Full wwPDB X-ray Structure Validation Report (i)

Jan 31, 2016 – 07:49 PM GMT

PDB ID	:	1HBN
Title	:	METHYL-COENZYME M REDUCTASE
Authors	:	Ermler, U.; Grabarse, W.
Deposited on	:	2001-04-20
Resolution	:	1.16 Å(reported)

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

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

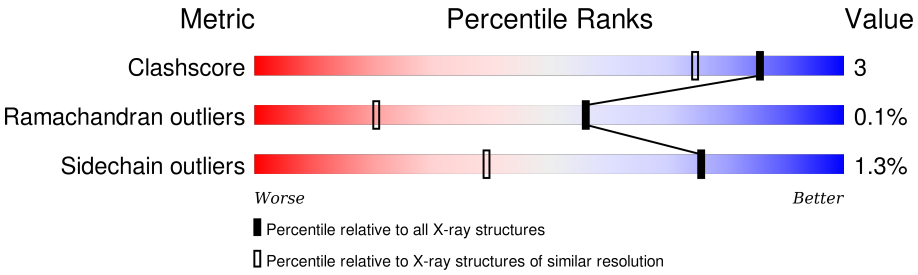
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)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

1 Overall quality at a glance

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

The reported resolution of this entry is 1.16 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	102246	1109 (1.20-1.12)
Ramachandran outliers	100387	1058 (1.20-1.12)
Sidechain outliers	100360	1058 (1.20-1.12)

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

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	549	90% 8% •
1	D	549	90% 9% •
2	B	442	89% 10% •
2	E	442	91% 8% •
3	C	248	88% 10% •
3	F	248	89% 9% •

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

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
4	F43	A	1550	X	-	-	-
4	F43	D	1550	X	-	-	-
5	TP7	A	1551	X	-	-	-
5	TP7	D	1551	X	-	-	-

2 Entry composition

There are 12 unique types of molecules in this entry. The entry contains 21962 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called METHYL-COENZYME M REDUCTASE I ALPHA SUBUNIT.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	548	Total	C	N	O	S	23	13	0
			4292	2712	723	837	20			
1	D	548	Total	C	N	O	S	23	16	0
			4297	2717	721	839	20			

There are 10 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	257	MHS	HIS	MODIFIED RESIDUE	UNP P11558
A	271	AGM	ARG	MODIFIED RESIDUE	UNP P11558
A	400	MGN	GLN	MODIFIED RESIDUE	UNP P11558
A	445	GL3	GLY	MODIFIED RESIDUE	UNP P11558
A	452	SMC	CYS	MODIFIED RESIDUE	UNP P11558
D	257	MHS	HIS	MODIFIED RESIDUE	UNP P11558
D	271	AGM	ARG	MODIFIED RESIDUE	UNP P11558
D	400	MGN	GLN	MODIFIED RESIDUE	UNP P11558
D	445	GL3	GLY	MODIFIED RESIDUE	UNP P11558
D	452	SMC	CYS	MODIFIED RESIDUE	UNP P11558

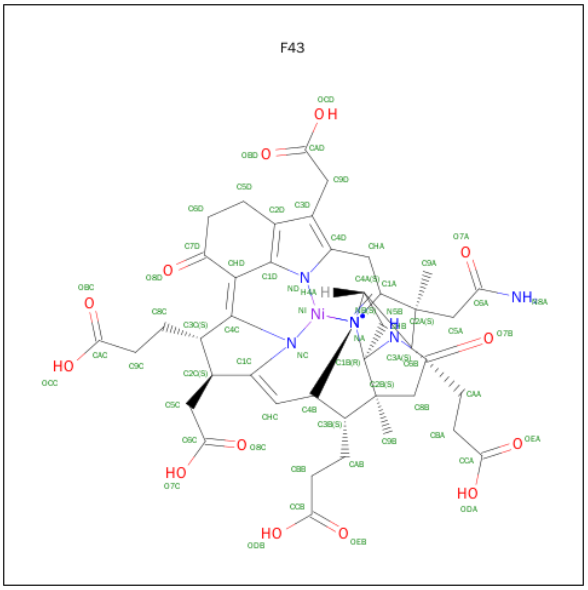
- Molecule 2 is a protein called METHYL-COENZYME M REDUCTASE I BETA SUBUNIT.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	442	Total	C	N	O	S	26	15	0
			3348	2115	557	654	22			
2	E	442	Total	C	N	O	S	41	12	0
			3340	2115	551	653	21			

- Molecule 3 is a protein called METHYL-COENZYME M REDUCTASE I GAMMA SUBUNIT.

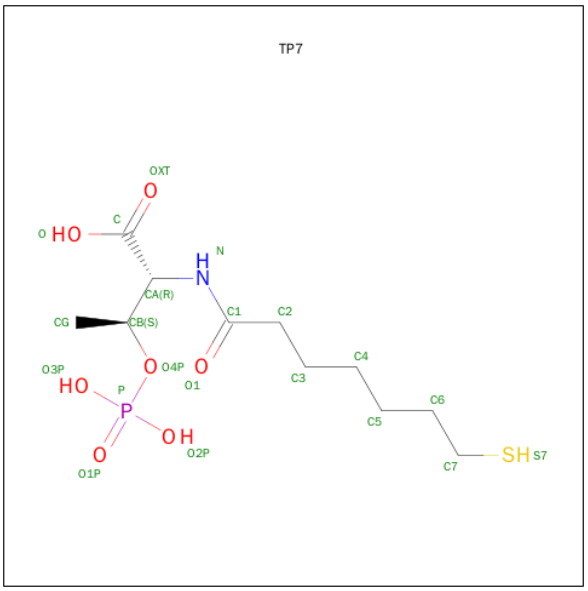
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	247	Total	C	N	O	S	39	5	0
			2008	1242	355	399	12			
3	F	247	Total	C	N	O	S	45	5	0
			2007	1242	354	399	12			

- Molecule 4 is FACTOR 430 (three-letter code: F43) (formula: $C_{42}H_{49}N_6NiO_{13}$).



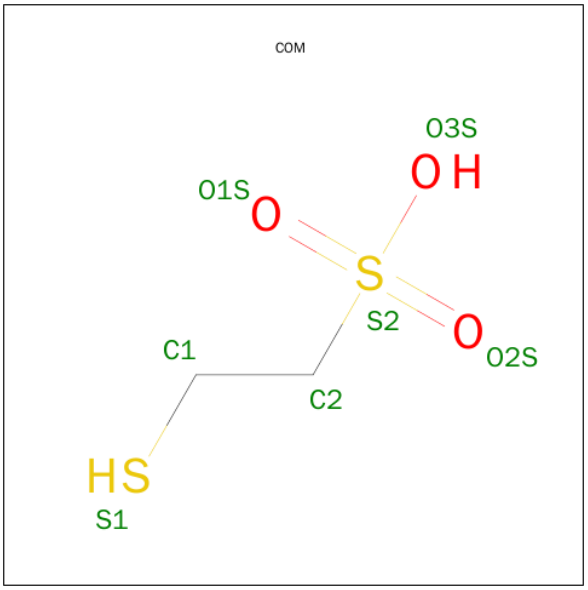
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	A	1	Total	C	N	Ni	O	0	0
			62	42	6	1	13		
4	D	1	Total	C	N	Ni	O	0	0
			62	42	6	1	13		

- Molecule 5 is COENZYME B (three-letter code: TP7) (formula: $C_{11}H_{22}NO_7PS$).



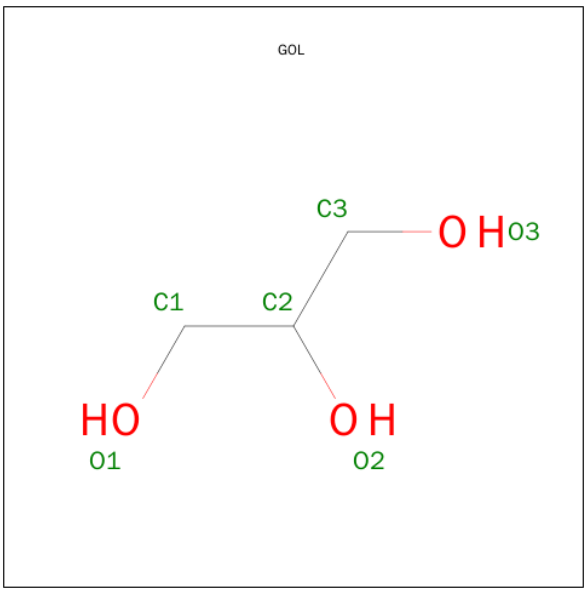
Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
5	A	1	Total	C	N	O	P	S	0	0
			21	11	1	7	1	1		
5	D	1	Total	C	N	O	P	S	0	0
			21	11	1	7	1	1		

- Molecule 6 is 1-THIOETHANESULFONIC ACID (three-letter code: COM) (formula: $C_2H_6O_3S_2$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
6	A	1	Total	C	O	S	0	0
			7	2	3	2		
6	D	1	Total	C	O	S	0	0
			7	2	3	2		

- Molecule 7 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	A	1	Total C O 6 3 3	0	0
7	A	1	Total C O 6 3 3	0	0
7	A	1	Total C O 6 3 3	0	0
7	A	1	Total C O 6 3 3	0	0
7	B	1	Total C O 6 3 3	0	0
7	C	1	Total C O 6 3 3	0	0
7	D	1	Total C O 6 3 3	0	0
7	D	1	Total C O 6 3 3	0	0
7	D	1	Total C O 6 3 3	0	0
7	D	1	Total C O 6 3 3	0	0
7	E	1	Total C O 6 3 3	0	0

- Molecule 8 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
8	A	1	Total Zn 1 1	0	1

- Molecule 9 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
9	D	2	Total Mg 2 2	0	0
9	E	5	Total Mg 5 5	0	0
9	B	2	Total Mg 2 2	0	0
9	C	2	Total Mg 2 2	0	0
9	A	5	Total Mg 5 5	0	0
9	F	2	Total Mg 2 2	0	0

- Molecule 10 is SODIUM ION (three-letter code: NA) (formula: Na).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
10	B	2	Total Na 2 2	0	0
10	A	5	Total Na 5 5	0	0
10	D	3	Total Na 3 3	0	0

- Molecule 11 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
11	B	1	Total Cl 1 1	0	0
11	E	1	Total Cl 1 1	0	0

- Molecule 12 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
12	A	489	Total O 489 489	0	29

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
12	B	423	Total O 423 423	0	31
12	C	294	Total O 294 294	0	25
12	D	510	Total O 510 510	0	37
12	E	402	Total O 402 402	0	33
12	F	275	Total O 275 275	0	15

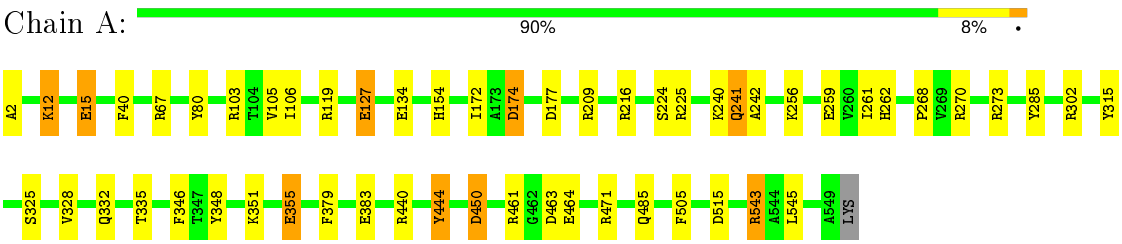
3 Residue-property plots (i)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density (RSRZ > 2). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

Note EDS was not executed.

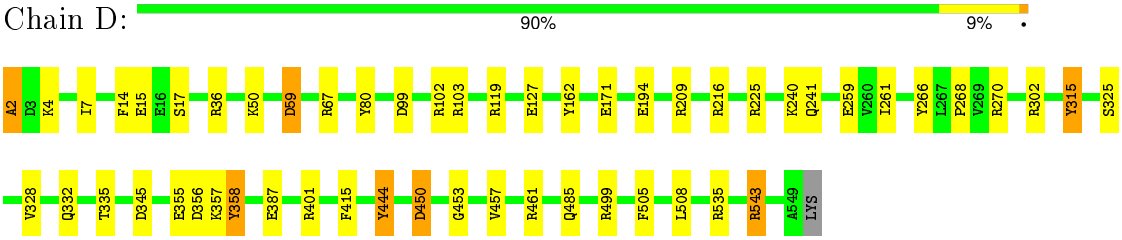
• Molecule 1: METHYL-COENZYME M REDUCTASE I ALPHA SUBUNIT

Chain A:



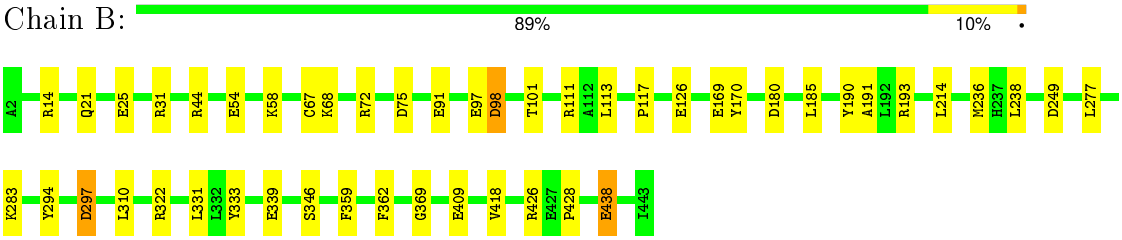
• Molecule 1: METHYL-COENZYME M REDUCTASE I ALPHA SUBUNIT

Chain D:



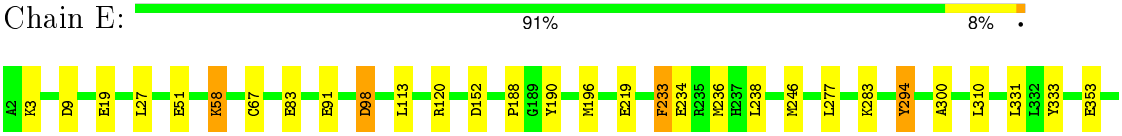
• Molecule 2: METHYL-COENZYME M REDUCTASE I BETA SUBUNIT

Chain B:



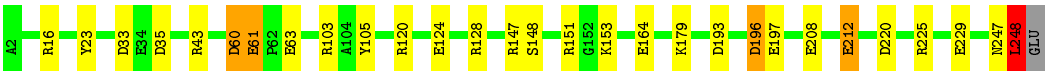
• Molecule 2: METHYL-COENZYME M REDUCTASE I BETA SUBUNIT

Chain E:



• Molecule 3: METHYL-COENZYME M REDUCTASE I GAMMA SUBUNIT

Chain C:



• Molecule 3: METHYL-COENZYME M REDUCTASE I GAMMA SUBUNIT

Chain F:

4 Data and refinement statistics (i)

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

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	81.72Å 116.88Å 122.58Å 90.00° 92.02° 90.00°	Depositor
Resolution (Å)	30.00 – 1.16	Depositor
% Data completeness (in resolution range)	93.1 (30.00-1.16)	Depositor
R_{merge}	0.07	Depositor
R_{sym}	0.07	Depositor
Refinement program	REFMAC	Depositor
R, R_{free}	0.124 , 0.190	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	21962	wwPDB-VP
Average B, all atoms (Å^2)	18.0	wwPDB-VP

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: GOL, MG, CL, ZN, NA, AGM, F43, MGN, TP7, SMC, GL3, COM, MHS

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	0.78	3/4412 (0.1%)	1.25	45/5986 (0.8%)
1	D	0.93	7/4433 (0.2%)	1.23	44/6015 (0.7%)
2	B	0.76	3/3493 (0.1%)	1.22	31/4724 (0.7%)
2	E	1.65	6/3459 (0.2%)	1.19	20/4682 (0.4%)
3	C	0.98	8/2073 (0.4%)	1.47	31/2790 (1.1%)
3	F	0.78	7/2071 (0.3%)	1.37	25/2789 (0.9%)
All	All	1.03	34/19941 (0.2%)	1.27	196/26986 (0.7%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1
1	D	0	1
2	B	0	1
2	E	0	1
3	C	0	1
All	All	0	5

All (34) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	E	438	GLU	CG-CD	83.79	2.77	1.51
2	E	83	GLU	CG-CD	28.40	1.94	1.51
1	D	355	GLU	CG-CD	26.78	1.92	1.51
1	D	127	GLU	CG-CD	-25.44	1.13	1.51
3	C	179	LYS	CD-CE	16.63	1.92	1.51
3	C	164	GLU	CG-CD	15.36	1.75	1.51
2	B	91	GLU	CG-CD	15.15	1.74	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	438	GLU	CG-CD	14.75	1.74	1.51
1	A	240	LYS	CE-NZ	-14.30	1.13	1.49
3	C	212	GLU	CG-CD	-14.20	1.30	1.51
1	A	127	GLU	CG-CD	13.20	1.71	1.51
3	C	60	ASP	CG-OD1	12.76	1.54	1.25
3	F	207	GLU	CG-CD	12.14	1.70	1.51
3	F	164	GLU	CG-CD	10.00	1.67	1.51
1	A	12	LYS	CG-CD	-9.39	1.20	1.52
1	D	240	LYS	CE-NZ	-9.15	1.26	1.49
3	C	63	GLU	CB-CG	-9.02	1.35	1.52
2	E	91[A]	GLU	CG-CD	8.36	1.64	1.51
2	E	91[B]	GLU	CG-CD	8.36	1.64	1.51
1	D	15	GLU	CB-CG	-8.11	1.36	1.52
3	C	208	GLU	CB-CG	-7.69	1.37	1.52
3	F	10	LYS	CG-CD	-7.57	1.26	1.52
2	B	283	LYS	CG-CD	7.26	1.77	1.52
1	D	2	ALA	CA-C	6.66	1.70	1.52
3	F	63	GLU	CB-CG	-6.45	1.39	1.52
3	F	248	LEU	CA-C	6.41	1.69	1.52
3	F	194	GLU	CB-CG	6.25	1.64	1.52
3	C	60	ASP	CG-OD2	-6.25	1.10	1.25
3	F	132	LYS	CG-CD	6.10	1.73	1.52
3	C	197	GLU	CG-CD	-6.01	1.43	1.51
2	E	98	ASP	CA-CB	-5.99	1.40	1.53
2	E	58	LYS	CG-CD	5.65	1.71	1.52
1	D	50	LYS	CD-CE	5.32	1.64	1.51
1	D	450	ASP	CA-CB	-5.15	1.42	1.53

All (196) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	C	60	ASP	CB-CG-OD1	-22.90	97.69	118.30
2	E	438	GLU	CB-CG-CD	-20.86	57.87	114.20
3	F	196	ASP	CB-CG-OD2	18.44	134.90	118.30
2	B	98	ASP	CA-CB-CG	-16.64	76.78	113.40
3	C	120	ARG	NE-CZ-NH2	-15.87	112.36	120.30
3	F	120	ARG	NE-CZ-NH2	-15.15	112.72	120.30
3	F	196	ASP	CB-CG-OD1	-15.15	104.67	118.30
3	F	120	ARG	NE-CZ-NH1	14.35	127.47	120.30
3	C	60	ASP	CB-CG-OD2	14.27	131.14	118.30
3	C	120	ARG	NE-CZ-NH1	13.89	127.25	120.30
2	B	98	ASP	CB-CG-OD2	13.15	130.14	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	D	266	TYR	CB-CG-CD1	12.09	128.25	121.00
1	A	12	LYS	CG-CD-CE	12.08	148.15	111.90
3	F	23	TYR	CB-CG-CD1	11.39	127.83	121.00
1	A	209[A]	ARG	NE-CZ-NH2	11.09	125.84	120.30
1	A	209[B]	ARG	NE-CZ-NH2	11.09	125.84	120.30
1	D	266	TYR	CB-CG-CD2	-11.05	114.37	121.00
2	B	98	ASP	CB-CG-OD1	-10.95	108.44	118.30
1	A	67[A]	ARG	NE-CZ-NH2	10.90	125.75	120.30
1	A	67[B]	ARG	NE-CZ-NH2	10.90	125.75	120.30
1	A	240	LYS	CD-CE-NZ	10.86	136.68	111.70
3	C	103	ARG	NE-CZ-NH1	-10.74	114.93	120.30
1	D	499	ARG	NE-CZ-NH1	-10.27	115.16	120.30
3	F	23	TYR	CB-CG-CD2	-10.04	114.98	121.00
3	C	147	ARG	NE-CZ-NH2	9.97	125.28	120.30
2	E	83	GLU	CB-CG-CD	-9.91	87.44	114.20
1	D	461	ARG	NE-CZ-NH1	-9.89	115.35	120.30
1	A	12	LYS	CB-CG-CD	9.82	137.14	111.60
1	A	177	ASP	CB-CG-OD2	9.65	126.99	118.30
1	D	543	ARG	NE-CZ-NH1	-9.40	115.60	120.30
2	E	426	ARG	NE-CZ-NH2	9.33	124.97	120.30
3	F	248	LEU	CB-CA-C	-9.19	92.74	110.20
2	E	120	ARG	NE-CZ-NH2	9.18	124.89	120.30
2	B	359	PHE	CB-CG-CD2	9.01	127.11	120.80
2	B	438	GLU	CB-CG-CD	-8.94	90.05	114.20
3	C	61	GLU	CA-CB-CG	8.93	133.04	113.40
1	D	355	GLU	CB-CG-CD	-8.90	90.17	114.20
1	D	444	TYR	CB-CG-CD2	8.67	126.20	121.00
1	D	127	GLU	CG-CD-OE1	8.64	135.58	118.30
1	D	127	GLU	CB-CG-CD	8.45	137.00	114.20
2	B	31[A]	ARG	NE-CZ-NH1	-8.35	116.13	120.30
2	B	31[B]	ARG	NE-CZ-NH1	-8.35	116.13	120.30
3	C	128	ARG	NE-CZ-NH1	-8.14	116.23	120.30
3	F	225	ARG	NE-CZ-NH2	-8.12	116.24	120.30
1	A	119	ARG	NE-CZ-NH2	-8.12	116.24	120.30
2	B	409	GLU	OE1-CD-OE2	-8.04	113.66	123.30
3	C	61	GLU	OE1-CD-OE2	-7.93	113.79	123.30
3	C	196	ASP	CB-CG-OD1	7.92	125.43	118.30
1	A	355	GLU	CA-CB-CG	7.91	130.79	113.40
1	D	461	ARG	NE-CZ-NH2	7.80	124.20	120.30
2	E	423	ASP	CB-CG-OD2	-7.71	111.36	118.30
1	A	67[A]	ARG	NE-CZ-NH1	-7.70	116.45	120.30
1	A	67[B]	ARG	NE-CZ-NH1	-7.70	116.45	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	D	67	ARG	NE-CZ-NH2	7.67	124.14	120.30
2	B	190	TYR	CB-CG-CD2	-7.66	116.41	121.00
1	D	444	TYR	CB-CG-CD1	-7.61	116.44	121.00
1	D	270	ARG	NE-CZ-NH1	-7.57	116.52	120.30
1	A	273	ARG	NE-CZ-NH2	7.55	124.07	120.30
1	D	225	ARG	NE-CZ-NH2	7.50	124.05	120.30
2	B	322	ARG	NE-CZ-NH2	7.49	124.05	120.30
1	D	36	ARG	NE-CZ-NH1	-7.49	116.56	120.30
3	C	193	ASP	CB-CG-OD1	7.38	124.94	118.30
1	A	209[A]	ARG	NE-CZ-NH1	-7.37	116.61	120.30
1	A	209[B]	ARG	NE-CZ-NH1	-7.37	116.61	120.30
1	A	285	TYR	CB-CG-CD2	7.31	125.39	121.00
3	C	179	LYS	CG-CD-CE	-7.30	90.00	111.90
2	B	111	ARG	NE-CZ-NH1	-7.19	116.71	120.30
1	D	127	GLU	CG-CD-OE2	-7.18	103.95	118.30
1	A	346	PHE	CB-CG-CD2	7.17	125.82	120.80
1	A	80	TYR	CB-CG-CD2	-7.06	116.76	121.00
1	A	302	ARG	NE-CZ-NH1	-7.04	116.78	120.30
2	B	297	ASP	CB-CG-OD2	6.98	124.58	118.30
3	F	105	TYR	CB-CG-CD1	-6.97	116.82	121.00
3	F	103	ARG	NE-CZ-NH1	-6.93	116.83	120.30
3	C	60	ASP	OD1-CG-OD2	-6.90	110.18	123.30
1	A	471	ARG	NE-CZ-NH2	6.90	123.75	120.30
1	D	103	ARG	NE-CZ-NH1	-6.89	116.85	120.30
3	C	151	ARG	NE-CZ-NH1	-6.81	116.89	120.30
3	C	248	LEU	CB-CG-CD1	-6.78	99.48	111.00
3	C	220	ASP	CB-CG-OD2	6.78	124.40	118.30
2	B	190	TYR	CB-CG-CD1	6.68	125.01	121.00
1	A	216	ARG	NE-CZ-NH2	6.68	123.64	120.30
1	D	15	GLU	CA-CB-CG	6.67	128.08	113.40
3	F	236	ARG	NE-CZ-NH1	-6.63	116.98	120.30
3	C	225	ARG	NE-CZ-NH2	6.62	123.61	120.30
1	A	103	ARG	NE-CZ-NH1	-6.61	117.00	120.30
3	C	147	ARG	NE-CZ-NH1	-6.58	117.01	120.30
1	D	171	GLU	OE1-CD-OE2	-6.51	115.49	123.30
3	F	248	LEU	CA-C-O	6.48	133.71	120.10
2	E	409	GLU	OE1-CD-OE2	-6.48	115.53	123.30
3	C	33	ASP	CB-CG-OD2	6.47	124.13	118.30
2	B	91	GLU	CB-CG-CD	-6.42	96.88	114.20
1	A	127	GLU	CB-CG-CD	-6.38	96.96	114.20
2	B	297	ASP	CB-CG-OD1	-6.38	112.56	118.30
1	D	401	ARG	NE-CZ-NH2	6.37	123.48	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	D	209[A]	ARG	CD-NE-CZ	6.29	132.41	123.60
1	D	209[B]	ARG	CD-NE-CZ	6.29	132.41	123.60
1	D	119	ARG	NE-CZ-NH1	-6.29	117.16	120.30
3	C	208	GLU	CA-CB-CG	6.28	127.22	113.40
3	F	124	GLU	OE1-CD-OE2	-6.24	115.81	123.30
2	B	193	ARG	NE-CZ-NH1	-6.22	117.19	120.30
2	E	440	LYS	CA-CB-CG	6.22	127.08	113.40
3	C	105	TYR	CB-CG-CD1	-6.20	117.28	121.00
1	D	99	ASP	CB-CG-OD2	6.19	123.87	118.30
3	C	43	ARG	NE-CZ-NH1	6.15	123.38	120.30
2	E	9	ASP	CB-CG-OD2	-6.12	112.79	118.30
1	A	515	ASP	CB-CG-OD2	6.09	123.78	118.30
1	A	177	ASP	CB-CG-OD1	-6.08	112.83	118.30
3	F	151	ARG	NE-CZ-NH1	-6.07	117.27	120.30
1	A	259[A]	GLU	OE1-CD-OE2	6.06	130.57	123.30
1	A	259[B]	GLU	OE1-CD-OE2	6.06	130.57	123.30
3	F	248	LEU	N-CA-C	-6.06	94.64	111.00
1	A	270	ARG	NE-CZ-NH2	6.05	123.32	120.30
1	D	216	ARG	NE-CZ-NH1	-6.04	117.28	120.30
3	C	61	GLU	CB-CG-CD	6.02	130.45	114.20
1	A	440	ARG	NE-CZ-NH1	6.02	123.31	120.30
1	A	285	TYR	CB-CG-CD1	-5.97	117.42	121.00
1	D	59	ASP	CB-CG-OD1	5.95	123.66	118.30
1	D	450	ASP	CB-CG-OD2	5.95	123.66	118.30
2	E	294	TYR	CB-CG-CD1	5.94	124.56	121.00
1	D	450	ASP	N-CA-CB	5.93	121.28	110.60
2	E	426	ARG	NE-CZ-NH1	-5.93	117.34	120.30
1	A	450	ASP	N-CA-CB	5.88	121.19	110.60
2	E	233[A]	PHE	CB-CG-CD1	5.88	124.92	120.80
2	E	233[B]	PHE	CB-CG-CD1	5.88	124.92	120.80
1	D	102	ARG	NE-CZ-NH2	-5.86	117.37	120.30
1	D	67	ARG	NE-CZ-NH1	-5.85	117.38	120.30
3	C	23	TYR	CB-CG-CD2	-5.83	117.50	121.00
3	F	225	ARG	NH1-CZ-NH2	5.83	125.82	119.40
2	E	58	LYS	CB-CG-CD	-5.83	96.46	111.60
3	F	105	TYR	CB-CG-CD2	5.82	124.49	121.00
1	A	471	ARG	NE-CZ-NH1	-5.81	117.39	120.30
1	D	315	TYR	CB-CG-CD2	5.75	124.45	121.00
2	B	72	ARG	NE-CZ-NH1	-5.74	117.43	120.30
3	F	128	ARG	NE-CZ-NH1	-5.73	117.44	120.30
1	A	461	ARG	NE-CZ-NH1	-5.73	117.44	120.30
1	D	535	ARG	NE-CZ-NH1	-5.72	117.44	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	40	PHE	CB-CG-CD2	5.70	124.79	120.80
1	A	273	ARG	NE-CZ-NH1	-5.69	117.46	120.30
2	E	353	GLU	OE1-CD-OE2	5.68	130.12	123.30
3	F	185	GLU	OE1-CD-OE2	5.68	130.12	123.30
2	B	426	ARG	NE-CZ-NH2	5.66	123.13	120.30
2	B	54	GLU	OE1-CD-OE2	5.66	130.09	123.30
1	A	225	ARG	NE-CZ-NH2	5.65	123.12	120.30
2	B	180	ASP	CB-CG-OD2	-5.62	113.24	118.30
2	B	72	ARG	NE-CZ-NH2	5.60	123.10	120.30
2	B	283	LYS	CB-CG-CD	-5.58	97.08	111.60
1	A	134[A]	GLU	OE1-CD-OE2	5.58	129.99	123.30
1	A	134[B]	GLU	OE1-CD-OE2	5.58	129.99	123.30
2	B	14	ARG	NE-CZ-NH1	-5.57	117.52	120.30
3	C	247	ASN	O-C-N	-5.56	113.80	122.70
3	F	161	ARG	NE-CZ-NH2	-5.56	117.52	120.30
1	D	216	ARG	NE-CZ-NH2	5.55	123.08	120.30
1	A	543	ARG	NE-CZ-NH1	-5.54	117.53	120.30
3	C	103	ARG	NE-CZ-NH2	5.52	123.06	120.30
2	B	170	TYR	CB-CG-CD1	-5.51	117.69	121.00
3	C	124	GLU	OE1-CD-OE2	-5.51	116.68	123.30
1	D	358	TYR	CB-CG-CD1	-5.51	117.69	121.00
1	A	543	ARG	NE-CZ-NH2	5.50	123.05	120.30
1	D	241	GLN	CA-CB-CG	5.50	125.50	113.40
2	B	169	GLU	OE1-CD-OE2	-5.48	116.73	123.30
1	D	80	TYR	CB-CG-CD2	-5.47	117.72	121.00
1	D	302[A]	ARG	NE-CZ-NH1	-5.47	117.56	120.30
1	D	302[B]	ARG	NE-CZ-NH1	-5.47	117.56	120.30
2	E	190	TYR	CB-CG-CD1	5.47	124.28	121.00
1	A	463	ASP	CB-CG-OD1	5.47	123.22	118.30
2	B	426	ARG	NE-CZ-NH1	-5.42	117.59	120.30
1	A	461	ARG	NE-CZ-NH2	5.41	123.01	120.30
2	B	359	PHE	CB-CG-CD1	-5.40	117.02	120.80
2	E	233[A]	PHE	N-CA-CB	-5.35	100.97	110.60
2	E	233[B]	PHE	N-CA-CB	-5.35	100.97	110.60
1	A	241	GLN	CA-CB-CG	5.32	125.11	113.40
2	E	51	GLU	OE1-CD-OE2	-5.31	116.93	123.30
2	B	249	ASP	CB-CG-OD1	5.26	123.04	118.30
3	F	63	GLU	CA-CB-CG	5.26	124.98	113.40
2	B	31[A]	ARG	NH1-CZ-NH2	5.25	125.17	119.40
2	B	31[B]	ARG	NH1-CZ-NH2	5.25	125.17	119.40
1	D	14	PHE	CB-CG-CD1	-5.19	117.16	120.80
3	F	67	ARG	NE-CZ-NH1	-5.18	117.71	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	D	415	PHE	CB-CG-CD2	5.17	124.42	120.80
3	F	81	ARG	NE-CZ-NH2	-5.17	117.72	120.30
1	D	415	PHE	CB-CG-CD1	-5.16	117.19	120.80
2	E	388	PHE	CB-CG-CD1	5.12	124.39	120.80
1	D	270	ARG	NE-CZ-NH2	5.11	122.85	120.30
3	C	35	ASP	CB-CG-OD1	5.09	122.88	118.30
2	B	97	GLU	CB-CG-CD	-5.09	100.47	114.20
1	D	162	TYR	CB-CG-CD2	5.09	124.05	121.00
1	A	444	TYR	CB-CG-CD1	-5.08	117.95	121.00
3	F	151	ARG	CG-CD-NE	-5.07	101.16	111.80
1	D	450	ASP	CB-CA-C	5.06	120.53	110.40
3	C	23	TYR	CB-CG-CD1	5.06	124.03	121.00
1	A	464	GLU	OE1-CD-OE2	-5.06	117.23	123.30
3	F	174	ARG	NE-CZ-NH1	5.02	122.81	120.30
3	C	16	ARG	NE-CZ-NH1	-5.02	117.79	120.30
2	E	152	ASP	CB-CG-OD2	-5.02	113.78	118.30
3	C	229	GLU	OE1-CD-OE2	-5.01	117.29	123.30

There are no chirality outliers.

All (5) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	241	GLN	Peptide
2	B	333	TYR	Sidechain
3	C	60	ASP	Sidechain
1	D	2	ALA	Mainchain
2	E	333	TYR	Sidechain

5.2 Too-close contacts (i)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	4292	0	4093	24	0
1	D	4297	0	4108	16	1
2	B	3348	0	3331	31	0
2	E	3340	0	3325	28	0
3	C	2008	0	1937	9	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	F	2007	0	1937	3	0
4	A	62	0	43	1	0
4	D	62	0	43	1	0
5	A	21	0	19	0	0
5	D	21	0	19	0	0
6	A	7	0	5	0	0
6	D	7	0	5	0	0
7	A	24	0	31	7	0
7	B	6	0	7	1	0
7	C	6	0	8	0	0
7	D	24	0	31	2	0
7	E	6	0	8	0	0
8	A	1	0	0	0	0
9	A	5	0	0	0	0
9	B	2	0	0	0	0
9	C	2	0	0	0	0
9	D	2	0	0	0	0
9	E	5	0	0	0	0
9	F	2	0	0	0	0
10	A	5	0	0	0	0
10	B	2	0	0	0	0
10	D	3	0	0	0	0
11	B	1	0	0	0	0
11	E	1	0	0	0	0
12	A	489	0	0	10	0
12	B	423	0	0	10	0
12	C	294	0	0	3	0
12	D	510	0	0	6	0
12	E	402	0	0	6	0
12	F	275	0	0	0	0
All	All	21962	0	18950	106	1

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 3.

All (106) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:21[B]:GLN:OE1	12:B:2048[B]:HOH:O	1.58	1.20
2:E:196[B]:MET:HE1	2:E:374:ILE:HG22	1.39	1.01
2:B:236[B]:MET:CE	2:B:236[B]:MET:SD	2.53	0.97

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:236[B]:MET:HB2	3:C:248:LEU:HD11	1.51	0.92
2:B:236[A]:MET:HB2	3:C:248:LEU:HD11	1.53	0.91
1:A:262[B]:HIS:ND1	12:A:2294[B]:HOH:O	2.02	0.90
2:E:196[B]:MET:CE	2:E:374:ILE:HG22	2.00	0.90
2:E:246[A]:MET:CE	2:E:429:LEU:HD12	2.03	0.88
2:B:101:THR:HA	12:B:2076:HOH:O	1.77	0.83
2:E:219:GLU:CD	12:E:2265[B]:HOH:O	2.16	0.81
2:E:246[A]:MET:HE1	2:E:429:LEU:HD12	1.64	0.80
1:A:268:PRO:HG3	12:B:2256:HOH:O	1.82	0.80
1:D:387[B]:GLU:OE1	12:D:2396:HOH:O	2.01	0.77
1:A:256:LYS:O	7:A:1553:GOL:H31	1.88	0.73
2:B:236[B]:MET:CE	2:B:236[B]:MET:HG2	2.18	0.73
1:A:348:TYR:HB3	7:A:1556:GOL:H32	1.71	0.73
2:B:236[B]:MET:CE	2:B:236[B]:MET:CG	2.69	0.71
2:E:196[B]:MET:HE3	2:E:374:ILE:HA	1.73	0.71
2:B:277[B]:LEU:HD21	2:B:294:TYR:CE2	2.26	0.70
7:A:1555:GOL:H12	12:A:2449:HOH:O	1.91	0.70
2:B:236[B]:MET:SD	3:C:248:LEU:HD11	2.32	0.69
2:B:58[A]:LYS:HE3	2:B:75:ASP:OD1	1.93	0.69
2:E:219:GLU:OE1	12:E:2265[B]:HOH:O	2.09	0.68
2:B:236[B]:MET:HB2	3:C:248:LEU:CD1	2.26	0.64
2:E:196[B]:MET:HE1	2:E:374:ILE:CG2	2.22	0.64
2:E:27:LEU:HD22	2:E:246[B]:MET:SD	2.37	0.64
2:B:238:LEU:HD11	12:B:2421[B]:HOH:O	1.99	0.63
2:B:236[A]:MET:HB2	3:C:248:LEU:CD1	2.28	0.62
7:A:1556:GOL:H11	12:A:2008:HOH:O	2.00	0.62
2:B:113[A]:LEU:HD13	2:B:418:VAL:HG13	1.83	0.61
1:A:262[B]:HIS:HD2	12:A:2292[B]:HOH:O	1.83	0.61
1:D:261[B]:ILE:HD12	1:D:508:LEU:HD12	1.81	0.61
2:E:196[B]:MET:CE	2:E:374:ILE:HA	2.31	0.61
2:E:246[A]:MET:CE	2:E:429:LEU:CD1	2.79	0.60
2:E:238:LEU:HD11	12:E:2401[B]:HOH:O	1.99	0.60
1:A:2:ALA:HB3	12:A:2003:HOH:O	2.01	0.59
2:E:277[B]:LEU:HD21	2:E:294:TYR:CE2	2.37	0.59
1:A:315:TYR:HB3	1:A:485:GLN:HE21	1.68	0.59
2:E:58:LYS:HG3	12:E:2115:HOH:O	2.02	0.59
1:D:315:TYR:HB3	1:D:485:GLN:HE21	1.66	0.59
1:A:348:TYR:CB	7:A:1556:GOL:H32	2.33	0.58
2:B:277[B]:LEU:HD21	2:B:294:TYR:HE2	1.68	0.58
1:D:259[B]:GLU:OE2	12:D:2302[B]:HOH:O	0.58	0.58
1:D:4:LYS:HB2	1:D:7:ILE:HG12	1.85	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:44:ARG:NH2	12:B:2076:HOH:O	2.36	0.57
7:D:1556:GOL:H11	12:D:2001:HOH:O	2.05	0.56
1:A:105[B]:VAL:CG1	12:A:2294[B]:HOH:O	2.53	0.56
1:A:224:SER:OG	7:A:1553:GOL:H32	2.04	0.56
2:E:246[A]:MET:HE3	2:E:429:LEU:CD1	2.35	0.56
2:E:233[B]:PHE:CD2	2:E:236[B]:MET:HE2	2.41	0.55
3:C:212:GLU:HG3	12:C:2253:HOH:O	2.06	0.55
1:A:127:GLU:HG3	12:A:2196:HOH:O	2.06	0.55
1:A:15:GLU:HB3	12:A:2011:HOH:O	2.07	0.54
1:A:172:ILE:HD12	12:A:2263:HOH:O	2.08	0.54
1:A:379:PHE:O	1:A:383[B]:GLU:HG3	2.09	0.53
2:E:233[B]:PHE:HD2	2:E:236[B]:MET:HE2	1.74	0.53
1:D:356:ASP:HB3	12:D:2366:HOH:O	2.08	0.53
1:D:268:PRO:HG3	12:E:2248:HOH:O	2.08	0.53
3:C:61:GLU:HG3	12:C:2110:HOH:O	2.07	0.53
1:A:328:VAL:HB	4:A:1550:F43:H9A1	1.90	0.52
1:A:262[B]:HIS:CD2	12:A:2292[B]:HOH:O	2.59	0.51
2:E:233[B]:PHE:CD2	2:E:236[B]:MET:CE	2.94	0.51
1:D:328:VAL:HB	4:D:1550:F43:H9A1	1.93	0.51
3:C:153[B]:LYS:NZ	12:C:2188[B]:HOH:O	2.31	0.50
1:A:154:HIS:NE2	1:A:545:LEU:HD21	2.28	0.49
12:E:2364:HOH:O	3:F:52[B]:VAL:HG21	2.11	0.49
1:D:387[B]:GLU:CD	12:D:2396:HOH:O	2.48	0.49
1:A:351:LYS:NZ	1:A:355:GLU:OE2	2.36	0.48
2:E:246[B]:MET:HE1	2:E:432:VAL:HG12	1.97	0.47
2:E:277[B]:LEU:HD21	2:E:294:TYR:HE2	1.80	0.47
1:A:154:HIS:CE1	1:A:545:LEU:HD21	2.49	0.47
2:B:185[B]:LEU:CD2	2:B:191:ALA:HA	2.45	0.46
12:B:2228:HOH:O	2:E:188:PRO:HD3	2.14	0.46
2:B:68[A]:LYS:HE3	12:B:2114:HOH:O	2.15	0.46
2:B:25:GLU:HG2	7:B:1444:GOL:H32	1.98	0.46
2:B:58[A]:LYS:HE2	12:B:2092:HOH:O	2.16	0.45
1:D:261[B]:ILE:CD1	1:D:508:LEU:HD12	2.46	0.45
2:E:113[A]:LEU:HD13	2:E:418:VAL:HG13	1.98	0.44
1:A:106:ILE:HB	1:A:261:ILE:HB	1.99	0.43
1:D:345:ASP:OD2	7:D:1556:GOL:H12	2.18	0.43
1:A:174:ASP:CG	7:A:1554:GOL:H32	2.38	0.43
1:D:453:GLY:O	1:D:457:VAL:HG23	2.18	0.43
2:B:310:LEU:HD11	2:B:331:LEU:HD23	2.00	0.43
2:E:310:LEU:HD11	2:E:331:LEU:HD23	2.01	0.42
1:A:332:GLN:HA	1:A:335:THR:OG1	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:332:GLN:HA	1:D:335:THR:OG1	2.19	0.42
2:E:3:LYS:NZ	2:E:234:GLU:OE1	2.52	0.42
2:B:117:PRO:HA	12:B:2076:HOH:O	2.19	0.42
2:B:113[A]:LEU:CD1	2:B:418:VAL:HG13	2.48	0.42
2:B:214:LEU:HB2	2:B:428:PRO:HG3	2.02	0.42
2:E:424:GLU:CD	2:E:424:GLU:H	2.23	0.42
2:E:19:GLU:OE2	2:E:440:LYS:NZ	2.46	0.42
2:B:362:PHE:O	2:B:369:GLY:HA3	2.20	0.41
1:D:357:LYS:HE2	1:D:358:TYR:CZ	2.55	0.41
1:A:505:PHE:CE1	2:E:67:CYS:HB3	2.56	0.41
1:A:242:ALA:HB2	3:F:84:TYR:CE2	2.56	0.41
2:B:236[B]:MET:HE2	2:B:236[B]:MET:HG2	2.02	0.41
2:B:113[A]:LEU:HD13	2:B:418:VAL:CG1	2.48	0.41
2:B:67:CYS:HB3	1:D:505:PHE:CE1	2.55	0.41
1:D:194:GLU:HG3	12:D:2131:HOH:O	2.21	0.40
2:B:339:GLU:HG3	2:B:346:SER:HB3	2.03	0.40
2:B:185[B]:LEU:HD21	2:B:191:ALA:HA	2.03	0.40
2:E:300:ALA:HB2	3:F:248:LEU:CD1	2.51	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:59:ASP:OD2	1:D:357:LYS:NZ[2_644]	2.19	0.01

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	A	554/549 (101%)	535 (97%)	18 (3%)	1 (0%)	52 20
1	D	557/549 (102%)	539 (97%)	17 (3%)	1 (0%)	52 20

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	B	456/442 (103%)	447 (98%)	9 (2%)	0	100	100
2	E	452/442 (102%)	445 (98%)	7 (2%)	0	100	100
3	C	250/248 (101%)	245 (98%)	5 (2%)	0	100	100
3	F	250/248 (101%)	242 (97%)	8 (3%)	0	100	100
All	All	2519/2478 (102%)	2453 (97%)	64 (2%)	2 (0%)	56	21

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	325	SER
1	D	325	SER

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	446/434 (103%)	440 (99%)	6 (1%)	76	39
1	D	449/434 (104%)	445 (99%)	4 (1%)	84	55
2	B	357/341 (105%)	353 (99%)	4 (1%)	80	47
2	E	353/341 (104%)	350 (99%)	3 (1%)	86	59
3	C	220/216 (102%)	216 (98%)	4 (2%)	66	26
3	F	220/216 (102%)	215 (98%)	5 (2%)	58	17
All	All	2045/1982 (103%)	2019 (99%)	26 (1%)	76	39

All (26) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	12	LYS
1	A	15	GLU
1	A	174	ASP
1	A	444	TYR
1	A	450	ASP

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Mol	Chain	Res	Type
1	A	543	ARG
2	B	98	ASP
2	B	126	GLU
2	B	297	ASP
2	B	438	GLU
3	C	148[A]	SER
3	C	148[B]	SER
3	C	196	ASP
3	C	248	LEU
1	D	17	SER
1	D	444	TYR
1	D	450	ASP
1	D	543	ARG
2	E	98	ASP
2	E	283	LYS
2	E	438	GLU
3	F	10	LYS
3	F	186	MET
3	F	194	GLU
3	F	196	ASP
3	F	208	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (6) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	485	GLN
1	D	42	ASN
1	D	187	GLN
1	D	365	ASN
1	D	485	GLN
2	E	40	GLN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

10 non-standard protein/DNA/RNA residues are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
1	MHS	A	257	1	8,11,12	1.67	1 (12%)	7,14,16	1.65	2 (28%)
1	AGM	A	271	1	7,11,12	0.98	1 (14%)	5,13,15	1.37	1 (20%)
1	MGN	A	400	1	6,9,10	0.74	0	6,12,14	0.82	0
1	GL3	A	445	1	3,3,4	2.02	1 (33%)	2,2,4	0.72	0
1	SMC	A	452	1	5,6,7	0.61	0	2,6,8	1.94	1 (50%)
1	MHS	D	257	1	8,11,12	1.53	1 (12%)	7,14,16	2.16	3 (42%)
1	AGM	D	271	1	7,11,12	0.96	0	5,13,15	1.34	1 (20%)
1	MGN	D	400	1	6,9,10	1.27	1 (16%)	6,12,14	0.76	0
1	GL3	D	445	1	3,3,4	2.55	1 (33%)	2,2,4	0.96	0
1	SMC	D	452	1	5,6,7	1.06	0	2,6,8	1.30	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
1	MHS	A	257	1	-	0/4/6/8	0/1/1/1
1	AGM	A	271	1	-	0/7/11/13	0/0/0/0
1	MGN	A	400	1	-	0/6/9/12	0/0/0/0
1	GL3	A	445	1	-	0/1/1/2	0/0/0/0
1	SMC	A	452	1	-	0/3/5/7	0/0/0/0
1	MHS	D	257	1	-	0/4/6/8	0/1/1/1
1	AGM	D	271	1	-	0/7/11/13	0/0/0/0
1	MGN	D	400	1	-	0/6/9/12	0/0/0/0
1	GL3	D	445	1	-	0/1/1/2	0/0/0/0
1	SMC	D	452	1	-	0/3/5/7	0/0/0/0

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	445	GL3	C-S	-4.41	1.65	1.80
1	A	445	GL3	C-S	-3.46	1.68	1.80
1	D	400	MGN	CB1-CA	-2.48	1.52	1.55

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	271	AGM	CB-CA	-2.05	1.51	1.53
1	D	257	MHS	CM-ND1	3.29	1.54	1.47
1	A	257	MHS	CM-ND1	3.65	1.55	1.47

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	D	257	MHS	NE2-CE1-ND1	-3.68	107.30	112.28
1	A	257	MHS	O-C-CA	-2.87	118.01	125.49
1	D	271	AGM	CE2-CD-NE1	-2.83	106.67	112.05
1	A	452	SMC	O-C-CA	-2.67	118.52	125.49
1	D	257	MHS	O-C-CA	-2.30	119.50	125.49
1	A	271	AGM	CE2-CD-NE1	-2.29	107.70	112.05
1	A	257	MHS	CD2-NE2-CE1	2.04	108.93	105.71
1	D	257	MHS	CD2-NE2-CE1	2.97	110.40	105.71

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates (i)

There are no carbohydrates in this entry.

5.6 Ligand geometry (i)

Of 48 ligands modelled in this entry, 31 are monoatomic - leaving 17 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	$\#\|Z\| > 2$
4	F43	A	1550	1,6	42,71,71	3.38	14 (33%)	35,118,118	1.65	4 (11%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
5	TP7	A	1551	-	16,20,20	1.47	2 (12%)	16,26,26	1.39	3 (18%)
6	COM	A	1552	4	5,6,6	0.88	0	5,8,8	1.68	1 (20%)
7	GOL	A	1553	10	5,5,5	0.41	0	5,5,5	1.90	2 (40%)
7	GOL	A	1554	-	5,5,5	0.68	0	5,5,5	1.23	1 (20%)
7	GOL	A	1555	-	5,5,5	0.95	0	5,5,5	0.97	0
7	GOL	A	1556	-	5,5,5	1.10	0	5,5,5	0.93	0
7	GOL	B	1444	-	5,5,5	1.24	1 (20%)	5,5,5	1.21	0
7	GOL	C	1249	-	5,5,5	0.55	0	5,5,5	0.30	0
4	F43	D	1550	1,6	42,71,71	3.44	13 (30%)	35,118,118	1.75	6 (17%)
5	TP7	D	1551	-	16,20,20	1.62	2 (12%)	16,26,26	1.29	3 (18%)
6	COM	D	1552	4	5,6,6	0.96	1 (20%)	5,8,8	0.49	0
7	GOL	D	1553	-	5,5,5	0.87	0	5,5,5	0.91	0
7	GOL	D	1554	10	5,5,5	0.67	0	5,5,5	0.59	0
7	GOL	D	1555	-	5,5,5	0.73	0	5,5,5	0.97	0
7	GOL	D	1556	-	5,5,5	1.11	1 (20%)	5,5,5	1.59	2 (40%)
7	GOL	E	1444	-	5,5,5	0.90	0	5,5,5	0.83	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
4	F43	A	1550	1,6	1/1/25/27	0/18/165/165	0/0/10/10
5	TP7	A	1551	-	1/1/5/6	0/20/24/24	0/0/0/0
6	COM	A	1552	4	-	0/4/4/4	0/0/0/0
7	GOL	A	1553	10	-	0/4/4/4	0/0/0/0
7	GOL	A	1554	-	-	0/4/4/4	0/0/0/0
7	GOL	A	1555	-	-	0/4/4/4	0/0/0/0
7	GOL	A	1556	-	-	0/4/4/4	0/0/0/0
7	GOL	B	1444	-	-	0/4/4/4	0/0/0/0
7	GOL	C	1249	-	-	0/4/4/4	0/0/0/0
4	F43	D	1550	1,6	1/1/25/27	0/18/165/165	0/0/10/10
5	TP7	D	1551	-	1/1/5/6	0/20/24/24	0/0/0/0
6	COM	D	1552	4	-	0/4/4/4	0/0/0/0
7	GOL	D	1553	-	-	0/4/4/4	0/0/0/0
7	GOL	D	1554	10	-	0/4/4/4	0/0/0/0
7	GOL	D	1555	-	-	0/4/4/4	0/0/0/0
7	GOL	D	1556	-	-	0/4/4/4	0/0/0/0
7	GOL	E	1444	-	-	0/4/4/4	0/0/0/0

All (34) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	D	1550	F43	C4B-NB	-14.36	1.27	1.49
4	A	1550	F43	C4B-NB	-13.51	1.28	1.49
5	D	1551	TP7	C2-C1	-4.70	1.42	1.51
5	A	1551	TP7	C2-C1	-4.29	1.43	1.51
4	A	1550	F43	C4A-NA	-3.56	1.43	1.49
4	D	1550	F43	C4A-NA	-2.87	1.44	1.49
4	D	1550	F43	C1D-ND	-2.72	1.31	1.36
7	B	1444	GOL	O2-C2	-2.51	1.36	1.43
4	A	1550	F43	C1D-ND	-2.42	1.31	1.36
7	D	1556	GOL	O2-C2	-2.07	1.37	1.43
4	D	1550	F43	NI-ND	2.03	2.05	1.92
6	D	1552	COM	O3S-S2	2.11	1.51	1.46
4	A	1550	F43	C1C-NC	2.17	1.41	1.37
4	A	1550	F43	CAB-C3B	2.24	1.58	1.53
4	A	1550	F43	CAA-C3A	2.26	1.58	1.53
4	D	1550	F43	CHD-C7D	2.41	1.51	1.46
4	A	1550	F43	C1B-N5B	2.50	1.51	1.45
5	D	1551	TP7	O1-C1	2.51	1.28	1.23
4	A	1550	F43	CHD-C7D	2.57	1.52	1.46
5	A	1551	TP7	C1-N	2.69	1.39	1.34
4	D	1550	F43	C2B-C3B	2.88	1.59	1.54
4	D	1550	F43	NI-NC	2.88	2.03	1.90
4	A	1550	F43	C2B-C3B	3.20	1.60	1.54
4	D	1550	F43	C1C-NC	3.25	1.44	1.37
4	D	1550	F43	C6D-C7D	3.88	1.56	1.50
4	D	1550	F43	C2A-C1A	3.99	1.56	1.51
4	A	1550	F43	NI-NC	4.60	2.10	1.90
4	A	1550	F43	C1D-C2D	4.87	1.53	1.40
4	D	1550	F43	C1D-C2D	5.03	1.54	1.40
4	A	1550	F43	C2A-C1A	5.36	1.58	1.51
4	A	1550	F43	C3D-C2D	6.94	1.54	1.39
4	D	1550	F43	C3D-C2D	7.52	1.56	1.39
4	A	1550	F43	C4D-C3D	9.57	1.50	1.37
4	D	1550	F43	C4D-C3D	9.87	1.50	1.37

All (22) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	D	1550	F43	C9D-C3D-C4D	-7.28	114.74	127.01
4	A	1550	F43	C9D-C3D-C4D	-6.59	115.91	127.01
5	A	1551	TP7	O1-C1-N	-3.51	117.05	123.01
6	A	1552	COM	O1S-S2-C2	-3.32	104.07	106.91

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
7	A	1553	GOL	O3-C3-C2	-3.24	94.49	110.18
5	D	1551	TP7	O1-C1-N	-3.00	117.93	123.01
5	D	1551	TP7	C-CA-N	-2.58	108.34	113.51
7	D	1556	GOL	C3-C2-C1	-2.58	101.02	111.12
5	A	1551	TP7	C-CA-N	-2.49	108.53	113.51
4	D	1550	F43	O8D-C7D-C6D	-2.39	116.42	120.76
7	A	1554	GOL	O3-C3-C2	-2.34	98.84	110.18
7	D	1556	GOL	O3-C3-C2	-2.28	99.12	110.18
7	A	1553	GOL	C3-C2-C1	-2.10	102.87	111.12
4	D	1550	F43	C3C-C4C-NC	2.26	112.40	109.13
4	A	1550	F43	C9A-C2A-C3A	2.35	116.76	112.94
5	A	1551	TP7	O1-C1-C2	2.39	126.10	121.98
5	D	1551	TP7	O1-C1-C2	2.43	126.17	121.98
4	A	1550	F43	C9B-C2B-C3B	2.44	116.62	111.81
4	D	1550	F43	C3A-C4A-NA	2.44	106.21	102.27
4	D	1550	F43	C9B-C2B-C3B	3.15	118.02	111.81
4	D	1550	F43	C3B-C4B-NB	3.33	116.42	106.03
4	A	1550	F43	C3B-C4B-NB	3.59	117.24	106.03

All (4) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
5	D	1551	TP7	C1
4	A	1550	F43	C4B
5	A	1551	TP7	C1
4	D	1550	F43	C4B

There are no torsion outliers.

There are no ring outliers.

8 monomers are involved in 12 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	1550	F43	1	0
7	A	1553	GOL	2	0
7	A	1554	GOL	1	0
7	A	1555	GOL	1	0
7	A	1556	GOL	3	0
7	B	1444	GOL	1	0
4	D	1550	F43	1	0
7	D	1556	GOL	2	0

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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

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

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

6.3 Carbohydrates

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

6.4 Ligands

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

6.5 Other polymers

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