21	UNL	P	4089	1/-	0.45	15.86	63,63,63,63	0
21	UNL	D	4067	1/-	0.58	15.51	58,58,58,58	0
21	UNL	E	4050	1/-	0.39	15.29	65,65,65,65	0
21	UNL	G	4053	1/-	0.21	14.51	77,77,77,77	0
11	BHG	S	2012	18/18	0.43	14.46	89,103,106,107	0
11	BHG	C	2011	18/18	0.47	13.47	106,118,123,125	0
21	UNL	P	4058	1/-	0.28	12.06	61,61,61,61	0
21	UNL	T	4065	1/-	0.72	11.68	66,66,66,66	0
12	AZI	P	3005	3/3	0.33	10.27	54,54,59,63	0
22	GOL	E	4007	5/6	0.45	10.16	97,100,101,102	0
22	GOL	O	4005	6/6	0.90	9.16	166,167,167,168	0
21	UNL	O	4071	1/-	0.82	8.84	70,70,70,70	0
21	UNL	V	4090	1/-	0.96	8.67	74,74,74,74	0
11	BHG	P	3011	18/18	0.38	8.52	99,107,109,109	0
12	AZI	A	4002	3/3	0.63	8.03	48,48,58,65	0
21	UNL	D	4036	1/-	0.34	7.74	83,83,83,83	0
13	PO4	R	4013	5/5	0.26	7.73	114,114,116,116	0
22	GOL	P	3008	6/6	0.49	7.12	83,84,85,88	0
21	UNL	U	4049	1/-	0.68	6.18	77,77,77,77	0
21	UNL	A	4048	1/-	0.35	6.04	72,72,72,72	0
12	AZI	C	2005	3/3	0.30	5.71	41,41,55,60	0
21	UNL	D	4027	1/-	0.31	5.02	87,87,87,87	0
21	UNL	P	4040	1/-	0.31	5.01	73,73,73,73	0
21	UNL	O	4037	1/-	0.78	4.98	62,62,62,62	0
21	UNL	D	4054	1/-	0.49	4.85	76,76,76,76	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(Å ²)	Q<0.9
13	PO4	D	4011	5/5	0.31	4.82	130,130,130,131	0
20	PEE	B	4017	8/51	0.40	4.77	85,88,91,92	0
20	PEE	D	2006	51/51	0.32	4.49	85,98,115,118	0
22	GOL	E	4006	6/6	0.25	4.21	67,71,72,75	0
22	GOL	C	2008	6/6	0.29	4.16	60,63,63,70	0
21	UNL	O	4041	1/-	0.31	4.11	71,71,71,71	0
21	UNL	B	4034	1/-	0.68	4.08	87,87,87,87	0
13	PO4	B	3009	5/5	0.12	3.80	97,99,100,101	0
21	UNL	O	4031	1/-	0.46	3.47	86,86,86,86	0
21	UNL	C	4086	1/-	0.21	3.44	50,50,50,50	0
21	UNL	P	4021	2/-	0.20	3.14	71,71,71,73	0
21	UNL	P	4060	1/-	0.34	2.61	88,88,88,88	0
21	UNL	A	4038	1/-	0.59	2.60	85,85,85,85	0
21	UNL	P	4074	1/-	0.15	2.37	59,59,59,59	0
22	GOL	P	4009	6/6	0.34	2.18	67,70,71,72	0
20	PEE	C	2007	49/51	0.25	2.14	33,58,74,74	0
20	PEE	Q	3006	51/51	0.22	2.13	53,65,110,110	0
13	PO4	A	2010	5/5	0.22	2.12	133,133,134,134	0
21	UNL	B	4051	1/-	0.19	2.11	78,78,78,78	0
12	AZI	G	4001	3/3	0.21	2.07	47,47,57,59	0
20	PEE	P	3007	49/51	0.23	2.00	35,58,75,76	0
13	PO4	Q	4012	5/5	0.20	1.95	108,109,110,110	0
21	UNL	G	4070	1/-	0.29	1.65	67,67,67,67	0
19	CDL	P	3004	49/100	0.29	1.57	54,81,117,120	0
13	PO4	I	4015	5/5	0.31	1.34	122,122,123,123	0
21	UNL	N	4073	1/-	0.17	1.21	69,69,69,69	0
21	UNL	B	4052	1/-	0.16	0.93	60,60,60,60	0
18	UQ	C	2002	18/63	0.29	0.92	61,73,76,76	0
19	CDL	C	2004	44/100	0.21	0.92	54,83,104,106	0
17	SMA	C	2001	37/37	0.15	0.64	25,33,44,46	0
19	CDL	D	2003	39/100	0.20	0.61	64,84,106,107	0
18	UQ	P	3002	18/63	0.24	0.36	60,82,85,86	0
22	GOL	C	4008	6/6	0.23	0.29	53,55,60,60	0
15	HEC	D	501	43/43	0.14	0.17	26,33,37,38	0
21	UNL	O	4043	1/-	0.22	0.13	80,80,80,80	0
14	HEM	P	501	43/43	0.15	0.13	22,26,33,40	0
19	CDL	Q	3003	39/100	0.22	0.12	54,90,96,96	0
16	FES	E	501	4/4	0.14	0.11	38,39,40,40	0
14	HEM	C	502	43/43	0.17	0.11	23,26,33,36	0
11	BHG	A	4004	18/18	0.13	0.10	29,36,42,44	0
21	UNL	O	4082	1/-	0.16	0.07	73,73,73,73	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(Å ²)	Q<0.9
14	HEM	C	501	43/43	0.14	-0.01	21,27,34,38	0
17	SMA	P	3001	37/37	0.14	-0.05	30,39,47,52	0
13	PO4	P	3010	5/5	0.18	-0.30	115,115,115,116	0
15	HEC	Q	501	43/43	0.12	-0.45	29,36,41,45	0
14	HEM	P	502	43/43	0.12	-0.70	23,27,37,39	0
16	FES	R	501	4/4	0.13	-0.76	27,29,30,30	0
13	PO4	T	4016	5/5	0.09	-1.17	107,108,108,108	0
13	PO4	O	2009	5/5	0.09	-1.56	76,79,81,81	0
21	UNL	W	4077	1/-	0.11	-2.44	60,60,60,60	0
21	UNL	T	4066	1/-	0.07	-5.76	70,70,70,70	0
21	UNL	R	4055	1/-	0.13	-	73,73,73,73	0
21	UNL	D	4062	1/-	0.39	-	90,90,90,90	0
13	PO4	D	4010	5/5	0.35	-	169,169,170,170	0
21	UNL	A	4081	1/-	0.48	-	71,71,71,71	0
21	UNL	B	4042	1/-	0.35	-	81,81,81,81	0
21	UNL	O	4020	2/-	0.22	-	96,96,96,97	0
21	UNL	V	4024	1/-	1.25	-	96,96,96,96	0
21	UNL	V	4088	1/-	0.90	-	80,80,80,80	0
21	UNL	D	4059	1/-	0.85	-	57,57,57,57	0
21	UNL	E	4061	1/-	0.16	-	79,79,79,79	0
21	UNL	S	4047	1/-	0.58	-	71,71,71,71	0
21	UNL	A	4085	1/-	0.20	-	56,56,56,56	0

6.5 Other polymers ⓘ

There are no such residues in this entry.