



Full wwPDB X-ray Structure Validation Report ⓘ

Jan 31, 2016 – 08:50 PM GMT

PDB ID : 1M1N
Title : Nitrogenase MoFe protein from Azotobacter vinelandii
Authors : Einsle, O.; Tezcan, F.A.; Andrade, S.L.A.; Schmid, B.; Yoshida, M.; Howard, J.B.; Rees, D.C.
Deposited on : 2002-06-19
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 ⓘ symbol.

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

MolProbity : 4.02b-467
Mogul : 1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix) : **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

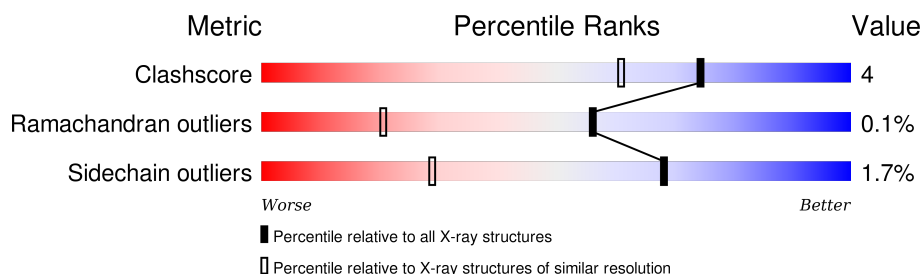
1 Overall quality at a glance

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 $\leq 5\%$. 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	491	
1	C	491	
1	E	491	
1	G	491	
2	B	522	
2	D	522	
2	F	522	

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
2	H	522	 87% 12% •

2 Entry composition [i](#)

There are 7 unique types of molecules in this entry. The entry contains 37384 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 Nitrogenase molybdenum-iron protein alpha chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	477	Total	C	N	O	S	0	6	0
			3810	2423	647	713	27			
1	C	477	Total	C	N	O	S	0	6	0
			3814	2424	652	710	28			
1	E	477	Total	C	N	O	S	0	7	0
			3815	2426	647	715	27			
1	G	477	Total	C	N	O	S	0	7	0
			3819	2428	653	710	28			

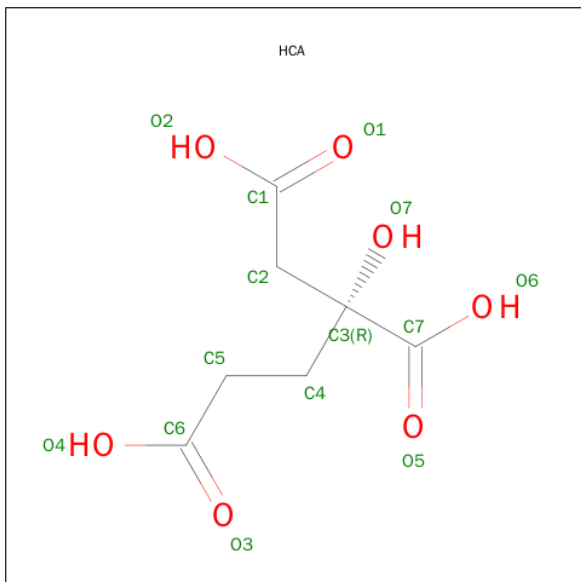
- Molecule 2 is a protein called Nitrogenase molybdenum-iron protein beta chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	522	Total	C	N	O	S	0	18	0
			4236	2710	707	784	35			
2	D	522	Total	C	N	O	S	0	15	0
			4225	2701	707	782	35			
2	F	522	Total	C	N	O	S	0	17	0
			4234	2709	707	783	35			
2	H	522	Total	C	N	O	S	0	13	0
			4218	2696	707	780	35			

- Molecule 3 is CALCIUM ION (three-letter code: CA) (formula: Ca).

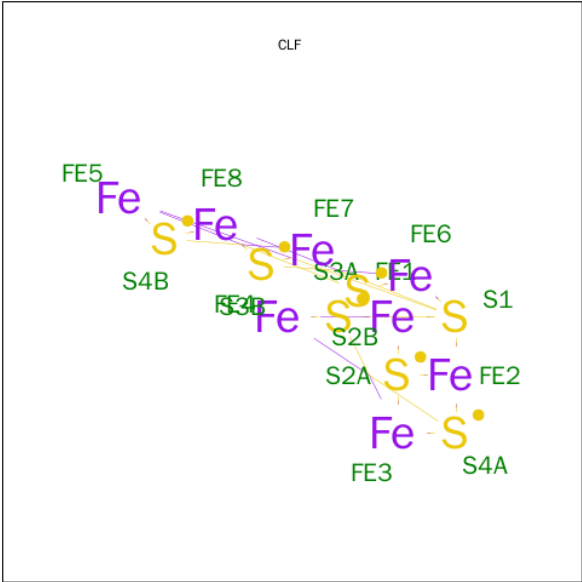
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	H	1	Total	Ca	0	0
			1	1		
3	B	1	Total	Ca	0	0
			1	1		
3	D	1	Total	Ca	0	0
			1	1		
3	F	1	Total	Ca	0	0
			1	1		

- Molecule 4 is 3-HYDROXY-3-CARBOXY-ADIPIC ACID (three-letter code: HCA) (formula: $C_7H_{10}O_7$).



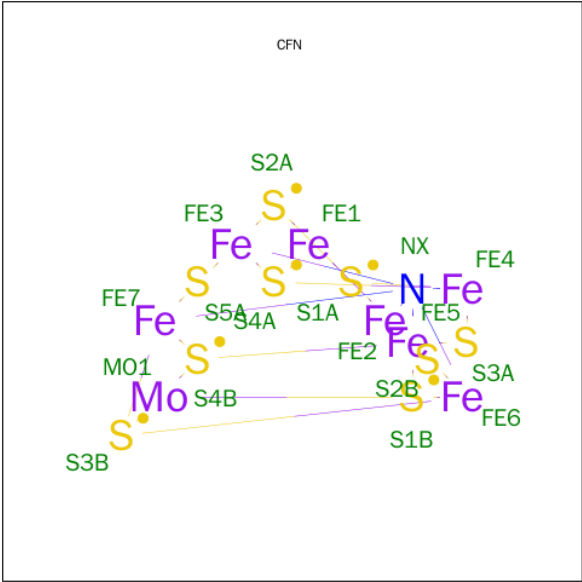
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			14	7	7		
4	C	1	Total	C	O	0	0
			14	7	7		
4	E	1	Total	C	O	0	0
			14	7	7		
4	G	1	Total	C	O	0	0
			14	7	7		

- Molecule 5 is FE(8)-S(7) CLUSTER (three-letter code: CLF) (formula: Fe_8S_7).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	B	1	Total	Fe	S	0	0
			15	8	7		
5	D	1	Total	Fe	S	0	0
			15	8	7		
5	F	1	Total	Fe	S	0	0
			15	8	7		
5	H	1	Total	Fe	S	0	0
			15	8	7		

- Molecule 6 is FE(7)-MO-S(9)-N CLUSTER (three-letter code: CFN) (formula: Fe₇MoNS₉).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
6	A	1	Total 18	Fe 7	Mo 1	N 1	S 9	0	0
6	C	1	Total 18	Fe 7	Mo 1	N 1	S 9	0	0
6	E	1	Total 18	Fe 7	Mo 1	N 1	S 9	0	0
6	G	1	Total 18	Fe 7	Mo 1	N 1	S 9	0	0

- Molecule 7 is water.

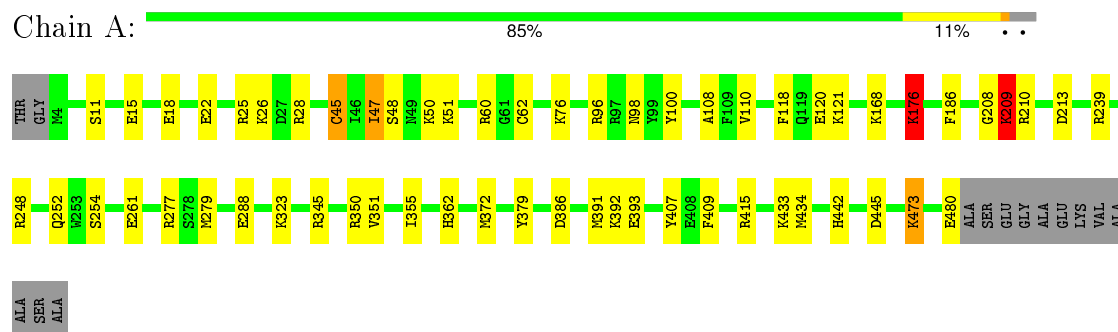
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	553	Total 553	O 553	0	0
7	B	723	Total 723	O 723	0	0
7	C	570	Total 570	O 570	0	0
7	D	704	Total 704	O 704	0	0
7	E	536	Total 536	O 536	0	0
7	F	708	Total 708	O 708	0	0
7	G	533	Total 533	O 533	0	0
7	H	694	Total 694	O 694	0	0

3 Residue-property plots [i](#)

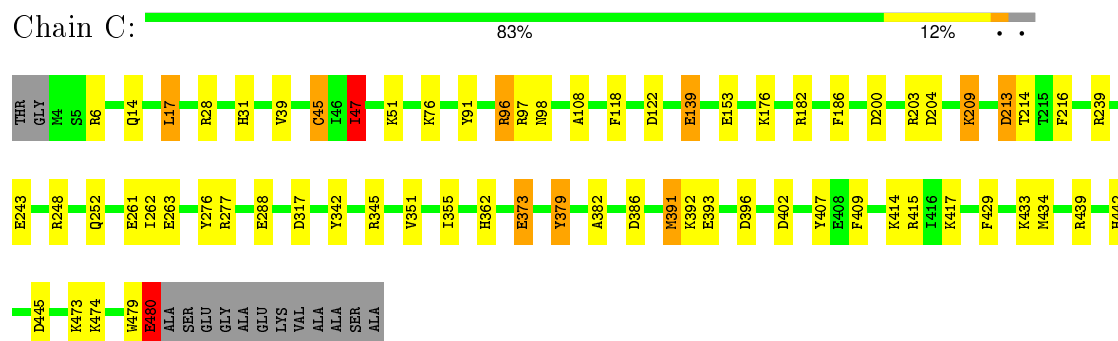
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according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

Note EDS was not executed.

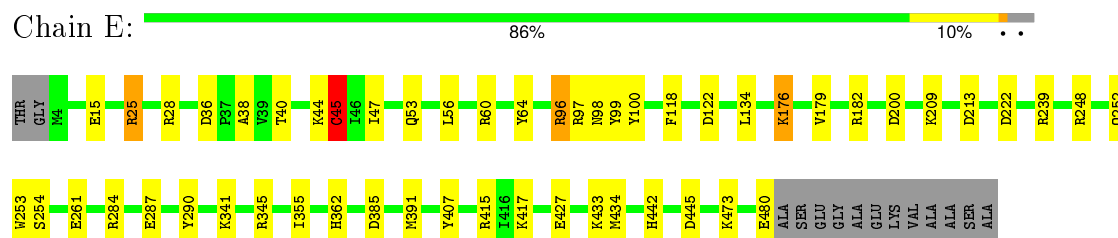
- Molecule 1: Nitrogenase molybdenum-iron protein alpha chain



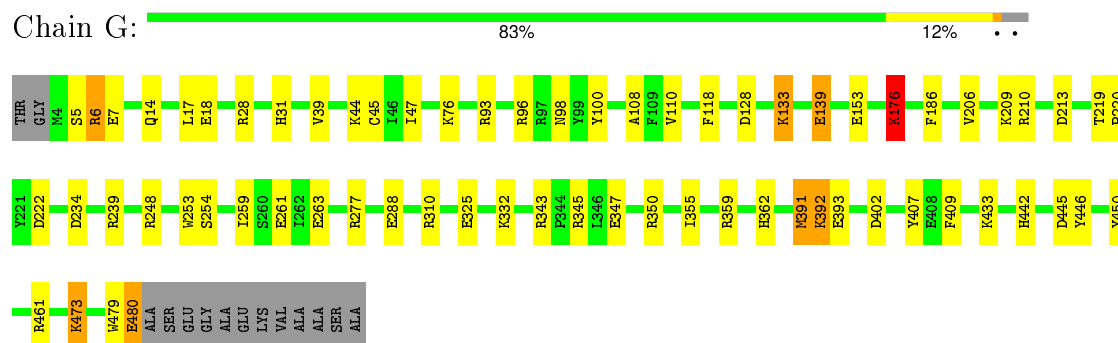
- Molecule 1: Nitrogenase molybdenum-iron protein alpha chain



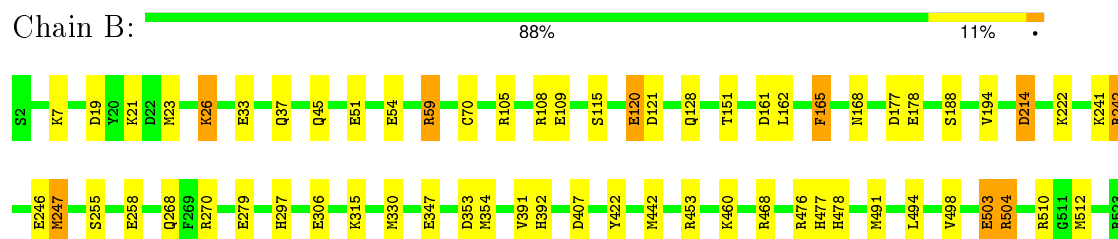
- Molecule 1: Nitrogenase molybdenum-iron protein alpha chain



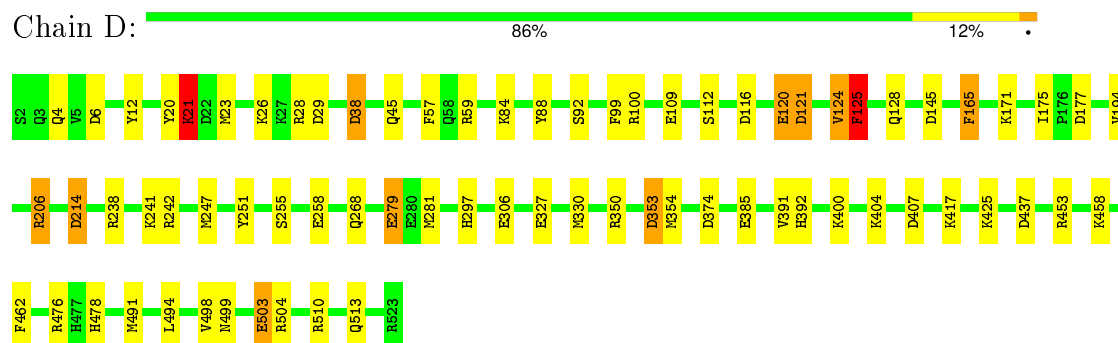
- Molecule 1: Nitrogenase molybdenum-iron protein alpha chain



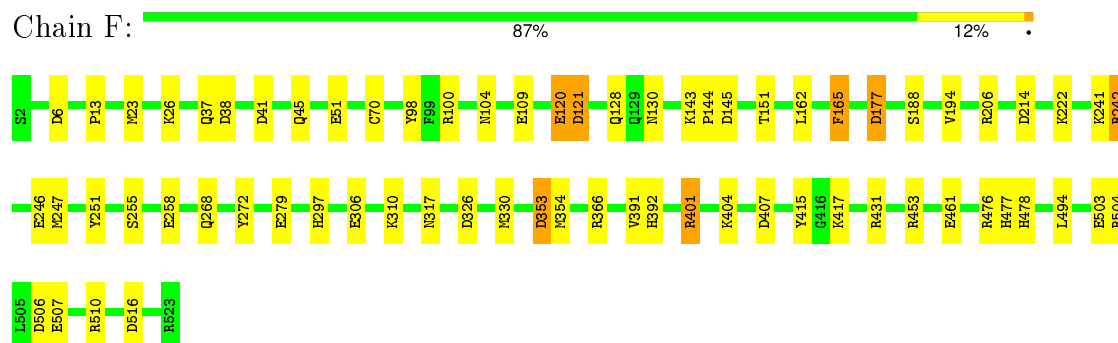
- Molecule 2: Nitrogenase molybdenum-iron protein beta chain



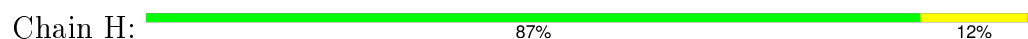
- Molecule 2: Nitrogenase molybdenum-iron protein beta chain



- Molecule 2: Nitrogenase molybdenum-iron protein beta chain



- Molecule 2: Nitrogenase molybdenum-iron protein beta chain





4 Data and refinement statistics

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	108.31Å 131.63Å 159.16Å 90.00° 108.37° 90.00°	Depositor
Resolution (Å)	50.00 – 1.16	Depositor
% Data completeness (in resolution range)	95.6 (50.00-1.16)	Depositor
R_{merge}	0.09	Depositor
R_{sym}	0.08	Depositor
Refinement program	REFMAC 5	Depositor
R, R_{free}	0.123 , 0.149	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	37384	wwPDB-VP
Average B, all atoms (Å ²)	19.0	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: CFN, CLF, HCA, CA

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# $ Z > 5$	RMSZ	# $ Z > 5$
1	A	1.27	21/3922 (0.5%)	1.20	25/5286 (0.5%)
1	C	1.32	28/3926 (0.7%)	1.26	34/5291 (0.6%)
1	E	1.25	15/3931 (0.4%)	1.19	27/5298 (0.5%)
1	G	1.23	18/3935 (0.5%)	1.16	27/5302 (0.5%)
2	B	1.29	29/4414 (0.7%)	1.19	25/5960 (0.4%)
2	D	1.29	29/4391 (0.7%)	1.23	42/5930 (0.7%)
2	F	1.21	22/4408 (0.5%)	1.12	21/5952 (0.4%)
2	H	1.24	25/4376 (0.6%)	1.18	30/5909 (0.5%)
All	All	1.26	187/33303 (0.6%)	1.19	231/44928 (0.5%)

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	2
1	C	0	2
1	E	0	1
1	G	0	2
2	B	0	3
2	H	0	1
All	All	0	11

All (187) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	391	MET	CG-SD	-11.51	1.51	1.81
1	C	407	TYR	CE1-CZ	-10.23	1.25	1.38
2	D	503	GLU	CD-OE1	10.23	1.36	1.25
1	G	391	MET	CG-SD	-10.04	1.55	1.81

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	92	SER	CB-OG	-9.96	1.29	1.42
1	A	261	GLU	CB-CG	-9.93	1.33	1.52
1	E	261	GLU	CB-CG	-9.85	1.33	1.52
1	C	393	GLU	CD-OE1	9.79	1.36	1.25
2	D	279	GLU	CG-CD	9.51	1.66	1.51
2	F	306	GLU	CD-OE1	9.41	1.35	1.25
2	B	306	GLU	CD-OE1	9.22	1.35	1.25
2	D	120	GLU	CD-OE1	9.10	1.35	1.25
2	B	330	MET	SD-CE	-9.09	1.26	1.77
2	B	222	LYS	CD-CE	8.95	1.73	1.51
2	H	503	GLU	CD-OE1	8.72	1.35	1.25
2	B	178	GLU	CD-OE1	8.66	1.35	1.25
2	F	51	GLU	CD-OE2	8.60	1.35	1.25
2	H	391	VAL	CB-CG2	-8.53	1.34	1.52
2	B	503	GLU	CD-OE1	8.44	1.34	1.25
2	F	279	GLU	CD-OE2	8.28	1.34	1.25
2	B	279	GLU	CD-OE2	8.27	1.34	1.25
1	C	209	LYS	CE-NZ	8.17	1.69	1.49
1	C	393	GLU	CD-OE2	-8.11	1.16	1.25
2	D	453	ARG	NE-CZ	8.03	1.43	1.33
1	A	51	LYS	CB-CG	-7.94	1.31	1.52
2	D	109	GLU	CD-OE1	-7.93	1.17	1.25
2	F	279	GLU	CG-CD	7.85	1.63	1.51
2	B	51	GLU	CD-OE2	7.78	1.34	1.25
1	G	393	GLU	CD-OE1	7.76	1.34	1.25
1	C	391	MET	CB-CG	7.73	1.76	1.51
2	B	306	GLU	CD-OE2	-7.61	1.17	1.25
1	A	391	MET	CG-SD	-7.61	1.61	1.81
1	E	45	CYS	CB-SG	-7.52	1.69	1.82
1	G	332	LYS	CD-CE	7.44	1.69	1.51
2	D	145	ASP	CB-CG	7.44	1.67	1.51
2	F	330	MET	SD-CE	-7.43	1.36	1.77
2	B	268	GLN	CB-CG	-7.41	1.32	1.52
1	G	261	GLU	CD-OE1	7.39	1.33	1.25
1	G	325	GLU	CD-OE1	7.38	1.33	1.25
2	H	109	GLU	CD-OE2	7.37	1.33	1.25
1	E	407	TYR	CE1-CZ	-7.32	1.29	1.38
1	C	407	TYR	CZ-OH	7.27	1.50	1.37
2	B	51	GLU	CD-OE1	7.26	1.33	1.25
2	H	461	GLU	CD-OE2	7.21	1.33	1.25
2	H	330	MET	SD-CE	-7.17	1.37	1.77
1	C	153	GLU	CD-OE1	7.16	1.33	1.25

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	H	268	GLN	CB-CG	-7.11	1.33	1.52
2	F	242	ARG	CG-CD	-7.11	1.34	1.51
1	E	434	MET	SD-CE	-7.08	1.38	1.77
1	C	139	GLU	CD-OE2	-7.07	1.17	1.25
1	A	261	GLU	CG-CD	7.03	1.62	1.51
2	D	330	MET	SD-CE	-7.00	1.38	1.77
2	B	242	ARG	CG-CD	-6.92	1.34	1.51
1	A	45	CYS	CB-SG	-6.87	1.70	1.82
1	A	186	PHE	CB-CG	-6.87	1.39	1.51
2	F	51	GLU	CD-OE1	6.87	1.33	1.25
1	C	434	MET	SD-CE	-6.82	1.39	1.77
2	F	120	GLU	CD-OE1	6.80	1.33	1.25
2	F	121	ASP	CB-CG	6.69	1.65	1.51
2	D	268	GLN	CB-CG	-6.64	1.34	1.52
1	G	139	GLU	CD-OE2	-6.64	1.18	1.25
1	C	45[A]	CYS	CB-SG	-6.56	1.71	1.82
1	C	45[B]	CYS	CB-SG	-6.56	1.71	1.82
2	F	109	GLU	CD-OE2	6.53	1.32	1.25
1	G	261	GLU	CG-CD	6.53	1.61	1.51
2	D	491	MET	SD-CE	-6.50	1.41	1.77
1	C	261	GLU	CD-OE1	6.49	1.32	1.25
2	D	109	GLU	CD-OE2	6.46	1.32	1.25
2	D	121	ASP	CB-CG	6.45	1.65	1.51
2	F	453	ARG	NE-CZ	6.43	1.41	1.33
2	H	6	ASP	CB-CG	6.42	1.65	1.51
2	F	306	GLU	CD-OE2	-6.39	1.18	1.25
1	A	62	CYS	CB-SG	6.39	1.93	1.82
1	E	290	TYR	CD2-CE2	-6.39	1.29	1.39
2	D	171	LYS	CD-CE	6.36	1.67	1.51
1	C	407	TYR	CD2-CE2	6.34	1.48	1.39
2	D	112	SER	CB-OG	6.31	1.50	1.42
1	C	17	LEU	CG-CD2	-6.31	1.28	1.51
2	H	482	SER	CB-OG	-6.29	1.34	1.42
2	B	279	GLU	CG-CD	6.25	1.61	1.51
1	A	176	LYS	CE-NZ	-6.25	1.33	1.49
1	E	209	LYS	CE-NZ	6.22	1.64	1.49
1	C	373	GLU	CD-OE1	6.20	1.32	1.25
1	C	342	TYR	CE1-CZ	-6.19	1.30	1.38
2	B	491	MET	SD-CE	-6.18	1.43	1.77
2	F	268	GLN	CB-CG	-6.15	1.35	1.52
1	C	51	LYS	CB-CG	-6.13	1.36	1.52
2	H	241	LYS	CE-NZ	6.06	1.64	1.49

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	G	407	TYR	CD2-CE2	6.06	1.48	1.39
1	E	100	TYR	CE2-CZ	6.03	1.46	1.38
1	G	17	LEU	CG-CD2	-6.02	1.29	1.51
2	D	327	GLU	CD-OE2	6.02	1.32	1.25
1	E	252	GLN	CB-CG	-5.96	1.36	1.52
2	D	6	ASP	CB-CG	5.95	1.64	1.51
1	C	409	PHE	CG-CD2	-5.94	1.29	1.38
2	B	347	GLU	CD-OE2	-5.93	1.19	1.25
1	E	261	GLU	CG-CD	5.92	1.60	1.51
2	D	242	ARG	CG-CD	-5.88	1.37	1.51
1	A	393	GLU	CD-OE1	5.87	1.32	1.25
2	B	241	LYS	CE-NZ	5.86	1.63	1.49
2	D	385	GLU	CD-OE1	-5.86	1.19	1.25
2	H	503	GLU	CG-CD	5.84	1.60	1.51
2	B	109	GLU	CD-OE2	5.83	1.32	1.25
1	G	392	LYS	CB-CG	5.82	1.68	1.52
2	B	247[A]	MET	SD-CE	5.79	2.10	1.77
2	B	247[B]	MET	SD-CE	5.79	2.10	1.77
2	D	241	LYS	CE-NZ	5.78	1.63	1.49
2	F	98	TYR	CG-CD2	-5.78	1.31	1.39
2	H	109	GLU	CD-OE1	-5.78	1.19	1.25
2	B	120	GLU	CD-OE2	5.77	1.31	1.25
2	D	491	MET	CG-SD	5.75	1.96	1.81
2	B	54	GLU	CD-OE1	5.72	1.31	1.25
1	C	409	PHE	CE2-CZ	-5.71	1.26	1.37
2	H	300	LYS	CD-CE	-5.68	1.37	1.51
2	B	422	TYR	CE2-CZ	-5.68	1.31	1.38
2	H	241	LYS	CD-CE	-5.67	1.37	1.51
2	D	171	LYS	CE-NZ	5.64	1.63	1.49
2	F	306	GLU	CG-CD	5.63	1.60	1.51
2	H	347	GLU	CD-OE2	-5.62	1.19	1.25
2	F	241	LYS	CD-CE	-5.61	1.37	1.51
1	G	407	TYR	CE1-CZ	-5.59	1.31	1.38
1	G	261	GLU	CD-OE2	-5.57	1.19	1.25
1	G	391	MET	CB-CG	5.56	1.69	1.51
2	B	453	ARG	NE-CZ	5.56	1.40	1.33
2	D	12	TYR	CE1-CZ	-5.55	1.31	1.38
1	C	186	PHE	CA-CB	5.49	1.66	1.53
2	F	177	ASP	CB-CG	-5.46	1.40	1.51
1	E	287	GLU	CB-CG	5.46	1.62	1.52
1	C	47	ILE	CB-CG2	-5.45	1.35	1.52
2	B	460	LYS	CD-CE	-5.43	1.37	1.51

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	491	MET	CG-SD	5.43	1.95	1.81
2	H	280	GLU	CD-OE2	5.42	1.31	1.25
2	H	453	ARG	NE-CZ	5.42	1.40	1.33
1	A	288	GLU	CG-CD	5.41	1.60	1.51
1	C	261	GLU	CG-CD	5.41	1.60	1.51
2	H	145	ASP	CB-CG	5.41	1.63	1.51
2	H	279	GLU	CG-CD	5.39	1.60	1.51
2	D	125	PHE	CD1-CE1	5.38	1.50	1.39
2	B	120	GLU	CD-OE1	5.37	1.31	1.25
1	A	288	GLU	CD-OE2	5.36	1.31	1.25
1	A	434	MET	SD-CE	-5.36	1.47	1.77
2	F	461	GLU	CD-OE1	5.34	1.31	1.25
2	B	121	ASP	C-O	5.33	1.33	1.23
2	H	231	GLU	CG-CD	-5.32	1.44	1.51
2	B	498	VAL	CB-CG1	-5.32	1.41	1.52
2	B	33	GLU	CD-OE1	-5.32	1.19	1.25
2	H	247	MET	CB-CG	-5.31	1.34	1.51
1	G	433	LYS	CG-CD	-5.29	1.34	1.52
2	F	109	GLU	CD-OE1	-5.26	1.19	1.25
1	A	18	GLU	CD-OE2	5.25	1.31	1.25
1	A	254	SER	CB-OG	-5.25	1.35	1.42
1	E	182	ARG	CG-CD	-5.25	1.38	1.51
2	H	171	LYS	CD-CE	5.21	1.64	1.51
1	C	414	LYS	CE-NZ	5.19	1.62	1.49
2	F	415	TYR	CE2-CZ	-5.17	1.31	1.38
1	C	433	LYS	CG-CD	-5.17	1.34	1.52
1	A	252	GLN	CB-CG	-5.16	1.38	1.52
2	H	171	LYS	CE-NZ	5.15	1.61	1.49
2	D	251	TYR	CE2-CZ	-5.15	1.31	1.38
1	E	427	GLU	CD-OE2	5.15	1.31	1.25
2	H	242	ARG	CG-CD	-5.14	1.39	1.51
1	C	243	GLU	CD-OE2	5.13	1.31	1.25
2	H	461	GLU	CD-OE1	5.13	1.31	1.25
2	F	507	GLU	CD-OE1	-5.13	1.20	1.25
1	A	209	LYS	CG-CD	5.13	1.69	1.52
1	G	407	TYR	CZ-OH	5.12	1.46	1.37
1	C	414	LYS	CD-CE	-5.12	1.38	1.51
2	D	498	VAL	CB-CG1	-5.11	1.42	1.52
2	H	12	TYR	CE1-CZ	-5.11	1.31	1.38
1	A	279[A]	MET	CG-SD	-5.11	1.67	1.81
1	A	279[B]	MET	CG-SD	-5.11	1.67	1.81
1	A	407	TYR	CZ-OH	5.11	1.46	1.37

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	26	LYS	CE-NZ	5.11	1.61	1.49
1	C	252	GLN	CB-CG	-5.11	1.38	1.52
2	D	281[A]	MET	SD-CE	-5.11	1.49	1.77
2	D	281[B]	MET	SD-CE	-5.11	1.49	1.77
2	D	425	LYS	CD-CE	5.10	1.64	1.51
1	A	433	LYS	CG-CD	-5.10	1.35	1.52
1	A	407	TYR	CE1-CZ	-5.09	1.31	1.38
1	G	153	GLU	CD-OE1	5.09	1.31	1.25
2	D	21	LYS	CE-NZ	5.08	1.61	1.49
1	G	347	GLU	CG-CD	-5.07	1.44	1.51
1	G	186	PHE	CB-CG	-5.07	1.42	1.51
1	E	179	VAL	CB-CG2	-5.06	1.42	1.52
1	E	47	ILE	CB-CG2	-5.04	1.37	1.52
1	E	433	LYS	CB-CG	5.01	1.66	1.52
2	F	251	TYR	CD2-CE2	-5.01	1.31	1.39

All (231) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	H	247	MET	CG-SD-CE	14.08	122.72	100.20
2	H	38	ASP	CB-CG-OD2	13.25	130.23	118.30
2	B	491	MET	CG-SD-CE	-12.97	79.44	100.20
2	B	510	ARG	NE-CZ-NH1	12.90	126.75	120.30
2	D	491	MET	CG-SD-CE	-12.35	80.44	100.20
2	B	59	ARG	NE-CZ-NH2	-11.92	114.34	120.30
1	C	213	ASP	CB-CG-OD2	11.77	128.89	118.30
2	H	510	ARG	NE-CZ-NH1	11.68	126.14	120.30
2	F	510	ARG	NE-CZ-NH1	11.40	126.00	120.30
1	G	248	ARG	NE-CZ-NH2	-11.21	114.70	120.30
1	G	248	ARG	NE-CZ-NH1	11.03	125.81	120.30
2	D	510	ARG	NE-CZ-NH1	10.34	125.47	120.30
1	E	96	ARG	NE-CZ-NH1	9.74	125.17	120.30
2	B	59	ARG	NE-CZ-NH1	9.66	125.13	120.30
1	C	277	ARG	NE-CZ-NH2	-9.48	115.56	120.30
1	C	45[A]	CYS	N-CA-CB	-9.37	93.73	110.60
1	C	45[B]	CYS	N-CA-CB	-9.37	93.73	110.60
2	D	476	ARG	NE-CZ-NH1	9.24	124.92	120.30
2	H	206	ARG	NE-CZ-NH1	-9.08	115.76	120.30
2	B	19	ASP	CB-CG-OD1	8.97	126.38	118.30
1	C	17	LEU	CA-CB-CG	-8.85	94.95	115.30
2	D	109	GLU	OE1-CD-OE2	-8.82	112.72	123.30
2	D	177	ASP	CB-CG-OD1	8.78	126.20	118.30

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	96	ARG	NE-CZ-NH2	8.72	124.66	120.30
2	F	121	ASP	CB-CG-OD2	8.70	126.13	118.30
1	A	350	ARG	NE-CZ-NH2	-8.62	115.99	120.30
1	A	277	ARG	NE-CZ-NH2	-8.48	116.06	120.30
1	A	480	GLU	CA-C-O	8.43	137.80	120.10
2	D	279	GLU	OE1-CD-OE2	-8.36	113.27	123.30
2	D	350	ARG	NE-CZ-NH1	8.35	124.47	120.30
2	D	206	ARG	NE-CZ-NH2	8.29	124.45	120.30
1	E	248	ARG	NE-CZ-NH1	8.24	124.42	120.30
1	C	480	GLU	CA-C-O	8.18	137.28	120.10
1	A	28	ARG	NE-CZ-NH2	-8.16	116.22	120.30
2	H	504	ARG	NE-CZ-NH1	-8.16	116.22	120.30
1	A	248	ARG	NE-CZ-NH1	7.95	124.27	120.30
1	E	25	ARG	NE-CZ-NH2	-7.84	116.38	120.30
1	E	248	ARG	NE-CZ-NH2	-7.77	116.42	120.30
1	E	25	ARG	NE-CZ-NH1	7.74	124.17	120.30
2	H	19	ASP	CB-CG-OD1	7.72	125.25	118.30
2	H	491	MET	CG-SD-CE	-7.72	87.85	100.20
1	C	248	ARG	NE-CZ-NH2	-7.61	116.50	120.30
1	C	122	ASP	CB-CG-OD2	7.60	125.14	118.30
2	D	353	ASP	CB-CG-OD1	-7.57	111.48	118.30
2	H	357	ASP	CB-CG-OD1	7.57	125.11	118.30
2	B	121	ASP	CB-CG-OD2	7.55	125.10	118.30
1	E	213	ASP	CB-CG-OD2	7.54	125.09	118.30
2	B	109	GLU	OE1-CD-OE2	-7.50	114.30	123.30
2	D	504	ARG	NE-CZ-NH1	-7.50	116.55	120.30
2	F	504	ARG	NE-CZ-NH1	-7.49	116.56	120.30
2	F	476	ARG	NE-CZ-NH1	7.46	124.03	120.30
1	A	323	LYS	CD-CE-NZ	-7.44	94.58	111.70
2	B	177	ASP	CB-CG-OD2	7.36	124.93	118.30
1	C	28	ARG	NE-CZ-NH2	-7.33	116.63	120.30
2	D	6	ASP	CB-CG-OD1	7.33	124.89	118.30
2	H	109	GLU	OE1-CD-OE2	-7.31	114.53	123.30
2	D	242	ARG	NE-CZ-NH1	-7.27	116.67	120.30
2	D	214	ASP	CB-CG-OD2	7.25	124.83	118.30
1	G	210	ARG	NE-CZ-NH1	7.10	123.85	120.30
1	E	118	PHE	CB-CG-CD1	7.07	125.75	120.80
1	G	213	ASP	CB-CG-OD2	7.07	124.67	118.30
2	D	28	ARG	NE-CZ-NH2	-7.07	116.77	120.30
1	C	182	ARG	NE-CZ-NH2	-7.04	116.78	120.30
2	H	206	ARG	NE-CZ-NH2	7.04	123.82	120.30
1	A	345	ARG	NE-CZ-NH1	7.02	123.81	120.30

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	385	ASP	CB-CG-OD1	7.01	124.61	118.30
1	E	284	ARG	NE-CZ-NH2	7.01	123.81	120.30
2	D	247	MET	CG-SD-CE	6.97	111.35	100.20
2	D	242	ARG	NE-CZ-NH2	6.93	123.77	120.30
1	E	284	ARG	NE-CZ-NH1	-6.91	116.84	120.30
1	A	209	LYS	CB-CG-CD	6.91	129.57	111.60
2	F	38	ASP	CB-CG-OD1	6.87	124.49	118.30
1	A	45	CYS	CA-CB-SG	6.85	126.33	114.00
2	D	28	ARG	NE-CZ-NH1	6.82	123.71	120.30
2	H	214	ASP	CB-CG-OD2	6.81	124.43	118.30
2	B	476	ARG	NE-CZ-NH1	6.81	123.70	120.30
2	H	145	ASP	CB-CG-OD2	6.79	124.41	118.30
2	H	6	ASP	CB-CG-OD1	6.79	124.41	118.30
2	H	38	ASP	CB-CG-OD1	-6.77	112.21	118.30
1	A	288	GLU	OE1-CD-OE2	-6.74	115.21	123.30
2	F	41	ASP	CB-CG-OD1	6.72	124.34	118.30
1	E	45	CYS	N-CA-CB	-6.71	98.53	110.60
2	D	38[A]	ASP	CB-CG-OD2	6.67	124.31	118.30
2	D	38[B]	ASP	CB-CG-OD2	6.67	124.31	118.30
1	C	118	PHE	CB-CG-CD1	6.67	125.47	120.80
1	E	96	ARG	NE-CZ-NH2	-6.62	116.99	120.30
1	E	415	ARG	NE-CZ-NH1	6.60	123.60	120.30
2	B	407	ASP	CB-CG-OD2	6.60	124.24	118.30
2	D	165	PHE	CB-CG-CD1	6.60	125.42	120.80
2	H	507	GLU	OE1-CD-OE2	-6.57	115.41	123.30
1	E	200	ASP	CB-CG-OD1	6.57	124.21	118.30
1	E	28	ARG	NE-CZ-NH2	-6.54	117.03	120.30
1	A	60	ARG	NE-CZ-NH2	-6.54	117.03	120.30
1	G	277	ARG	NE-CZ-NH2	-6.54	117.03	120.30
2	D	59	ARG	NE-CZ-NH1	6.50	123.55	120.30
2	F	206	ARG	NE-CZ-NH2	6.47	123.54	120.30
1	C	17	LEU	CB-CG-CD1	6.47	122.00	111.00
1	G	350	ARG	NE-CZ-NH2	-6.46	117.07	120.30
1	A	60	ARG	NE-CZ-NH1	6.45	123.52	120.30
1	C	396	ASP	CB-CG-OD2	6.45	124.10	118.30
2	F	109	GLU	OE1-CD-OE2	-6.43	115.58	123.30
1	G	450	TYR	CB-CG-CD1	6.39	124.84	121.00
1	E	64	TYR	CB-CG-CD2	6.37	124.82	121.00
1	A	409	PHE	CB-CG-CD1	6.36	125.25	120.80
2	F	431	ARG	NE-CZ-NH2	-6.33	117.13	120.30
1	G	359	ARG	NE-CZ-NH2	-6.32	117.14	120.30
1	C	434	MET	CG-SD-CE	-6.32	90.09	100.20

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	270	ARG	NE-CZ-NH2	6.30	123.45	120.30
1	C	439	ARG	NE-CZ-NH1	6.29	123.44	120.30
1	A	118	PHE	CB-CG-CD1	6.28	125.19	120.80
2	D	20	TYR	CB-CG-CD2	6.28	124.77	121.00
1	E	290	TYR	CB-CG-CD1	6.26	124.75	121.00
2	H	21	LYS	CD-CE-NZ	6.24	126.04	111.70
1	E	480	GLU	CA-C-O	6.22	133.16	120.10
2	D	59	ARG	NE-CZ-NH2	-6.19	117.20	120.30
1	C	379	TYR	CD1-CE1-CZ	6.18	125.37	119.80
1	C	345	ARG	NE-CZ-NH1	6.18	123.39	120.30
2	H	120	GLU	OE1-CD-OE2	-6.14	115.93	123.30
1	C	248	ARG	NE-CZ-NH1	6.13	123.36	120.30
2	H	242	ARG	NE-CZ-NH1	-6.13	117.24	120.30
1	C	345	ARG	NE-CZ-NH2	-6.10	117.25	120.30
2	H	59	ARG	NE-CZ-NH2	-6.10	117.25	120.30
1	A	213	ASP	CB-CG-OD2	6.08	123.77	118.30
2	F	353	ASP	CB-CG-OD2	6.07	123.77	118.30
1	C	393	GLU	CG-CD-OE2	-6.05	106.19	118.30
1	G	118	PHE	CB-CG-CD1	6.05	125.04	120.80
1	C	393	GLU	CG-CD-OE1	6.02	130.34	118.30
1	C	391	MET	CB-CA-C	5.99	122.39	110.40
1	C	200	ASP	CB-CG-OD1	5.91	123.62	118.30
2	D	121	ASP	CB-CA-C	5.88	122.16	110.40
2	D	385	GLU	OE1-CD-OE2	-5.88	116.25	123.30
1	G	17	LEU	CA-CB-CG	-5.88	101.78	115.30
1	E	99	TYR	CB-CG-CD1	5.87	124.52	121.00
1	A	261	GLU	CB-CA-C	5.87	122.13	110.40
2	F	165	PHE	CB-CG-CD1	5.85	124.89	120.80
1	G	6	ARG	NE-CZ-NH2	-5.84	117.38	120.30
2	B	504	ARG	NE-CZ-NH1	-5.83	117.39	120.30
1	E	434	MET	CG-SD-CE	-5.83	90.87	100.20
2	B	330	MET	CG-SD-CE	-5.80	90.91	100.20
1	G	17	LEU	CB-CG-CD1	5.80	120.86	111.00
1	G	128	ASP	CB-CG-OD1	5.79	123.51	118.30
2	F	100	ARG	NE-CZ-NH2	-5.79	117.41	120.30
1	G	343	ARG	NE-CZ-NH2	-5.77	117.42	120.30
1	C	277	ARG	NE-CZ-NH1	5.76	123.18	120.30
2	F	326	ASP	CB-CG-OD1	5.75	123.48	118.30
2	F	366	ARG	NE-CZ-NH2	-5.74	117.43	120.30
1	A	209	LYS	CD-CE-NZ	5.74	124.90	111.70
1	A	434	MET	CG-SD-CE	-5.74	91.02	100.20
2	D	374	ASP	CB-CG-OD1	-5.74	113.14	118.30

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	209	LYS	CG-CD-CE	5.72	129.06	111.90
2	D	116	ASP	CB-CG-OD2	-5.71	113.16	118.30
2	D	21	LYS	CD-CE-NZ	5.71	124.82	111.70
1	G	234	ASP	CB-CG-OD2	-5.70	113.17	118.30
2	H	476	ARG	NE-CZ-NH1	5.63	123.12	120.30
2	H	20	TYR	CB-CG-CD2	5.63	124.38	121.00
2	F	121	ASP	OD1-CG-OD2	-5.61	112.63	123.30
2	D	437	ASP	CB-CG-OD1	5.61	123.35	118.30
2	B	105	ARG	NE-CZ-NH1	5.60	123.10	120.30
1	C	28	ARG	NE-CZ-NH1	5.59	123.09	120.30
1	G	210	ARG	NE-CZ-NH2	-5.59	117.51	120.30
2	B	121	ASP	N-CA-CB	-5.58	100.55	110.60
2	D	206	ARG	NE-CZ-NH1	-5.58	117.51	120.30
1	E	122	ASP	CB-CG-OD2	5.58	123.32	118.30
2	D	88	TYR	CB-CG-CD1	5.58	124.35	121.00
1	C	216	PHE	CB-CG-CD1	-5.57	116.90	120.80
1	C	91	TYR	CB-CG-CD1	5.56	124.34	121.00
1	A	25	ARG	NE-CZ-NH1	5.56	123.08	120.30
2	B	161	ASP	CB-CG-OD2	5.55	123.29	118.30
1	A	386	ASP	CB-CG-OD2	5.53	123.27	118.30
2	D	99	PHE	CB-CG-CD1	5.52	124.66	120.80
2	H	366	ARG	NE-CZ-NH2	-5.50	117.55	120.30
2	B	222	LYS	CD-CE-NZ	5.47	124.29	111.70
1	G	345	ARG	CD-NE-CZ	5.46	131.24	123.60
1	C	429	PHE	CB-CG-CD1	-5.44	116.99	120.80
2	H	366	ARG	NE-CZ-NH1	5.44	123.02	120.30
2	F	206	ARG	NE-CZ-NH1	-5.43	117.58	120.30
2	B	468	ARG	NE-CZ-NH1	-5.43	117.59	120.30
2	D	175	ILE	CG1-CB-CG2	5.43	123.34	111.40
1	A	407	TYR	CG-CD1-CE1	5.42	125.64	121.30
2	B	214	ASP	CB-CG-OD2	5.42	123.17	118.30
2	D	121	ASP	CB-CG-OD2	5.41	123.17	118.30
1	G	461	ARG	NE-CZ-NH1	-5.40	117.60	120.30
1	C	97	ARG	NE-CZ-NH1	5.39	123.00	120.30
1	G	176	LYS	CD-CE-NZ	5.38	124.08	111.70
2	D	407	ASP	CB-CG-OD2	5.37	123.13	118.30
1	G	93	ARG	NE-CZ-NH1	-5.36	117.62	120.30
1	E	60	ARG	NE-CZ-NH2	-5.35	117.62	120.30
2	D	29	ASP	CB-CG-OD1	5.34	123.11	118.30
1	E	44	LYS	CD-CE-NZ	5.33	123.97	111.70
1	G	310	ARG	NE-CZ-NH2	-5.33	117.64	120.30
1	E	290	TYR	CZ-CE2-CD2	5.32	124.59	119.80

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	100	ARG	NE-CZ-NH2	-5.32	117.64	120.30
2	H	59	ARG	NE-CZ-NH1	5.30	122.95	120.30
1	E	222	ASP	CB-CG-OD2	5.28	123.05	118.30
2	D	238	ARG	NE-CZ-NH1	-5.27	117.66	120.30
2	D	177	ASP	OD1-CG-OD2	-5.26	113.30	123.30
1	C	317	ASP	CB-CG-OD2	5.25	123.03	118.30
1	G	222	ASP	CB-CG-OD1	5.25	123.03	118.30
2	D	57	PHE	CB-CG-CD1	5.24	124.47	120.80
2	H	26	LYS	CD-CE-NZ	5.23	123.73	111.70
1	C	276	TYR	CB-CG-CD2	-5.23	117.86	121.00
2	B	510	ARG	NE-CZ-NH2	-5.23	117.69	120.30
2	F	506	ASP	CB-CG-OD1	5.22	123.00	118.30
1	G	28	ARG	NE-CZ-NH2	-5.22	117.69	120.30
2	H	508	GLU	OE1-CD-OE2	-5.22	117.04	123.30
2	F	516	ASP	CB-CG-OD1	5.19	122.97	118.30
2	F	401	ARG	NE-CZ-NH2	-5.18	117.71	120.30
1	E	345	ARG	NE-CZ-NH1	5.17	122.88	120.30
2	H	512[A]	MET	N-CA-CB	-5.16	101.31	110.60
2	H	512[B]	MET	N-CA-CB	-5.16	101.31	110.60
2	F	407	ASP	CB-CG-OD2	5.15	122.94	118.30
1	C	415	ARG	NE-CZ-NH1	5.15	122.88	120.30
2	F	272	TYR	CB-CG-CD1	5.15	124.09	121.00
2	B	165	PHE	CB-CG-CD1	5.14	124.40	120.80
1	A	210	ARG	NE-CZ-NH2	-5.14	117.73	120.30
1	G	47	ILE	CA-CB-CG2	5.14	121.18	110.90
1	G	409	PHE	CB-CG-CD1	5.13	124.39	120.80
1	A	11[A]	SER	N-CA-CB	5.11	118.17	110.50
1	A	11[B]	SER	N-CA-CB	5.11	118.17	110.50
2	B	512[A]	MET	N-CA-CB	-5.11	101.39	110.60
2	B	512[B]	MET	N-CA-CB	-5.11	101.39	110.60
2	D	121	ASP	N-CA-CB	-5.11	101.40	110.60
2	H	320	MET	CG-SD-CE	5.11	108.38	100.20
1	C	351	VAL	CG1-CB-CG2	5.10	119.07	110.90
1	G	288	GLU	OE1-CD-OE2	-5.08	117.20	123.30
2	B	442	MET	CG-SD-CE	5.05	108.28	100.20
2	H	26	LYS	CA-CB-CG	5.04	124.48	113.40
2	B	121	ASP	CB-CA-C	5.04	120.47	110.40
1	G	409	PHE	CB-CG-CD2	-5.03	117.28	120.80
2	D	353	ASP	CB-CG-OD2	5.01	122.81	118.30
1	E	97	ARG	NE-CZ-NH2	5.00	122.80	120.30

There are no chirality outliers.

All (11) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	379	TYR	Sidechain
1	A	96	ARG	Sidechain
2	B	108	ARG	Sidechain
2	B	315	LYS	Mainchain
2	B	59	ARG	Sidechain
1	C	379	TYR	Sidechain
1	C	96	ARG	Sidechain
1	E	96	ARG	Sidechain
1	G	446	TYR	Sidechain
1	G	96	ARG	Sidechain
2	H	109	GLU	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	3810	0	3748	30	0
1	C	3814	0	3755	40	2
1	E	3815	0	3750	15	0
1	G	3819	0	3764	32	0
2	B	4236	0	4156	31	0
2	D	4225	0	4141	46	0
2	F	4234	0	4155	38	0
2	H	4218	0	4136	43	0
3	B	1	0	0	1	0
3	D	1	0	0	1	0
3	F	1	0	0	0	0
3	H	1	0	0	0	0
4	A	14	0	6	2	0
4	C	14	0	6	2	0
4	E	14	0	6	1	0
4	G	14	0	6	2	0
5	B	15	0	0	0	0
5	D	15	0	0	0	0
5	F	15	0	0	0	0
5	H	15	0	0	0	0
6	A	18	0	0	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	C	18	0	0	0	0
6	E	18	0	0	0	0
6	G	18	0	0	0	0
7	A	553	0	0	12	5
7	B	723	0	0	15	2
7	C	570	0	0	10	12
7	D	704	0	0	24	6
7	E	536	0	0	5	0
7	F	708	0	0	14	4
7	G	533	0	0	7	4
7	H	694	0	0	17	5
All	All	37384	0	31629	258	20

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 4.

All (258) 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)
1:C:209:LYS:NZ	1:C:209:LYS:CE	1.69	1.56
1:C:391:MET:CG	1:C:391:MET:CB	1.76	1.55
2:F:247[A]:MET:CE	2:F:247[A]:MET:SD	2.01	1.48
2:B:247[A]:MET:SD	2:B:247[A]:MET:CE	2.10	1.38
2:D:124:VAL:HG13	7:D:8044:HOH:O	1.35	1.20
7:B:7790:HOH:O	1:C:474:LYS:HE2	1.02	1.17
2:H:461:GLU:HG3	7:H:4510:HOH:O	1.45	1.14
1:C:373:GLU:HG3	7:C:8065:HOH:O	1.42	1.13
2:D:124:VAL:HG23	7:D:7966:HOH:O	1.48	1.11
2:B:214:ASP:OD1	7:B:8171:HOH:O	1.66	1.10
2:D:214:ASP:OD1	7:D:8144:HOH:O	1.67	1.09
2:H:178:GLU:OE1	7:H:4929:HOH:O	1.69	1.09
1:A:47:ILE:CD1	7:A:7032:HOH:O	1.99	1.08
2:F:214:ASP:OD1	7:F:4919:HOH:O	1.73	1.04
1:G:480:GLU:OE2	1:G:480:GLU:HA	1.56	1.03
2:H:306:GLU:OE2	7:H:4859:HOH:O	1.77	1.00
2:D:45[A]:GLN:HG2	7:D:7809:HOH:O	1.59	1.00
1:A:209:LYS:HG2	7:A:7046:HOH:O	1.59	0.99
1:G:239:ARG:HD3	2:H:23[B]:MET:SD	2.03	0.98
1:C:391:MET:SD	1:C:391:MET:CB	2.52	0.97
2:D:84:LYS:NZ	7:D:8029:HOH:O	1.96	0.95
2:D:121:ASP:O	7:D:8044:HOH:O	1.85	0.95

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:45[A]:GLN:HG2	7:H:3646:HOH:O	1.64	0.95
2:H:214:ASP:OD1	7:H:3806:HOH:O	1.85	0.95
2:F:477:HIS:H	2:H:499:ASN:HD21	1.15	0.94
2:B:45[B]:GLN:HG2	7:B:8147:HOH:O	1.65	0.94
2:B:477:HIS:H	2:D:499:ASN:HD21	1.10	0.92
1:A:47:ILE:HD13	1:A:48:SER:H	1.35	0.91
1:C:473:LYS:HG2	7:C:7955:HOH:O	1.72	0.89
1:C:47:ILE:HG13	7:C:7989:HOH:O	1.73	0.89
1:E:239:ARG:HD3	2:F:23[B]:MET:SD	2.11	0.89
1:G:473:LYS:HG2	7:G:4558:HOH:O	1.70	0.89
1:C:391:MET:CE	1:C:391:MET:CB	2.50	0.89
1:C:391:MET:HB2	1:C:391:MET:CE	2.03	0.88
1:A:239:ARG:HD3	2:B:23[B]:MET:SD	2.14	0.88
1:A:47:ILE:CD1	1:A:50:LYS:HE2	2.04	0.87
2:F:404:LYS:NZ	7:F:4299:HOH:O	2.08	0.85
1:C:239:ARG:HD3	2:D:23[B]:MET:SD	2.18	0.83
1:G:479:TRP:O	1:G:480:GLU:HB2	1.77	0.83
1:G:480:GLU:OE2	1:G:480:GLU:CA	2.25	0.83
1:E:45:CYS:SG	1:E:391:MET:HE1	2.19	0.83
2:B:503:GLU:OE2	7:B:7745:HOH:O	1.97	0.82
1:G:473:LYS:HA	1:G:473:LYS:HE2	1.61	0.81
1:C:391:MET:HB2	1:C:391:MET:HE2	1.63	0.79
1:A:47:ILE:HD11	1:A:50:LYS:HE2	1.65	0.78
1:C:213:ASP:OD1	7:C:8007:HOH:O	2.00	0.77
2:D:84:LYS:CE	7:D:8029:HOH:O	2.31	0.77
1:C:139:GLU:OE2	1:C:176:LYS:HE3	1.83	0.77
3:D:6492:CA:CA	7:D:7499:HOH:O	1.62	0.76
2:D:306:GLU:OE2	7:D:8158:HOH:O	2.04	0.75
2:F:310:LYS:NZ	7:F:3777:HOH:O	2.20	0.75
1:A:47:ILE:HD11	7:A:7032:HOH:O	1.74	0.74
2:F:503:GLU:CD	7:F:4246:HOH:O	2.25	0.73
2:D:124:VAL:CG2	2:D:124:VAL:O	2.37	0.73
2:D:279:GLU:OE1	7:D:7961:HOH:O	2.08	0.72
2:B:503:GLU:CD	7:B:7976:HOH:O	2.26	0.72
1:A:47:ILE:HD13	1:A:48:SER:N	2.06	0.71
2:H:306:GLU:OE1	7:H:4032:HOH:O	2.06	0.71
2:H:54:GLU:OE1	7:H:4132:HOH:O	2.08	0.71
2:D:125:PHE:N	7:D:8044:HOH:O	2.22	0.71
1:C:479:TRP:O	1:C:480:GLU:HB2	1.91	0.71
1:A:120:GLU:OE1	7:A:6934:HOH:O	2.07	0.71
2:D:353:ASP:OD2	7:D:8199:HOH:O	2.08	0.70

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:45[B]:GLN:HG2	7:F:4821:HOH:O	1.89	0.70
2:B:353:ASP:OD2	7:B:8212:HOH:O	2.09	0.70
2:D:124:VAL:HG22	2:D:124:VAL:O	1.92	0.69
1:G:31:HIS:HE1	7:G:3017:HOH:O	1.75	0.69
1:A:47:ILE:HD13	7:A:7032:HOH:O	1.78	0.68
2:H:353:ASP:OD2	7:H:5005:HOH:O	2.10	0.68
2:D:84:LYS:HE3	7:D:8029:HOH:O	1.90	0.68
2:D:503:GLU:CG	7:D:8131:HOH:O	2.40	0.68
2:D:4:GLN:OE1	7:D:8128:HOH:O	2.12	0.67
2:H:177:ASP:OD1	7:H:4511:HOH:O	2.13	0.67
2:H:124:VAL:HG22	2:H:124:VAL:O	1.94	0.66
1:G:209:LYS:HZ1	1:G:259:ILE:HD11	1.59	0.66
1:G:18:GLU:HG2	7:G:4205:HOH:O	1.93	0.66
2:B:120:GLU:OE2	7:B:7587:HOH:O	2.13	0.66
1:G:39:VAL:HG12	1:G:391:MET:HE1	1.77	0.66
1:G:209:LYS:NZ	1:G:263:GLU:OE2	2.28	0.65
1:A:47:ILE:HD12	1:A:50:LYS:HE2	1.78	0.65
1:G:206:VAL:HA	1:G:209:LYS:HE2	1.78	0.65
2:F:37:GLN:HE22	2:H:513:GLN:HE22	1.45	0.65
2:F:145:ASP:OD2	7:F:3900:HOH:O	2.14	0.64
2:F:222:LYS:HE2	7:F:4730:HOH:O	1.98	0.64
2:F:391[A]:VAL:HG12	2:F:392:HIS:CE1	2.32	0.64
1:A:176:LYS:HE3	7:A:6831:HOH:O	1.97	0.64
2:D:124:VAL:CG1	7:D:8044:HOH:O	2.13	0.63
2:H:124:VAL:CG2	2:H:124:VAL:O	2.47	0.62
2:B:37:GLN:HE22	2:D:513:GLN:HE22	1.46	0.62
1:E:36:ASP:OD1	1:E:38:ALA:HB3	1.99	0.62
1:E:45:CYS:SG	1:E:391:MET:CE	2.87	0.62
3:B:7492:CA:CA	7:B:7493:HOH:O	1.77	0.62
2:F:503:GLU:CG	7:F:4226:HOH:O	2.50	0.60
1:C:6:ARG:NE	7:C:7884:HOH:O	1.77	0.60
1:E:25:ARG:HD3	7:E:3407:HOH:O	2.01	0.59
2:H:45[B]:GLN:HE22	2:H:458[B]:LYS:NZ	2.01	0.59
1:G:133:LYS:HE3	7:G:3883:HOH:O	2.02	0.59
1:G:44:LYS:NZ	7:G:3100:HOH:O	2.36	0.58
1:G:209:LYS:NZ	1:G:259:ILE:HD11	2.18	0.58
2:F:478:HIS:NE2	2:H:354[B]:MET:HG3	2.19	0.58
2:B:115[B]:SER:HB2	7:B:7562:HOH:O	2.02	0.58
1:A:47:ILE:HG12	7:A:7032:HOH:O	1.97	0.57
1:C:31:HIS:HD2	1:C:402:ASP:OD2	1.87	0.57
1:A:473:LYS:HG2	7:A:6912:HOH:O	2.04	0.57

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:242:ARG:HD3	2:H:246:GLU:OE2	2.05	0.56
1:C:31:HIS:HE1	7:C:7601:HOH:O	1.87	0.55
1:A:209:LYS:HE2	1:A:209:LYS:N	2.22	0.55
2:H:503:GLU:CG	7:H:4772:HOH:O	2.54	0.55
7:B:7790:HOH:O	1:C:474:LYS:CE	1.89	0.55
1:E:36:ASP:OD1	1:E:38:ALA:N	2.39	0.55
1:E:15[B]:GLU:OE2	7:E:4952:HOH:O	2.18	0.54
2:F:353:ASP:OD2	7:F:5006:HOH:O	2.18	0.54
2:F:120:GLU:OE2	7:F:3364:HOH:O	2.18	0.54
2:B:354[B]:MET:HG3	2:D:478:HIS:NE2	2.23	0.53
1:C:480:GLU:HA	1:C:480:GLU:OE2	2.06	0.53
1:E:417:LYS:NZ	7:E:4120:HOH:O	2.37	0.53
2:D:120:GLU:OE2	7:D:7539:HOH:O	2.19	0.53
1:A:176:LYS:NZ	7:A:6983:HOH:O	2.42	0.53
1:G:473:LYS:HE2	1:G:473:LYS:CA	2.35	0.52
2:B:478:HIS:NE2	2:D:354[B]:MET:HG3	2.25	0.52
2:H:417:LYS:NZ	7:H:4638:HOH:O	1.95	0.52
1:G:31:HIS:HD2	1:G:402:ASP:OD2	1.92	0.52
2:F:478:HIS:CD2	2:H:354[B]:MET:HG3	2.45	0.52
1:C:14:GLN:NE2	7:C:7763:HOH:O	2.43	0.52
2:F:354[B]:MET:HG3	2:H:478:HIS:NE2	2.25	0.52
2:B:503:GLU:CG	7:B:7976:HOH:O	2.58	0.51
1:A:473:LYS:CG	7:A:6912:HOH:O	2.57	0.51
7:B:7790:HOH:O	1:C:474:LYS:CD	2.43	0.51
2:H:461:GLU:CG	7:H:4510:HOH:O	2.26	0.51
2:H:214:ASP:OD1	7:H:4825:HOH:O	2.19	0.51
2:D:354[B]:MET:SD	2:D:494:LEU:HD22	2.51	0.51
2:F:354[B]:MET:SD	2:F:494:LEU:HD22	2.51	0.51
2:B:151:THR:HG23	2:B:162:LEU:HD11	1.92	0.51
2:D:458[A]:LYS:HG2	2:D:462:PHE:CD2	2.46	0.51
1:C:473:LYS:HA	1:C:473:LYS:HE2	1.92	0.51
1:E:341:LYS:NZ	7:E:4543:HOH:O	2.37	0.51
2:F:354[B]:MET:HG2	2:F:494:LEU:HD22	1.93	0.50
1:C:139:GLU:CD	1:C:176:LYS:HE3	2.30	0.50
2:B:21:LYS:HE2	7:B:8088:HOH:O	2.10	0.50
2:H:458[A]:LYS:HE2	2:H:462:PHE:CD1	2.47	0.50
1:C:417:LYS:NZ	7:C:7846:HOH:O	2.44	0.50
1:E:442:HIS:HB3	4:E:8494:HCA:O5	2.12	0.50
2:D:354[B]:MET:HG2	2:D:494:LEU:HD22	1.94	0.49
1:C:480:GLU:CA	1:C:480:GLU:OE2	2.61	0.49
1:G:206:VAL:HA	1:G:209:LYS:CE	2.41	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:478:HIS:CD2	2:D:354[B]:MET:HG3	2.47	0.49
1:G:39:VAL:HG12	1:G:391:MET:CE	2.41	0.49
2:H:354[B]:MET:HG2	2:H:494:LEU:HD22	1.94	0.48
2:H:151:THR:HG23	2:H:162:LEU:HD11	1.94	0.48
2:D:391[A]:VAL:HG12	2:D:392:HIS:CE1	2.48	0.48
2:D:206:ARG:HG2	7:D:8053:HOH:O	2.12	0.48
2:B:391[A]:VAL:HG12	2:B:392:HIS:CE1	2.48	0.48
2:H:354[B]:MET:SD	2:H:494:LEU:HD22	2.53	0.48
2:B:354[B]:MET:HG2	2:B:494:LEU:HD22	1.96	0.48
1:A:415:ARG:HD2	7:A:7036:HOH:O	2.13	0.48
2:F:151:THR:HG23	2:F:162:LEU:HD11	1.94	0.48
2:F:128:GLN:HE22	2:F:165:PHE:HA	1.78	0.48
1:C:479:TRP:O	1:C:480:GLU:CB	2.60	0.47
1:A:351:VAL:CG2	1:A:372:MET:CE	2.92	0.47
1:C:214:THR:HG21	7:C:7911:HOH:O	2.15	0.47
1:G:442:HIS:HB3	4:G:9494:HCA:O5	2.14	0.47
2:F:194:VAL:HB	2:F:297:HIS:CG	2.50	0.47
2:D:503:GLU:CD	7:D:8131:HOH:O	2.52	0.47
2:H:411:ALA:HB3	7:H:3114:HOH:O	2.15	0.47
1:C:391:MET:HB2	1:C:391:MET:HE3	1.94	0.47
2:F:503:GLU:HG3	7:F:4226:HOH:O	2.13	0.47
1:C:203[A]:ARG:HD2	1:C:204:ASP:OD1	2.14	0.47
2:B:354[B]:MET:HG3	2:D:478:HIS:CD2	2.51	0.46
2:H:45[B]:GLN:HE22	2:H:458[B]:LYS:HZ1	1.63	0.46
1:A:22:GLU:HG3	1:A:26:LYS:HE3	1.97	0.46
1:C:39:VAL:O	1:C:391:MET:HE3	2.15	0.46
1:A:76:LYS:O	1:A:108:ALA:HA	2.16	0.46
1:G:14:GLN:NE2	7:G:3719:HOH:O	2.45	0.46
2:D:417:LYS:NZ	7:D:8090:HOH:O	1.96	0.45
2:H:354[B]:MET:HG2	2:H:494:LEU:CD2	2.46	0.45
1:E:176:LYS:NZ	7:E:4742:HOH:O	2.49	0.45
1:C:391:MET:HE2	1:C:391:MET:CB	2.30	0.45
2:B:128:GLN:HE22	2:B:165:PHE:HA	1.81	0.45
2:B:354[B]:MET:CG	2:B:494:LEU:HD22	2.47	0.45
2:B:354[B]:MET:SD	2:B:494:LEU:HD22	2.57	0.45
2:F:354[B]:MET:HG2	2:F:494:LEU:CD2	2.46	0.45
2:F:45[B]:GLN:CG	7:F:4821:HOH:O	2.59	0.45
2:D:128:GLN:HE22	2:D:165:PHE:HA	1.82	0.45
1:G:139:GLU:CD	1:G:176:LYS:HE3	2.37	0.45
2:H:128:GLN:HE22	2:H:165:PHE:HA	1.82	0.45
1:A:47:ILE:HD12	1:A:50:LYS:CE	2.47	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:194:VAL:HB	2:D:297:HIS:CG	2.52	0.44
2:H:458[A]:LYS:HE2	2:H:462:PHE:CE1	2.52	0.44
1:C:17:LEU:CD1	1:C:17:LEU:N	2.80	0.44
1:G:100:TYR:CE1	1:G:110:VAL:HB	2.52	0.44
1:A:100:TYR:CE1	1:A:110:VAL:HB	2.52	0.44
2:B:194:VAL:HB	2:B:297:HIS:CG	2.53	0.44
1:E:36:ASP:OD1	1:E:38:ALA:CB	2.66	0.44
1:C:6:ARG:NH2	7:C:7884:HOH:O	2.47	0.44
1:G:253:TRP:HA	1:G:254:SER:HA	1.78	0.44
2:D:21:LYS:HB2	2:D:21:LYS:HE2	1.56	0.44
2:B:242:ARG:HD3	2:B:246:GLU:OE2	2.18	0.44
1:G:219:THR:HB	1:G:220:PRO:HD2	1.99	0.43
1:C:76:LYS:O	1:C:108:ALA:HA	2.18	0.43
2:D:503:GLU:HG3	7:D:8131:HOH:O	2.10	0.43
2:D:391[A]:VAL:HG13	7:D:7918:HOH:O	2.18	0.43
1:A:351:VAL:CG2	1:A:372:MET:HE1	2.49	0.43
1:A:168:LYS:NZ	7:A:6647:HOH:O	2.52	0.43
1:G:39:VAL:O	1:G:391:MET:HE3	2.19	0.43
2:D:121:ASP:O	2:D:125:PHE:CE1	2.72	0.43
2:B:478:HIS:CE1	2:D:354[B]:MET:HG3	2.54	0.43
1:G:442:HIS:CG	4:G:9494:HCA:H52	2.54	0.43
1:A:442:HIS:CG	4:A:6494:HCA:H52	2.54	0.43
2:D:400:LYS:HB3	7:D:8152:HOH:O	2.18	0.43
2:B:168:ASN:ND2	7:B:8105:HOH:O	2.52	0.42
1:G:7:GLU:CD	1:G:7:GLU:H	2.23	0.42
1:C:442:HIS:CG	4:C:7494:HCA:H52	2.54	0.42
1:C:209:LYS:NZ	1:C:263:GLU:OE2	2.43	0.42
2:B:354[B]:MET:HG2	2:B:494:LEU:CD2	2.49	0.42
2:D:354[B]:MET:HG2	2:D:494:LEU:CD2	2.48	0.42
1:A:208:GLY:C	1:A:209:LYS:HE2	2.40	0.42
2:H:168:ASN:ND2	2:H:171:LYS:NZ	2.67	0.42
1:C:391:MET:CG	1:C:391:MET:CA	2.81	0.42
2:F:478:HIS:CE1	2:H:354[B]:MET:HG3	2.55	0.42
2:F:130:ASN:HD22	2:F:130:ASN:H	1.67	0.42
2:H:503:GLU:CD	7:H:4772:HOH:O	2.57	0.42
2:H:376:VAL:HG21	2:H:395[B]:CYS:SG	2.60	0.42
2:F:417:LYS:CG	7:F:4979:HOH:O	2.67	0.42
2:D:124:VAL:HG23	2:D:124:VAL:O	2.19	0.42
2:H:21:LYS:HE2	2:H:21:LYS:HB2	1.49	0.42
2:B:504:ARG:NH2	7:B:7973:HOH:O	2.52	0.42
1:C:262:ILE:HG21	1:C:262:ILE:HD13	1.83	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:382:ALA:HB1	1:C:386:ASP:HB2	2.02	0.42
2:F:317:ASN:ND2	7:F:2832:HOH:O	2.47	0.42
1:E:253:TRP:HA	1:E:254:SER:HA	1.86	0.42
1:E:53:GLN:HB2	1:E:56:LEU:HD12	2.02	0.42
2:H:354[B]:MET:CG	2:H:494:LEU:HD22	2.49	0.41
1:A:442:HIS:HB3	4:A:6494:HCA:O5	2.20	0.41
1:C:442:HIS:HB3	4:C:7494:HCA:O5	2.21	0.41
2:F:70:CYS:HB2	2:F:188:SER:HB2	2.02	0.41
2:H:45[A]:GLN:CG	7:H:3646:HOH:O	2.42	0.41
2:F:354[B]:MET:CG	2:F:494:LEU:HD22	2.50	0.41
2:F:354[B]:MET:HG3	2:H:478:HIS:CD2	2.55	0.41
2:B:70:CYS:HB2	2:B:188:SER:HB2	2.03	0.41
1:G:480:GLU:OE2	1:G:480:GLU:N	2.53	0.41
2:F:401:ARG:HH11	2:F:401:ARG:HD2	1.69	0.41
1:E:134:LEU:C	1:E:134:LEU:HD23	2.41	0.41
2:H:503:GLU:HG3	7:H:4772:HOH:O	2.19	0.41
2:F:242:ARG:HD3	2:F:246:GLU:OE2	2.21	0.41
2:D:45[A]:GLN:CG	7:D:7809:HOH:O	2.37	0.41
2:B:37:GLN:NE2	2:D:513:GLN:HE22	2.17	0.41
1:G:76:LYS:O	1:G:108:ALA:HA	2.20	0.40
2:D:404:LYS:HE3	2:D:404:LYS:HB3	1.31	0.40
1:G:133:LYS:CE	7:G:3883:HOH:O	2.66	0.40
2:H:194:VAL:HB	2:H:297:HIS:CG	2.57	0.40
2:F:143:LYS:N	2:F:144:PRO:CD	2.84	0.40
1:G:479:TRP:O	1:G:480:GLU:CB	2.58	0.40
2:D:354[B]:MET:CG	2:D:494:LEU:HD22	2.50	0.40
1:A:351:VAL:CG2	1:A:372:MET:HE2	2.52	0.40
2:F:26:LYS:HB3	2:F:26:LYS:HE3	1.80	0.40

All (20) 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)
7:G:3329:HOH:O	7:H:4423:HOH:O[2_756]	0.55	1.65
7:C:8019:HOH:O	7:D:8052:HOH:O[2_545]	0.56	1.64
7:A:6891:HOH:O	7:B:8141:HOH:O[2_655]	0.71	1.49
7:C:7897:HOH:O	7:F:4626:HOH:O[1_454]	0.84	1.36
7:C:7978:HOH:O	7:H:4816:HOH:O[1_454]	0.98	1.22
7:C:8023:HOH:O	7:H:4818:HOH:O[1_454]	1.11	1.09
7:C:8014:HOH:O	7:D:7911:HOH:O[2_545]	1.28	0.92

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:G:4892:HOH:O	7:H:4841:HOH:O[2_756]	1.30	0.90
1:C:288:GLU:OE2	7:A:6735:HOH:O[1_455]	1.33	0.87
7:A:6860:HOH:O	7:B:8174:HOH:O[2_655]	1.42	0.78
7:C:8015:HOH:O	7:F:4519:HOH:O[1_454]	1.57	0.63
7:C:8051:HOH:O	7:D:8116:HOH:O[2_545]	1.61	0.59
7:C:7911:HOH:O	7:F:4562:HOH:O[1_454]	1.64	0.56
7:G:4874:HOH:O	7:H:4641:HOH:O[2_756]	1.67	0.53
7:C:7808:HOH:O	7:D:8152:HOH:O[2_545]	1.72	0.48
7:C:8028:HOH:O	7:D:7858:HOH:O[2_545]	1.83	0.37
7:A:7018:HOH:O	7:C:7937:HOH:O[1_655]	1.90	0.30
1:C:288:GLU:CD	7:A:6735:HOH:O[1_455]	2.11	0.09
7:D:8175:HOH:O	7:G:5020:HOH:O[1_455]	2.16	0.04
7:C:7911:HOH:O	7:F:4799:HOH:O[1_454]	2.18	0.02

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	481/491 (98%)	463 (96%)	18 (4%)	0	100	100
1	C	481/491 (98%)	461 (96%)	20 (4%)	0	100	100
1	E	482/491 (98%)	462 (96%)	20 (4%)	0	100	100
1	G	482/491 (98%)	462 (96%)	20 (4%)	0	100	100
2	B	538/522 (103%)	529 (98%)	8 (2%)	1 (0%)	52	20
2	D	535/522 (102%)	525 (98%)	9 (2%)	1 (0%)	52	20
2	F	537/522 (103%)	527 (98%)	9 (2%)	1 (0%)	52	20
2	H	533/522 (102%)	524 (98%)	8 (2%)	1 (0%)	52	20
All	All	4069/4052 (100%)	3953 (97%)	112 (3%)	4 (0%)	56	21

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	255	SER
2	D	255	SER
2	F	255	SER
2	H	255	SER

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	413/414 (100%)	402 (97%)	11 (3%)	52	11
1	C	413/414 (100%)	404 (98%)	9 (2%)	60	18
1	E	414/414 (100%)	406 (98%)	8 (2%)	65	24
1	G	414/414 (100%)	401 (97%)	13 (3%)	47	9
2	B	472/454 (104%)	469 (99%)	3 (1%)	90	69
2	D	469/454 (103%)	462 (98%)	7 (2%)	72	34
2	F	471/454 (104%)	466 (99%)	5 (1%)	80	47
2	H	467/454 (103%)	463 (99%)	4 (1%)	84	55
All	All	3533/3472 (102%)	3473 (98%)	60 (2%)	68	29

All (60) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	45	CYS
1	A	47	ILE
1	A	98	ASN
1	A	121	LYS
1	A	176	LYS
1	A	209	LYS
1	A	355	ILE
1	A	362	HIS
1	A	392	LYS
1	A	445	ASP
1	A	473	LYS
2	B	7	LYS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	B	26	LYS
2	B	258	GLU
1	C	45[A]	CYS
1	C	45[B]	CYS
1	C	47	ILE
1	C	98	ASN
1	C	355	ILE
1	C	362	HIS
1	C	392	LYS
1	C	445	ASP
1	C	480	GLU
2	D	21	LYS
2	D	26	LYS
2	D	38[A]	ASP
2	D	38[B]	ASP
2	D	124	VAL
2	D	125	PHE
2	D	258	GLU
1	E	40	THR
1	E	45	CYS
1	E	98	ASN
1	E	176	LYS
1	E	355	ILE
1	E	362	HIS
1	E	445	ASP
1	E	473	LYS
2	F	6	ASP
2	F	13	PRO
2	F	121	ASP
2	F	177	ASP
2	F	258	GLU
1	G	5	SER
1	G	6	ARG
1	G	45[A]	CYS
1	G	45[B]	CYS
1	G	98	ASN
1	G	133	LYS
1	G	176	LYS
1	G	355	ILE
1	G	362	HIS
1	G	392	LYS
1	G	445	ASP

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	G	473	LYS
1	G	480	GLU
2	H	21	LYS
2	H	88	TYR
2	H	178	GLU
2	H	258	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (46) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	14	GLN
1	A	29	ASN
1	A	35	ASN
1	A	271	ASN
1	A	476	GLN
2	B	37	GLN
2	B	104	ASN
2	B	128	GLN
2	B	130	ASN
2	B	168	ASN
2	B	317	ASN
2	B	518	ASN
1	C	14	GLN
1	C	29	ASN
1	C	31	HIS
1	C	35	ASN
1	C	271	ASN
2	D	104	ASN
2	D	128	GLN
2	D	130	ASN
2	D	168	ASN
2	D	499	ASN
2	D	518	ASN
1	E	29	ASN
1	E	35	ASN
1	E	271	ASN
2	F	18	GLN
2	F	37	GLN
2	F	58	GLN
2	F	104	ASN
2	F	128	GLN
2	F	130	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	F	168	ASN
2	F	317	ASN
2	F	518	ASN
1	G	14	GLN
1	G	29	ASN
1	G	31	HIS
1	G	35	ASN
1	G	271	ASN
2	H	104	ASN
2	H	128	GLN
2	H	130	ASN
2	H	168	ASN
2	H	499	ASN
2	H	518	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

Of 16 ligands modelled in this entry, 4 are monoatomic - leaving 12 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	HCA	A	6494	-	4,13,13	0.94	0	3,18,18	1.42	1 (33%)
6	CFN	A	6496	1	6,30,30	1.34	1 (16%)	0,78,78	0.00	-
5	CLF	B	6498	1,2	0,24,24	0.00	-	0,57,57	0.00	-
4	HCA	C	7494	-	4,13,13	1.31	0	3,18,18	1.85	1 (33%)
6	CFN	C	7496	1	6,30,30	0.77	0	0,78,78	0.00	-
5	CLF	D	7498	1,2	0,24,24	0.00	-	0,57,57	0.00	-
4	HCA	E	8494	-	4,13,13	1.05	0	3,18,18	1.13	0
6	CFN	E	8496	1	6,30,30	0.79	0	0,78,78	0.00	-
5	CLF	F	8498	1,2	0,24,24	0.00	-	0,57,57	0.00	-
4	HCA	G	9494	-	4,13,13	1.42	1 (25%)	3,18,18	1.28	1 (33%)
6	CFN	G	9496	1	6,30,30	1.17	1 (16%)	0,78,78	0.00	-
5	CLF	H	9498	1,2	0,24,24	0.00	-	0,57,57	0.00	-

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	HCA	A	6494	-	-	0/7/17/17	0/0/0/0
6	CFN	A	6496	1	-	0/0/204/204	0/0/13/13
5	CLF	B	6498	1,2	-	0/0/132/132	0/12/10/10
4	HCA	C	7494	-	-	0/7/17/17	0/0/0/0
6	CFN	C	7496	1	-	0/0/204/204	0/0/13/13
5	CLF	D	7498	1,2	-	0/0/132/132	0/12/10/10
4	HCA	E	8494	-	-	0/7/17/17	0/0/0/0
6	CFN	E	8496	1	-	0/0/204/204	0/0/13/13
5	CLF	F	8498	1,2	-	0/0/132/132	0/12/10/10
4	HCA	G	9494	-	-	0/7/17/17	0/0/0/0
6	CFN	G	9496	1	-	0/0/204/204	0/0/13/13
5	CLF	H	9498	1,2	-	0/0/132/132	0/12/10/10

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	A	6496	CFN	S2B-FE6	-2.62	2.17	2.24
6	G	9496	CFN	S2B-FE6	-2.44	2.17	2.24
4	G	9494	HCA	O7-C3	2.23	1.46	1.43

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	C	7494	HCA	C3-C2-C1	-2.50	110.97	114.96
4	A	6494	HCA	C4-C5-C6	2.03	120.49	112.10
4	G	9494	HCA	C4-C5-C6	2.11	120.84	112.10

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

4 monomers are involved in 7 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	6494	HCA	2	0
4	C	7494	HCA	2	0
4	E	8494	HCA	1	0
4	G	9494	HCA	2	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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

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

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

6.3 Carbohydrates ⓘ

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

6.4 Ligands ⓘ

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

6.5 Other polymers ⓘ

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