



# Full wwPDB X-ray Structure Validation Report ⓘ

Jan 31, 2016 – 10:16 PM GMT

PDB ID : 1SS8  
Title : GroEL  
Authors : Chaudhry, C.; Horwich, A.L.; Brunger, A.T.; Adams, P.D.  
Deposited on : 2004-03-23  
Resolution : 2.70 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](mailto:validation@mail.wwpdb.org)  
A user guide is available at  
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>  
with specific help available everywhere you see the ⓘ symbol.

---

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

MolProbity : 4.02b-467  
Mogul : 1.7 (RC4), CSD as536be (2015)  
Xtriage (Phenix) : 1.9-1692  
EDS : rb-20026688  
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)  
Refmac : 5.8.0135  
CCP4 : 6.5.0  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : trunk26865

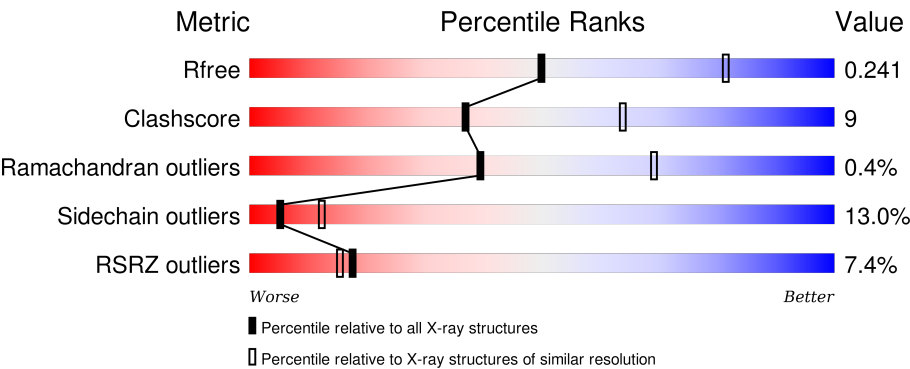
# 1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.70 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 <sub>free</sub>	91344	2103 (2.70-2.70)
Clashscore	102246	2422 (2.70-2.70)
Ramachandran outliers	100387	2382 (2.70-2.70)
Sidechain outliers	100360	2382 (2.70-2.70)
RSRZ outliers	91569	2107 (2.70-2.70)

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  $\geq 3$ , 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.

Mol	Chain	Length	Quality of chain
1	A	524	<div><div>6%</div><div><div></div><div></div><div></div><div></div></div><div>71%23%5% •</div></div>
1	B	524	<div><div>9%</div><div><div></div><div></div><div></div><div></div></div><div>71%22%5% •</div></div>
1	C	524	<div><div>6%</div><div><div></div><div></div><div></div><div></div></div><div>73%21% • •</div></div>
1	D	524	<div><div>6%</div><div><div></div><div></div><div></div><div></div></div><div>71%23%5% •</div></div>
1	E	524	<div><div>4%</div><div><div></div><div></div><div></div><div></div></div><div>72%22%6% •</div></div>

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain	
1	F	524	<div> <div style="width: 14%;"></div> <div style="width: 74%;"></div> <div style="width: 22%;"></div> </div>	..
1	G	524	<div> <div style="width: 6%;"></div> <div style="width: 72%;"></div> <div style="width: 23%;"></div> </div>	..

## 2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 27064 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 groEL protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	524	Total	C	N	O	S	0	0	0
			3851	2395	662	774	20			
1	B	524	Total	C	N	O	S	0	0	0
			3851	2395	662	774	20			
1	C	524	Total	C	N	O	S	0	0	0
			3851	2395	662	774	20			
1	D	524	Total	C	N	O	S	0	0	0
			3851	2395	662	774	20			
1	E	524	Total	C	N	O	S	0	0	0
			3851	2395	662	774	20			
1	F	524	Total	C	N	O	S	0	0	0
			3851	2395	662	774	20			
1	G	524	Total	C	N	O	S	0	0	0
			3851	2395	662	774	20			

There are 14 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	13	GLY	ARG	SEE REMARK 999	UNP P0A6F5
A	126	VAL	ALA	SEE REMARK 999	UNP P0A6F5
B	13	GLY	ARG	SEE REMARK 999	UNP P0A6F5
B	126	VAL	ALA	SEE REMARK 999	UNP P0A6F5
C	13	GLY	ARG	SEE REMARK 999	UNP P0A6F5
C	126	VAL	ALA	SEE REMARK 999	UNP P0A6F5
D	13	GLY	ARG	SEE REMARK 999	UNP P0A6F5
D	126	VAL	ALA	SEE REMARK 999	UNP P0A6F5
E	13	GLY	ARG	SEE REMARK 999	UNP P0A6F5
E	126	VAL	ALA	SEE REMARK 999	UNP P0A6F5
F	13	GLY	ARG	SEE REMARK 999	UNP P0A6F5
F	126	VAL	ALA	SEE REMARK 999	UNP P0A6F5
G	13	GLY	ARG	SEE REMARK 999	UNP P0A6F5
G	126	VAL	ALA	SEE REMARK 999	UNP P0A6F5

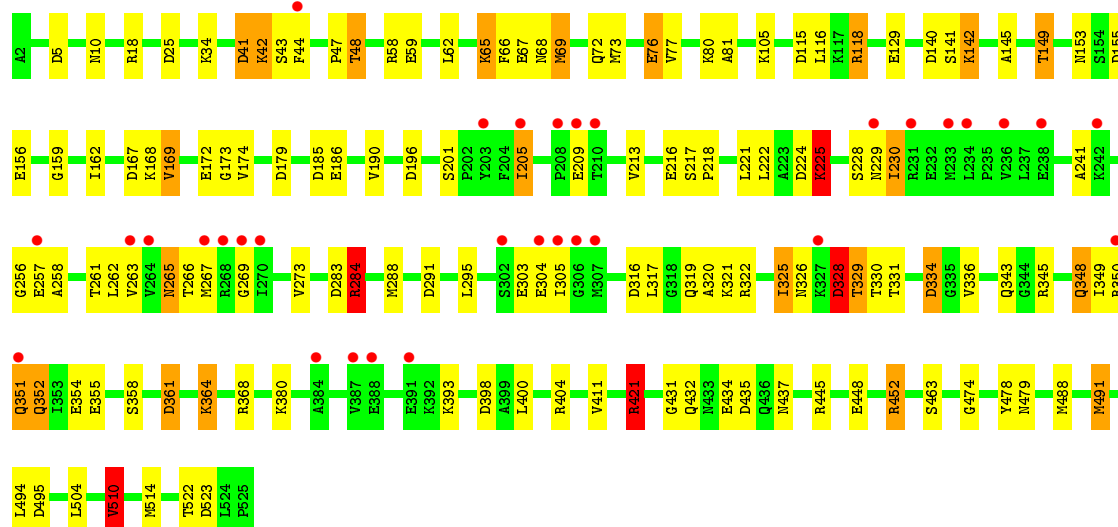
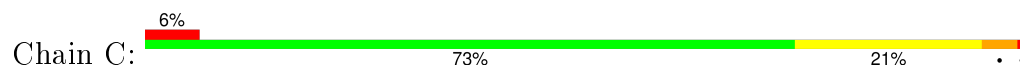
- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	18	Total 18	O 18	0	0
2	B	21	Total 21	O 21	0	0
2	C	15	Total 15	O 15	0	0
2	D	16	Total 16	O 16	0	0
2	E	17	Total 17	O 17	0	0
2	F	7	Total 7	O 7	0	0
2	G	13	Total 13	O 13	0	0

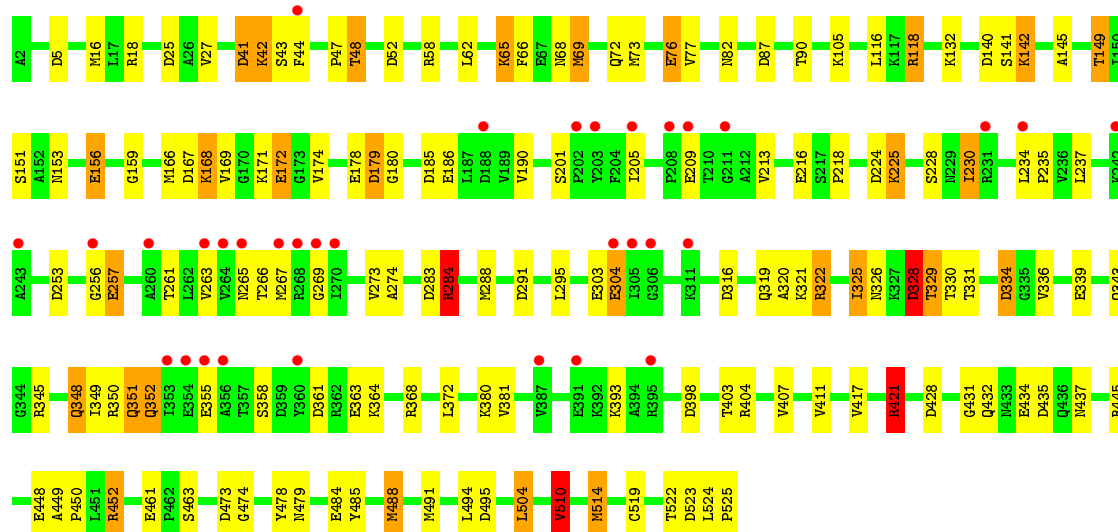




• Molecule 1: groEL protein

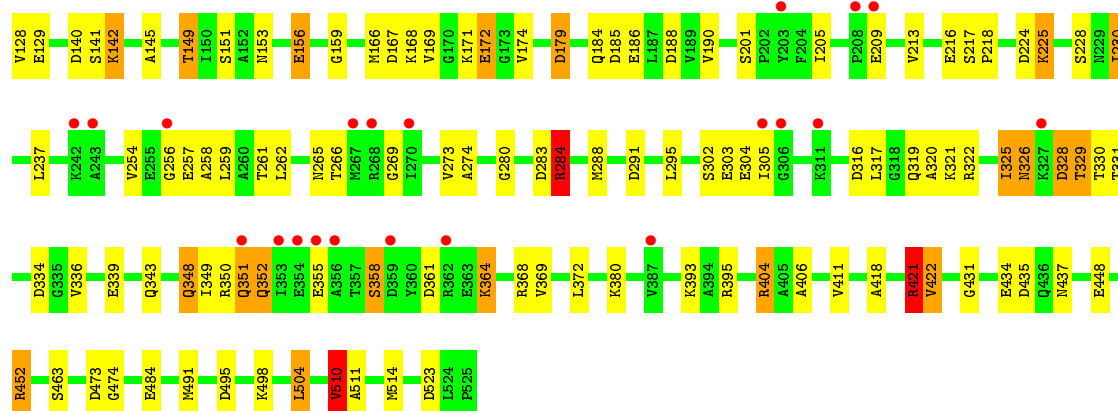


• Molecule 1: groEL protein

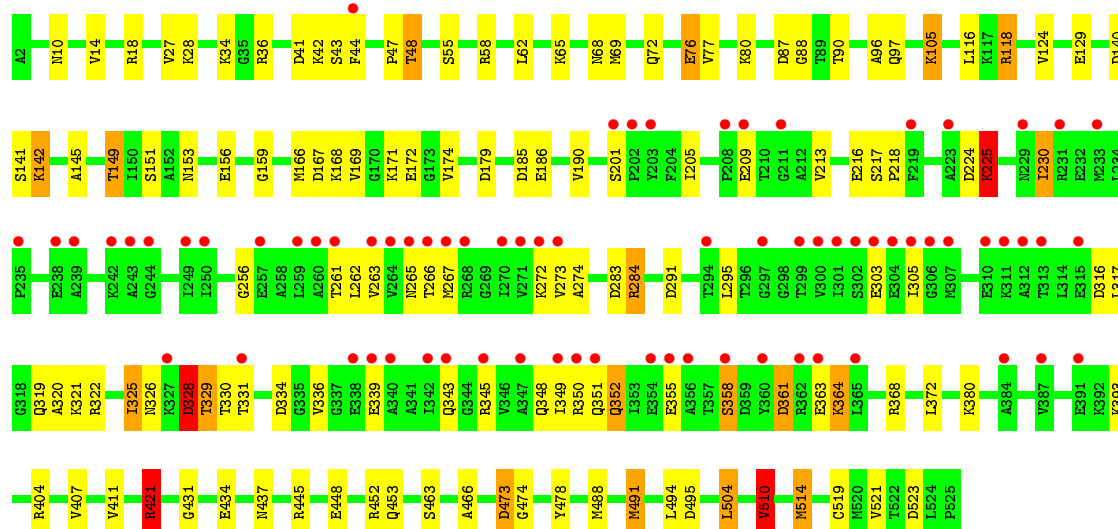
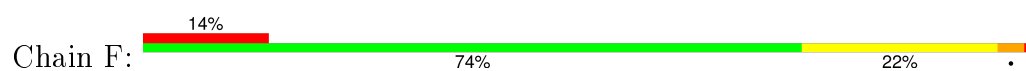


• Molecule 1: groEL protein

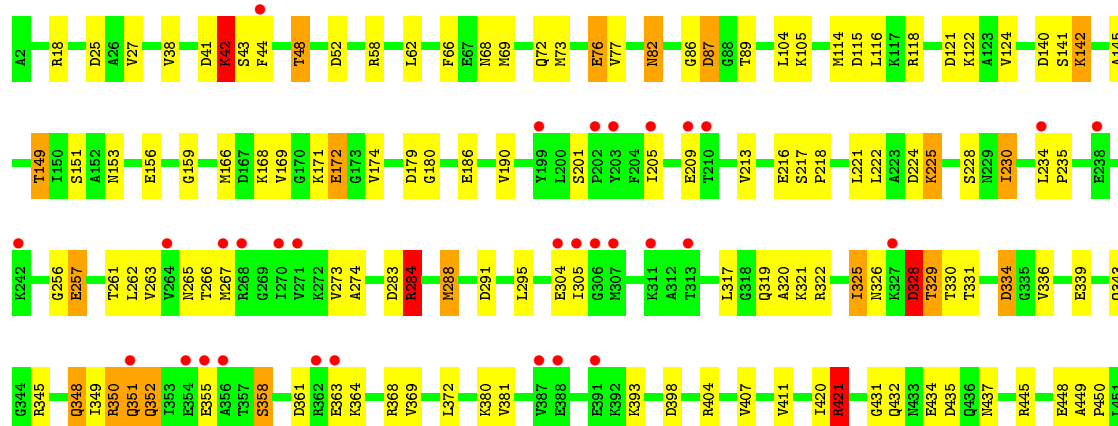




• Molecule 1: groEL protein



• Molecule 1: groEL protein







## 4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	178.38 Å   204.98 Å   280.98 Å 90.00°   90.00°   90.00°	Depositor
Resolution (Å)	30.00 – 2.70 29.96 – 2.70	Depositor EDS
% Data completeness (in resolution range)	(Not available) (30.00-2.70) 83.9 (29.96-2.70)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	0.59 (at 2.68 Å)	Xtriage
Refinement program	REFMAC 5	Depositor
R, $R_{free}$	0.215   ,   0.249 0.209   ,   0.241	Depositor DCC
$R_{free}$ test set	2966 reflections (2.58%)	DCC
Wilson B-factor (Å <sup>2</sup> )	38.5	Xtriage
Anisotropy	0.354	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.34 , 45.3	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.47$ , $\langle L^2 \rangle = 0.30$	Xtriage
Outliers	0 of 123506 reflections	Xtriage
$F_o, F_c$ correlation	0.92	EDS
Total number of atoms	27064	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	2.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.19% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical values of  $\langle |L| \rangle$ ,  $\langle L^2 \rangle$  for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 0.2 for perfectly twinned datasets.

## 5 Model quality ⓘ

### 5.1 Standard geometry ⓘ

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	1.24	28/3879 (0.7%)	1.11	22/5237 (0.4%)
1	B	1.28	33/3879 (0.9%)	1.15	27/5237 (0.5%)
1	C	1.19	30/3879 (0.8%)	1.13	26/5237 (0.5%)
1	D	1.19	27/3879 (0.7%)	1.14	31/5237 (0.6%)
1	E	1.34	35/3879 (0.9%)	1.21	30/5237 (0.6%)
1	F	1.09	22/3879 (0.6%)	1.08	18/5237 (0.3%)
1	G	1.21	21/3879 (0.5%)	1.11	19/5237 (0.4%)
All	All	1.22	196/27153 (0.7%)	1.13	173/36659 (0.5%)

All (196) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	E	129	GLU	CD-OE2	15.67	1.42	1.25
1	E	129	GLU	CD-OE1	15.50	1.42	1.25
1	E	156	GLU	CD-OE2	11.11	1.37	1.25
1	E	76	GLU	CD-OE1	11.03	1.37	1.25
1	B	473	ASP	CB-CG	11.01	1.74	1.51
1	A	44	PHE	CD1-CE1	10.82	1.60	1.39
1	B	44	PHE	CD2-CE2	9.93	1.59	1.39
1	B	76	GLU	CD-OE1	9.68	1.36	1.25
1	C	44	PHE	CD1-CE1	9.37	1.57	1.39
1	E	44	PHE	CD1-CE1	9.32	1.57	1.39
1	E	118	ARG	NE-CZ	9.16	1.45	1.33
1	E	44	PHE	CD2-CE2	9.12	1.57	1.39
1	F	44	PHE	CD1-CE1	9.06	1.57	1.39
1	A	114	MET	SD-CE	9.03	2.28	1.77
1	B	432	GLN	CG-CD	8.94	1.71	1.51
1	D	432	GLN	CG-CD	8.85	1.71	1.51
1	G	76	GLU	CD-OE2	8.84	1.35	1.25
1	B	118	ARG	NE-CZ	8.63	1.44	1.33
1	A	44	PHE	CD2-CE2	8.49	1.56	1.39
1	E	44	PHE	CE2-CZ	8.45	1.53	1.37
1	B	44	PHE	CD1-CE1	8.43	1.56	1.39

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	432	GLN	CG-CD	8.38	1.70	1.51
1	G	76	GLU	CD-OE1	8.32	1.34	1.25
1	A	118	ARG	NE-CZ	8.23	1.43	1.33
1	G	44	PHE	CD2-CE2	8.15	1.55	1.39
1	G	44	PHE	CD1-CE1	8.13	1.55	1.39
1	B	10	ASN	CB-CG	8.10	1.69	1.51
1	C	445	ARG	CG-CD	8.08	1.72	1.51
1	A	434	GLU	CD-OE2	8.06	1.34	1.25
1	E	10	ASN	CB-CG	8.03	1.69	1.51
1	F	76	GLU	CD-OE2	8.03	1.34	1.25
1	C	44	PHE	CD2-CE2	7.93	1.55	1.39
1	C	76	GLU	CD-OE1	7.92	1.34	1.25
1	C	118	ARG	NE-CZ	7.91	1.43	1.33
1	C	76	GLU	CD-OE2	7.90	1.34	1.25
1	A	44	PHE	CE2-CZ	7.87	1.52	1.37
1	E	129	GLU	CG-CD	7.84	1.63	1.51
1	A	18	ARG	CG-CD	7.83	1.71	1.51
1	D	44	PHE	CE2-CZ	7.64	1.51	1.37
1	D	18	ARG	CG-CD	7.62	1.71	1.51
1	C	10	ASN	CB-CG	7.54	1.68	1.51
1	D	473	ASP	CB-CG	7.52	1.67	1.51
1	D	44	PHE	CD1-CE1	7.52	1.54	1.39
1	F	44	PHE	CE2-CZ	7.46	1.51	1.37
1	D	445	ARG	CG-CD	7.44	1.70	1.51
1	C	44	PHE	CE2-CZ	7.38	1.51	1.37
1	G	445	ARG	CG-CD	7.29	1.70	1.51
1	G	434	GLU	CD-OE2	7.26	1.33	1.25
1	A	44	PHE	CG-CD2	7.25	1.49	1.38
1	G	44	PHE	CB-CG	7.19	1.63	1.51
1	F	44	PHE	CD2-CE2	7.12	1.53	1.39
1	B	44	PHE	CE2-CZ	7.11	1.50	1.37
1	G	432	GLN	CG-CD	7.04	1.67	1.51
1	A	434	GLU	CD-OE1	7.02	1.33	1.25
1	E	44	PHE	CG-CD1	6.99	1.49	1.38
1	F	69	MET	SD-CE	-6.96	1.38	1.77
1	A	58	ARG	CG-CD	6.95	1.69	1.51
1	C	59	GLU	CD-OE1	6.92	1.33	1.25
1	A	76	GLU	CD-OE1	6.86	1.33	1.25
1	B	58	ARG	CZ-NH1	6.84	1.42	1.33
1	D	284	ARG	CG-CD	6.81	1.69	1.51
1	A	44	PHE	CE1-CZ	6.75	1.50	1.37
1	E	434	GLU	CD-OE2	6.73	1.33	1.25

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	466	ALA	CA-CB	-6.67	1.38	1.52
1	E	434	GLU	CD-OE1	6.67	1.32	1.25
1	E	44	PHE	CG-CD2	6.64	1.48	1.38
1	G	118	ARG	NE-CZ	6.62	1.41	1.33
1	E	44	PHE	CE1-CZ	6.60	1.49	1.37
1	B	490	ASP	CB-CG	-6.58	1.38	1.51
1	B	44	PHE	CG-CD2	6.56	1.48	1.38
1	B	44	PHE	CB-CG	6.53	1.62	1.51
1	C	18	ARG	CZ-NH2	6.52	1.41	1.33
1	G	44	PHE	CE1-CZ	6.51	1.49	1.37
1	D	434	GLU	CG-CD	6.51	1.61	1.51
1	C	514	MET	CG-SD	6.49	1.98	1.81
1	A	44	PHE	CB-CG	6.48	1.62	1.51
1	D	156	GLU	CD-OE2	6.47	1.32	1.25
1	E	156	GLU	CD-OE1	6.41	1.32	1.25
1	C	434	GLU	CD-OE1	6.41	1.32	1.25
1	C	58	ARG	CZ-NH1	6.40	1.41	1.33
1	C	42	LYS	CD-CE	6.38	1.67	1.51
1	D	44	PHE	CD2-CE2	6.37	1.51	1.39
1	E	18	ARG	CZ-NH2	6.33	1.41	1.33
1	F	445	ARG	CG-CD	6.33	1.67	1.51
1	G	288	MET	SD-CE	6.33	2.13	1.77
1	B	76	GLU	CD-OE2	6.31	1.32	1.25
1	B	69	MET	SD-CE	-6.30	1.42	1.77
1	A	118	ARG	CZ-NH2	6.29	1.41	1.33
1	C	284	ARG	CG-CD	6.28	1.67	1.51
1	C	44	PHE	CG-CD1	6.25	1.48	1.38
1	D	44	PHE	CE1-CZ	6.25	1.49	1.37
1	G	44	PHE	CG-CD1	6.20	1.48	1.38
1	D	484	GLU	CD-OE1	6.19	1.32	1.25
1	D	118	ARG	CG-CD	6.17	1.67	1.51
1	E	76	GLU	CD-OE2	6.15	1.32	1.25
1	C	81	ALA	CA-CB	-6.12	1.39	1.52
1	A	127	ALA	CA-CB	-6.11	1.39	1.52
1	G	44	PHE	CE2-CZ	6.10	1.49	1.37
1	A	44	PHE	CG-CD1	6.08	1.47	1.38
1	G	484	GLU	CD-OE1	6.02	1.32	1.25
1	D	434	GLU	CD-OE1	6.00	1.32	1.25
1	G	434	GLU	CD-OE1	5.99	1.32	1.25
1	F	76	GLU	CD-OE1	5.96	1.32	1.25
1	F	514	MET	CG-SD	5.95	1.96	1.81
1	E	284	ARG	CG-CD	5.94	1.66	1.51

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	E	118	ARG	CZ-NH1	5.91	1.40	1.33
1	D	485	TYR	CE1-CZ	5.90	1.46	1.38
1	A	284	ARG	NE-CZ	5.90	1.40	1.33
1	E	114	MET	CG-SD	5.88	1.96	1.81
1	A	434	GLU	CG-CD	5.88	1.60	1.51
1	E	118	ARG	CZ-NH2	5.85	1.40	1.33
1	B	411	VAL	CB-CG2	-5.83	1.40	1.52
1	C	434	GLU	CD-OE2	5.82	1.32	1.25
1	A	118	ARG	CZ-NH1	5.81	1.40	1.33
1	G	18	ARG	CZ-NH2	5.80	1.40	1.33
1	B	118	ARG	CZ-NH2	5.80	1.40	1.33
1	A	18	ARG	CZ-NH2	5.79	1.40	1.33
1	F	18	ARG	CG-CD	5.78	1.66	1.51
1	B	44	PHE	CA-CB	5.78	1.66	1.53
1	D	44	PHE	CG-CD2	5.77	1.47	1.38
1	A	484	GLU	CD-OE1	5.75	1.31	1.25
1	G	44	PHE	CG-CD2	5.73	1.47	1.38
1	B	82	ASN	CG-OD1	5.73	1.36	1.24
1	B	44	PHE	CG-CD1	5.72	1.47	1.38
1	F	118	ARG	NE-CZ	5.72	1.40	1.33
1	B	164	GLU	CD-OE1	5.70	1.31	1.25
1	G	518	GLU	CD-OE2	-5.70	1.19	1.25
1	E	42	LYS	CD-CE	5.68	1.65	1.51
1	G	42	LYS	CD-CE	5.67	1.65	1.51
1	F	44	PHE	CG-CD2	5.66	1.47	1.38
1	B	284	ARG	CG-CD	5.65	1.66	1.51
1	E	484	GLU	CD-OE1	5.53	1.31	1.25
1	B	445	ARG	CG-CD	5.51	1.65	1.51
1	B	156	GLU	CD-OE2	5.49	1.31	1.25
1	C	118	ARG	CG-CD	5.47	1.65	1.51
1	D	42	LYS	CD-CE	5.47	1.65	1.51
1	F	44	PHE	CB-CG	5.46	1.60	1.51
1	F	58	ARG	CG-CD	5.46	1.65	1.51
1	B	102	GLU	CD-OE1	5.44	1.31	1.25
1	A	284	ARG	CG-CD	5.43	1.65	1.51
1	F	466	ALA	CA-CB	-5.42	1.41	1.52
1	C	44	PHE	CE1-CZ	5.42	1.47	1.37
1	G	44	PHE	CA-CB	5.42	1.65	1.53
1	D	168	LYS	CD-CE	5.41	1.64	1.51
1	E	77	VAL	CB-CG1	-5.40	1.41	1.52
1	C	44	PHE	CG-CD2	5.40	1.46	1.38
1	F	129	GLU	CD-OE2	5.39	1.31	1.25

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	76	GLU	CD-OE2	5.39	1.31	1.25
1	B	490	ASP	CG-OD1	5.38	1.37	1.25
1	F	434	GLU	CD-OE1	5.37	1.31	1.25
1	F	18	ARG	CZ-NH2	5.37	1.40	1.33
1	E	58	ARG	NE-CZ	5.36	1.40	1.33
1	D	514	MET	CG-SD	5.35	1.95	1.81
1	E	118	ARG	CG-CD	5.35	1.65	1.51
1	C	491	MET	SD-CE	5.34	2.07	1.77
1	E	71	ALA	CA-CB	-5.34	1.41	1.52
1	B	58	ARG	CZ-NH2	5.33	1.40	1.33
1	D	432	GLN	CB-CG	5.33	1.67	1.52
1	B	129	GLU	CD-OE2	5.32	1.31	1.25
1	C	58	ARG	NE-CZ	5.31	1.40	1.33
1	E	18	ARG	CG-CD	5.30	1.65	1.51
1	A	58	ARG	CZ-NH1	5.29	1.40	1.33
1	E	128	VAL	CB-CG2	-5.29	1.41	1.52
1	D	44	PHE	CG-CD1	5.25	1.46	1.38
1	C	69	MET	SD-CE	-5.25	1.48	1.77
1	C	18	ARG	NE-CZ	5.24	1.39	1.33
1	C	118	ARG	CZ-NH2	5.22	1.39	1.33
1	F	521	VAL	CB-CG2	-5.22	1.41	1.52
1	D	417	VAL	CB-CG1	-5.22	1.41	1.52
1	F	58	ARG	NE-CZ	5.21	1.39	1.33
1	B	422	VAL	CB-CG2	-5.20	1.42	1.52
1	D	18	ARG	CZ-NH1	5.17	1.39	1.33
1	B	490	ASP	CA-CB	-5.17	1.42	1.53
1	E	105	LYS	CE-NZ	5.16	1.61	1.49
1	A	463	SER	CB-OG	-5.15	1.35	1.42
1	E	422	VAL	CB-CG2	-5.15	1.42	1.52
1	D	118	ARG	NE-CZ	5.14	1.39	1.33
1	F	10	ASN	CB-CG	5.13	1.62	1.51
1	E	126	VAL	CB-CG2	-5.12	1.42	1.52
1	C	434	GLU	CG-CD	5.12	1.59	1.51
1	A	445	ARG	CG-CD	5.11	1.64	1.51
1	D	69	MET	SD-CE	-5.11	1.49	1.77
1	F	491	MET	SD-CE	5.11	2.06	1.77
1	E	406	ALA	CA-CB	-5.10	1.41	1.52
1	F	284	ARG	CG-CD	5.09	1.64	1.51
1	C	284	ARG	CB-CG	5.09	1.66	1.52
1	C	129	GLU	CD-OE1	5.08	1.31	1.25
1	A	92	ALA	CA-CB	-5.05	1.41	1.52
1	B	172	GLU	CD-OE2	5.05	1.31	1.25

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	G	284	ARG	CG-CD	5.04	1.64	1.51
1	A	156	GLU	CD-OE2	5.04	1.31	1.25
1	D	44	PHE	CA-CB	5.04	1.65	1.53
1	B	44	PHE	CA-C	5.04	1.66	1.52
1	E	18	ARG	CZ-NH1	5.04	1.39	1.33
1	B	489	ILE	CG1-CD1	5.03	1.85	1.50
1	C	432	GLN	CG-CD	5.02	1.62	1.51

All (173) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	421	ARG	NE-CZ-NH1	12.62	126.61	120.30
1	E	421	ARG	NE-CZ-NH2	-12.43	114.08	120.30
1	E	452	ARG	NE-CZ-NH1	12.14	126.37	120.30
1	B	491	MET	CG-SD-CE	-11.48	81.84	100.20
1	E	421	ARG	NE-CZ-NH1	11.13	125.86	120.30
1	D	167	ASP	CB-CG-OD2	11.08	128.27	118.30
1	A	421	ARG	NE-CZ-NH2	-11.05	114.77	120.30
1	A	435	ASP	CB-CG-OD2	10.11	127.40	118.30
1	C	452	ARG	NE-CZ-NH1	10.06	125.33	120.30
1	G	421	ARG	NE-CZ-NH2	-9.78	115.41	120.30
1	F	421	ARG	NE-CZ-NH1	9.71	125.16	120.30
1	G	115	ASP	CB-CG-OD2	9.65	126.98	118.30
1	G	495	ASP	CB-CG-OD2	9.61	126.95	118.30
1	E	452	ARG	NE-CZ-NH2	-8.99	115.81	120.30
1	B	490	ASP	CB-CG-OD2	-8.81	110.37	118.30
1	B	25	ASP	CB-CG-OD1	8.76	126.19	118.30
1	C	435	ASP	CB-CG-OD2	8.75	126.18	118.30
1	C	167	ASP	CB-CG-OD2	8.47	125.92	118.30
1	E	491	MET	CG-SD-CE	-8.36	86.83	100.20
1	C	421	ARG	NE-CZ-NH1	8.31	124.46	120.30
1	C	495	ASP	CB-CG-OD2	8.27	125.75	118.30
1	G	52	ASP	CB-CG-OD1	8.26	125.74	118.30
1	D	523	ASP	CB-CG-OD1	8.20	125.68	118.30
1	F	495	ASP	CB-CG-OD2	8.15	125.64	118.30
1	E	167	ASP	CB-CG-OD2	8.01	125.50	118.30
1	E	87	ASP	CB-CG-OD1	7.96	125.46	118.30
1	F	421	ARG	NE-CZ-NH2	-7.86	116.37	120.30
1	C	328	ASP	CB-CG-OD2	7.81	125.33	118.30
1	E	283	ASP	CB-CG-OD2	7.78	125.30	118.30
1	D	495	ASP	CB-CG-OD2	7.76	125.28	118.30
1	D	25	ASP	CB-CG-OD2	7.70	125.23	118.30

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	283	ASP	CB-CG-OD2	7.67	125.20	118.30
1	C	452	ARG	NE-CZ-NH2	-7.66	116.47	120.30
1	D	52	ASP	CB-CG-OD1	7.62	125.16	118.30
1	G	121	ASP	CB-CG-OD2	7.62	125.16	118.30
1	B	421	ARG	NE-CZ-NH2	-7.55	116.53	120.30
1	B	490	ASP	CB-CA-C	-7.50	95.41	110.40
1	A	510	VAL	CB-CA-C	-7.34	97.45	111.40
1	D	328	ASP	CB-CG-OD2	7.30	124.87	118.30
1	E	316	ASP	CB-CG-OD2	7.29	124.86	118.30
1	F	510	VAL	CB-CA-C	-7.29	97.56	111.40
1	D	167	ASP	CB-CG-OD1	-7.24	111.78	118.30
1	D	58	ARG	NE-CZ-NH2	-7.23	116.68	120.30
1	D	87	ASP	CB-CG-OD1	7.23	124.81	118.30
1	C	41	ASP	CB-CG-OD2	7.20	124.78	118.30
1	E	523	ASP	CB-CG-OD2	7.17	124.75	118.30
1	B	121	ASP	CB-CG-OD2	7.15	124.73	118.30
1	B	167	ASP	CB-CG-OD2	7.12	124.71	118.30
1	D	473	ASP	CB-CG-OD1	7.07	124.66	118.30
1	A	167	ASP	CB-CG-OD2	7.02	124.62	118.30
1	D	452	ARG	NE-CZ-NH1	7.00	123.80	120.30
1	B	36	ARG	NE-CZ-NH1	6.96	123.78	120.30
1	G	328	ASP	CB-CG-OD2	6.88	124.49	118.30
1	A	334	ASP	CB-CG-OD2	6.85	124.47	118.30
1	F	328	ASP	CB-CG-OD2	6.80	124.42	118.30
1	A	283	ASP	CB-CG-OD2	6.75	124.38	118.30
1	G	283	ASP	CB-CG-OD2	6.70	124.33	118.30
1	F	283	ASP	CB-CG-OD2	6.68	124.31	118.30
1	C	140	ASP	CB-CG-OD2	6.64	124.28	118.30
1	B	316	ASP	CB-CG-OD2	6.63	124.27	118.30
1	C	25	ASP	CB-CG-OD2	6.63	124.27	118.30
1	F	140	ASP	CB-CG-OD2	6.63	124.27	118.30
1	A	58	ARG	NE-CZ-NH2	-6.62	116.99	120.30
1	F	167	ASP	CB-CG-OD2	6.62	124.26	118.30
1	C	510	VAL	CB-CA-C	-6.59	98.88	111.40
1	D	461	GLU	OE1-CD-OE2	-6.58	115.41	123.30
1	E	115	ASP	CB-CG-OD2	6.56	124.20	118.30
1	D	334	ASP	CB-CG-OD2	6.55	124.20	118.30
1	E	395	ARG	NE-CZ-NH1	-6.55	117.02	120.30
1	B	510	VAL	CB-CA-C	-6.54	98.97	111.40
1	D	185	ASP	CB-CG-OD2	6.54	124.19	118.30
1	C	421	ARG	NE-CZ-NH2	-6.52	117.04	120.30
1	D	428	ASP	CB-CG-OD2	6.50	124.15	118.30

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	5	ASP	CB-CG-OD1	6.48	124.13	118.30
1	F	105	LYS	CD-CE-NZ	-6.48	96.80	111.70
1	B	421	ARG	NE-CZ-NH1	6.47	123.54	120.30
1	G	510	VAL	CB-CA-C	-6.43	99.18	111.40
1	D	5	ASP	CB-CG-OD2	6.43	124.09	118.30
1	C	316	ASP	CB-CG-OD2	6.41	124.07	118.30
1	E	185	ASP	CB-CG-OD2	6.40	124.06	118.30
1	A	495	ASP	CB-CG-OD1	-6.34	112.59	118.30
1	A	328	ASP	CB-CG-OD2	6.33	124.00	118.30
1	A	140	ASP	CB-CG-OD2	6.33	124.00	118.30
1	B	334	ASP	CB-CG-OD2	6.32	123.99	118.30
1	B	36	ARG	NE-CZ-NH2	-6.28	117.16	120.30
1	B	328	ASP	CB-CG-OD2	6.27	123.95	118.30
1	B	490	ASP	CB-CG-OD1	6.27	123.94	118.30
1	D	435	ASP	CB-CG-OD2	6.25	123.92	118.30
1	E	188	ASP	CB-CG-OD2	6.24	123.92	118.30
1	A	495	ASP	CB-CG-OD2	6.24	123.92	118.30
1	E	179	ASP	CB-CG-OD2	6.23	123.90	118.30
1	D	283	ASP	CB-CG-OD2	6.22	123.89	118.30
1	G	421	ARG	NE-CZ-NH1	6.21	123.41	120.30
1	G	495	ASP	CB-CG-OD1	-6.20	112.72	118.30
1	B	58	ARG	NE-CZ-NH2	-6.20	117.20	120.30
1	E	495	ASP	CB-CG-OD2	6.20	123.88	118.30
1	D	398	ASP	CB-CG-OD2	6.18	123.87	118.30
1	A	452	ARG	NE-CZ-NH1	6.18	123.39	120.30
1	C	196	ASP	CB-CG-OD2	6.17	123.86	118.30
1	A	316	ASP	CB-CG-OD2	6.16	123.84	118.30
1	D	179	ASP	CB-CG-OD2	6.15	123.83	118.30
1	E	52	ASP	CB-CG-OD2	6.12	123.80	118.30
1	C	495	ASP	CB-CG-OD1	-6.10	112.81	118.30
1	G	58	ARG	NE-CZ-NH2	-6.09	117.25	120.30
1	E	328	ASP	CB-CG-OD2	6.09	123.78	118.30
1	E	510	VAL	CB-CA-C	-6.08	99.86	111.40
1	E	404	ARG	NE-CZ-NH2	-6.07	117.27	120.30
1	A	41	ASP	CB-CG-OD1	6.05	123.74	118.30
1	D	140	ASP	CB-CG-OD2	6.03	123.73	118.30
1	B	283	ASP	CB-CG-OD2	6.01	123.71	118.30
1	E	435	ASP	CB-CG-OD2	6.01	123.71	118.30
1	D	316	ASP	CB-CG-OD2	6.00	123.70	118.30
1	A	504	LEU	CB-CG-CD2	5.99	121.19	111.00
1	A	491	MET	CG-SD-CE	-5.99	90.62	100.20
1	C	334	ASP	CB-CG-OD2	5.97	123.67	118.30

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	510	VAL	CB-CA-C	-5.93	100.14	111.40
1	A	52	ASP	CB-CG-OD2	5.92	123.63	118.30
1	F	185	ASP	CB-CG-OD2	5.91	123.62	118.30
1	B	185	ASP	CB-CG-OD2	5.90	123.61	118.30
1	G	25	ASP	CB-CG-OD2	5.90	123.61	118.30
1	B	523	ASP	CB-CG-OD1	5.86	123.58	118.30
1	D	504	LEU	CB-CG-CD2	5.86	120.96	111.00
1	D	488	MET	CG-SD-CE	-5.83	90.87	100.20
1	G	523	ASP	CB-CG-OD2	5.78	123.50	118.30
1	G	334	ASP	CB-CG-OD2	5.77	123.50	118.30
1	E	140	ASP	CB-CG-OD2	5.76	123.48	118.30
1	A	361	ASP	CB-CG-OD2	5.75	123.48	118.30
1	D	421	ARG	NE-CZ-NH2	-5.74	117.43	120.30
1	D	284	ARG	NE-CZ-NH1	5.73	123.17	120.30
1	G	140	ASP	CB-CG-OD2	5.70	123.43	118.30
1	C	523	ASP	CB-CG-OD2	5.69	123.42	118.30
1	E	116	LEU	CA-CB-CG	5.67	128.34	115.30
1	G	473	ASP	CB-CG-OD2	5.66	123.39	118.30
1	D	253	ASP	CB-CG-OD2	5.65	123.39	118.30
1	F	523	ASP	CB-CG-OD2	5.61	123.34	118.30
1	A	87	ASP	CB-CG-OD1	5.57	123.31	118.30
1	B	361	ASP	CB-CG-OD2	5.56	123.30	118.30
1	B	116	LEU	CA-CB-CG	5.55	128.07	115.30
1	F	140	ASP	OD1-CG-OD2	-5.53	112.80	123.30
1	E	498	LYS	CD-CE-NZ	5.51	124.38	111.70
1	G	435	ASP	CB-CG-OD2	5.50	123.25	118.30
1	E	172	GLU	CA-CB-CG	5.47	125.43	113.40
1	F	316	ASP	CB-CG-OD2	5.47	123.22	118.30
1	B	291	ASP	CB-CG-OD2	5.46	123.22	118.30
1	B	196	ASP	CB-CG-OD2	5.46	123.22	118.30
1	C	115	ASP	CB-CG-OD2	5.44	123.19	118.30
1	E	284	ARG	NE-CZ-NH1	5.43	123.02	120.30
1	C	361	ASP	CB-CG-OD2	5.41	123.17	118.30
1	E	64	ASP	CB-CG-OD2	5.40	123.16	118.30
1	D	361	ASP	CB-CG-OD2	5.40	123.16	118.30
1	B	253	ASP	CB-CG-OD2	5.39	123.15	118.30
1	A	253	ASP	CB-CG-OD2	5.37	123.13	118.30
1	C	80	LYS	CD-CE-NZ	-5.34	99.42	111.70
1	E	326	ASN	CB-CA-C	-5.34	99.73	110.40
1	B	140	ASP	CB-CG-OD2	5.33	123.10	118.30
1	G	398	ASP	CB-CG-OD2	5.31	123.08	118.30
1	A	185	ASP	CB-CG-OD2	5.28	123.06	118.30

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	G	87	ASP	CB-CG-OD1	5.28	123.06	118.30
1	C	155	ASP	CB-CG-OD2	5.28	123.05	118.30
1	C	185	ASP	CB-CG-OD2	5.27	123.04	118.30
1	F	361	ASP	CB-CG-OD2	5.25	123.03	118.30
1	B	473	ASP	CB-CG-OD2	5.24	123.01	118.30
1	D	87	ASP	OD1-CG-OD2	-5.23	113.36	123.30
1	D	41	ASP	CB-CG-OD2	5.21	122.99	118.30
1	F	140	ASP	CB-CG-OD1	5.15	122.94	118.30
1	F	48	THR	OG1-CB-CG2	-5.14	98.17	110.00
1	E	125	THR	OG1-CB-CG2	-5.14	98.18	110.00
1	E	473	ASP	CB-CG-OD2	5.13	122.92	118.30
1	C	25	ASP	OD1-CG-OD2	-5.07	113.67	123.30
1	F	473	ASP	CB-CG-OD1	5.06	122.86	118.30
1	F	36	ARG	NE-CZ-NH2	-5.05	117.77	120.30
1	B	432	GLN	CA-CB-CG	5.05	124.51	113.40
1	C	398	ASP	CB-CG-OD2	5.00	122.80	118.30

There are no chirality outliers.

There are no planarity outliers.

## 5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3851	0	3970	77	0
1	B	3851	0	3970	83	0
1	C	3851	0	3970	77	1
1	D	3851	0	3970	77	0
1	E	3851	0	3970	77	0
1	F	3851	0	3970	69	0
1	G	3851	0	3970	76	1
2	A	18	0	0	1	0
2	B	21	0	0	4	0
2	C	15	0	0	0	0
2	D	16	0	0	0	0
2	E	17	0	0	0	0
2	F	7	0	0	1	0

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	G	13	0	0	1	0
All	All	27064	0	27790	517	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 9.

All (517) 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:B:489:ILE:CD1	1:B:489:ILE:CG1	1.85	1.52
1:B:473:ASP:CG	1:B:473:ASP:CB	1.74	1.51
1:A:288:MET:CE	1:A:288:MET:SD	2.03	1.47
1:G:114:MET:SD	1:G:114:MET:CE	2.01	1.46
1:C:288:MET:CE	1:C:288:MET:SD	2.02	1.46
1:E:288:MET:CE	1:E:288:MET:SD	2.04	1.46
1:F:491:MET:SD	1:F:491:MET:CE	2.06	1.44
1:C:491:MET:CE	1:C:491:MET:SD	2.07	1.43
1:G:288:MET:CE	1:G:288:MET:SD	2.13	1.36
1:A:114:MET:SD	1:A:114:MET:CE	2.28	1.22
1:G:142:LYS:HD3	1:G:142:LYS:H	1.08	1.12
1:E:213:VAL:HB	1:E:325:ILE:HG12	1.40	1.04
1:B:142:LYS:HD3	1:B:142:LYS:H	1.25	0.98
1:G:142:LYS:HD3	1:G:142:LYS:N	1.77	0.98
1:E:142:LYS:HD3	1:E:142:LYS:H	1.29	0.97
1:B:142:LYS:HD3	1:B:142:LYS:N	1.81	0.95
1:B:473:ASP:OD1	2:B:528:HOH:O	1.84	0.94
1:F:213:VAL:HB	1:F:325:ILE:HG12	1.48	0.94
1:D:213:VAL:HB	1:D:325:ILE:HG12	1.48	0.94
1:C:142:LYS:HD3	1:C:142:LYS:H	1.32	0.93
1:A:213:VAL:HB	1:A:325:ILE:HG12	1.48	0.93
1:G:213:VAL:HB	1:G:325:ILE:HG12	1.48	0.93
1:F:142:LYS:H	1:F:142:LYS:HD3	1.34	0.92
1:B:213:VAL:HB	1:B:325:ILE:HG12	1.50	0.91
1:C:62:LEU:H	1:C:68:ASN:HD22	1.16	0.91
1:D:142:LYS:H	1:D:142:LYS:HD3	1.33	0.91
1:A:62:LEU:H	1:A:68:ASN:HD22	1.13	0.91
1:E:142:LYS:N	1:E:142:LYS:HD3	1.89	0.88
1:C:213:VAL:HB	1:C:325:ILE:HG12	1.53	0.87
1:G:149:THR:HG22	1:G:159:GLY:HA3	1.57	0.86
1:C:142:LYS:N	1:C:142:LYS:HD3	1.91	0.85
1:C:421:ARG:HD2	1:C:474:GLY:O	1.76	0.85

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:149:THR:HG22	1:B:159:GLY:HA3	1.57	0.85
1:A:62:LEU:H	1:A:68:ASN:ND2	1.75	0.84
1:A:142:LYS:H	1:A:142:LYS:HD3	1.41	0.84
1:B:490:ASP:OD2	2:B:536:HOH:O	1.95	0.84
1:C:149:THR:HG22	1:C:159:GLY:HA3	1.58	0.83
1:D:142:LYS:N	1:D:142:LYS:HD3	1.93	0.83
1:D:149:THR:HG22	1:D:159:GLY:HA3	1.58	0.83
1:A:42:LYS:HE2	1:A:48:THR:HG23	1.60	0.82
1:A:142:LYS:HD3	1:A:142:LYS:N	1.94	0.81
1:B:62:LEU:H	1:B:68:ASN:ND2	1.78	0.81
1:A:421:ARG:HD2	1:A:474:GLY:O	1.79	0.81
1:C:62:LEU:H	1:C:68:ASN:ND2	1.79	0.80
1:G:213:VAL:HB	1:G:325:ILE:CG1	2.12	0.80
1:D:421:ARG:HD2	1:D:474:GLY:O	1.82	0.79
1:C:42:LYS:HE2	1:C:48:THR:HG23	1.64	0.79
1:D:62:LEU:H	1:D:68:ASN:ND2	1.80	0.79
1:E:145:ALA:O	1:E:149:THR:CG2	2.31	0.79
1:D:145:ALA:O	1:D:149:THR:HG23	1.83	0.78
1:F:62:LEU:H	1:F:68:ASN:HD22	1.30	0.78
1:F:142:LYS:HD3	1:F:142:LYS:N	1.97	0.78
1:E:145:ALA:O	1:E:149:THR:HG23	1.82	0.78
1:A:149:THR:HG22	1:A:159:GLY:HA3	1.64	0.78
1:A:452:ARG:NH2	1:A:463:SER:HB3	1.98	0.78
1:D:213:VAL:HB	1:D:325:ILE:CG1	2.14	0.77
1:B:62:LEU:H	1:B:68:ASN:HD22	1.32	0.77
1:B:494:LEU:HD12	1:B:494:LEU:O	1.85	0.77
1:F:149:THR:HG22	1:F:159:GLY:HA3	1.64	0.77
1:F:452:ARG:NH2	1:F:463:SER:HB3	2.00	0.77
1:C:494:LEU:HD12	1:C:494:LEU:O	1.85	0.76
1:G:142:LYS:H	1:G:142:LYS:CD	1.95	0.76
1:D:42:LYS:HE2	1:D:48:THR:HG23	1.66	0.76
1:B:213:VAL:HB	1:B:325:ILE:CG1	2.16	0.76
1:A:145:ALA:O	1:A:149:THR:HG23	1.85	0.76
1:F:421:ARG:HD2	1:F:474:GLY:O	1.86	0.76
1:B:448:GLU:OE1	1:B:452:ARG:NH1	2.19	0.75
1:G:62:LEU:H	1:G:68:ASN:ND2	1.84	0.75
1:G:62:LEU:H	1:G:68:ASN:HD22	1.34	0.75
1:F:213:VAL:HB	1:F:325:ILE:CG1	2.17	0.74
1:D:62:LEU:H	1:D:68:ASN:HD22	1.35	0.74
1:C:213:VAL:HB	1:C:325:ILE:CG1	2.17	0.74
1:D:431:GLY:H	1:D:437:ASN:HD21	1.36	0.74

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:213:VAL:HB	1:E:325:ILE:CG1	2.17	0.74
1:F:473:ASP:OD1	2:F:527:HOH:O	2.05	0.74
1:D:452:ARG:NH2	1:D:463:SER:HB3	2.02	0.73
1:A:213:VAL:HB	1:A:325:ILE:CG1	2.18	0.73
1:A:231:ARG:NH1	1:B:241:ALA:HB1	2.03	0.73
1:F:62:LEU:H	1:F:68:ASN:ND2	1.88	0.72
1:E:431:GLY:H	1:E:437:ASN:HD21	1.35	0.72
1:F:145:ALA:O	1:F:149:THR:HG23	1.90	0.72
1:D:77:VAL:HG21	1:D:510:VAL:HG13	1.71	0.72
1:E:166:MET:HG2	1:E:171:LYS:HA	1.73	0.71
1:G:431:GLY:H	1:G:437:ASN:HD21	1.35	0.71
1:A:319:GLN:HB3	1:A:336:VAL:HG21	1.73	0.71
1:G:291:ASP:OD2	1:G:368:ARG:HD2	1.91	0.71
1:F:291:ASP:OD2	1:F:368:ARG:HD2	1.90	0.71
1:B:291:ASP:OD2	1:B:368:ARG:HD2	1.90	0.70
1:F:349:ILE:HA	1:F:352:GLN:HG3	1.73	0.70
1:C:431:GLY:H	1:C:437:ASN:ND2	1.90	0.70
1:F:179:ASP:OD1	1:F:393:LYS:HE3	1.91	0.70
1:C:42:LYS:HE2	1:C:48:THR:CG2	2.20	0.70
1:E:431:GLY:H	1:E:437:ASN:ND2	1.90	0.70
1:B:431:GLY:H	1:B:437:ASN:HD21	1.38	0.70
1:D:349:ILE:HA	1:D:352:GLN:HG3	1.74	0.69
1:A:448:GLU:OE1	1:A:452:ARG:NH1	2.25	0.69
1:G:421:ARG:HD2	1:G:474:GLY:O	1.93	0.69
1:C:431:GLY:H	1:C:437:ASN:HD21	1.40	0.69
1:A:291:ASP:OD2	1:A:368:ARG:HD2	1.92	0.69
1:G:145:ALA:O	1:G:149:THR:HG23	1.94	0.68
1:A:42:LYS:HE2	1:A:48:THR:CG2	2.23	0.68
1:B:349:ILE:HA	1:B:352:GLN:HG3	1.76	0.68
1:B:42:LYS:HE2	1:B:48:THR:HG23	1.76	0.67
1:A:269:GLY:HA3	1:G:257:GLU:HG3	1.77	0.67
1:G:41:ASP:O	1:G:42:LYS:HD3	1.95	0.67
1:E:149:THR:HG22	1:E:159:GLY:HA3	1.75	0.67
1:B:166:MET:HG2	1:B:171:LYS:HA	1.76	0.67
1:A:231:ARG:CZ	1:B:241:ALA:HB1	2.24	0.66
1:G:349:ILE:HA	1:G:352:GLN:HG3	1.77	0.66
1:F:42:LYS:HE2	1:F:48:THR:HG23	1.75	0.66
1:B:319:GLN:HB3	1:B:336:VAL:HG21	1.76	0.66
1:E:349:ILE:HA	1:E:352:GLN:HG3	1.76	0.66
1:A:431:GLY:H	1:A:437:ASN:HD21	1.43	0.66
1:E:326:ASN:HD22	1:E:329:THR:HB	1.61	0.66

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:145:ALA:O	1:A:149:THR:CG2	2.44	0.66
1:D:145:ALA:O	1:D:149:THR:CG2	2.43	0.66
1:B:145:ALA:O	1:B:149:THR:HG23	1.95	0.65
1:D:494:LEU:HD12	1:D:494:LEU:O	1.97	0.65
1:E:291:ASP:OD2	1:E:368:ARG:HD2	1.96	0.65
1:E:62:LEU:H	1:E:68:ASN:HD22	1.43	0.65
1:E:142:LYS:CD	1:E:142:LYS:H	2.08	0.65
1:B:431:GLY:H	1:B:437:ASN:ND2	1.95	0.65
1:E:62:LEU:H	1:E:68:ASN:ND2	1.95	0.65
1:C:321:LYS:HG3	1:C:334:ASP:HB3	1.80	0.64
1:F:27:VAL:CG1	1:F:90:THR:HG23	2.28	0.64
1:G:42:LYS:HE2	1:G:48:THR:HG23	1.80	0.64
1:C:291:ASP:OD2	1:C:368:ARG:HD2	1.98	0.64
1:D:431:GLY:H	1:D:437:ASN:ND2	1.95	0.64
1:C:145:ALA:O	1:C:149:THR:HG23	1.98	0.63
1:D:421:ARG:CD	1:D:474:GLY:O	2.47	0.63
1:E:421:ARG:HD2	1:E:474:GLY:O	1.98	0.63
1:B:224:ASP:O	1:B:225:LYS:HB3	1.99	0.63
1:F:68:ASN:ND2	1:F:72:GLN:HE21	1.97	0.63
1:D:257:GLU:HG3	1:E:269:GLY:O	1.98	0.63
1:E:452:ARG:NH2	1:E:463:SER:HB3	2.14	0.63
1:C:349:ILE:HA	1:C:352:GLN:HG3	1.80	0.62
1:D:291:ASP:OD2	1:D:368:ARG:HD2	1.99	0.62
1:F:321:LYS:HG3	1:F:334:ASP:HB3	1.81	0.62
1:G:452:ARG:NH2	1:G:463:SER:HB3	2.13	0.62
1:F:41:ASP:O	1:F:42:LYS:HD3	1.99	0.62
1:E:68:ASN:HD21	1:E:72:GLN:HE21	1.47	0.62
1:A:349:ILE:HA	1:A:352:GLN:HG3	1.82	0.62
1:F:145:ALA:O	1:F:149:THR:CG2	2.47	0.62
1:G:166:MET:HG2	1:G:171:LYS:HA	1.82	0.62
1:E:321:LYS:HG3	1:E:334:ASP:HB3	1.81	0.62
1:C:229:ASN:OD1	1:D:269:GLY:O	2.18	0.62
1:B:179:ASP:OD1	1:B:393:LYS:HE3	2.00	0.62
1:B:326:ASN:HD22	1:B:329:THR:HB	1.65	0.61
1:D:321:LYS:HG3	1:D:334:ASP:HB3	1.81	0.61
1:F:431:GLY:H	1:F:437:ASN:ND2	1.97	0.61
1:C:224:ASP:O	1:C:225:LYS:HB3	2.00	0.61
1:E:77:VAL:HG21	1:E:510:VAL:HG13	1.81	0.61
1:D:142:LYS:H	1:D:142:LYS:CD	2.11	0.61
1:C:77:VAL:HG21	1:C:510:VAL:HG13	1.82	0.61
1:F:224:ASP:O	1:F:225:LYS:HB3	2.01	0.61

*Continued on next page...*



*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:319:GLN:HB3	1:F:336:VAL:HG21	1.83	0.61
1:C:179:ASP:OD1	1:C:393:LYS:HE3	2.01	0.61
1:D:319:GLN:HB3	1:D:336:VAL:HG21	1.83	0.60
1:D:42:LYS:HE2	1:D:48:THR:CG2	2.31	0.60
1:A:326:ASN:HD22	1:A:329:THR:HB	1.66	0.60
1:E:42:LYS:CE	1:E:48:THR:HG23	2.31	0.60
1:B:142:LYS:H	1:B:142:LYS:CD	2.06	0.60
1:D:166:MET:HG2	1:D:171:LYS:HA	1.84	0.60
1:E:27:VAL:HG13	1:E:90:THR:HG23	1.82	0.60
1:C:491:MET:CE	1:C:491:MET:CG	2.79	0.60
1:C:142:LYS:H	1:C:142:LYS:CD	2.13	0.60
1:F:42:LYS:CE	1:F:48:THR:HG23	2.32	0.60
1:G:77:VAL:HG21	1:G:510:VAL:HG13	1.83	0.60
1:F:68:ASN:HD21	1:F:72:GLN:HE21	1.48	0.59
1:E:179:ASP:OD1	1:E:393:LYS:HE3	2.02	0.59
1:C:145:ALA:O	1:C:149:THR:CG2	2.50	0.59
1:A:124:VAL:HG13	1:A:504:LEU:HD13	1.83	0.59
1:D:42:LYS:CE	1:D:48:THR:CG2	2.81	0.59
1:A:224:ASP:O	1:A:225:LYS:HB3	2.03	0.59
1:B:494:LEU:HD12	1:B:494:LEU:C	2.23	0.58
1:G:66:PHE:HA	1:G:69:MET:HE3	1.85	0.58
1:E:66:PHE:HA	1:E:69:MET:HE3	1.86	0.58
1:G:326:ASN:HD22	1:G:329:THR:HB	1.69	0.58
1:E:68:ASN:ND2	1:E:72:GLN:HE21	2.00	0.58
1:G:420:ILE:HG13	1:G:448:GLU:HG2	1.84	0.58
1:C:421:ARG:CD	1:C:474:GLY:O	2.50	0.58
1:A:66:PHE:HA	1:A:69:MET:HE3	1.85	0.58
1:B:142:LYS:N	1:B:142:LYS:CD	2.63	0.57
1:E:42:LYS:HE2	1:E:48:THR:HG23	1.87	0.57
1:D:42:LYS:HE3	1:D:48:THR:HG21	1.86	0.57
1:G:68:ASN:O	1:G:72:GLN:HG2	2.04	0.57
1:F:27:VAL:HG13	1:F:90:THR:HG23	1.85	0.57
1:C:452:ARG:NH2	1:C:463:SER:HB3	2.20	0.57
1:C:284:ARG:O	1:C:288:MET:HG3	2.03	0.57
1:B:7:LYS:HE3	1:B:15:LYS:HE3	1.86	0.57
1:B:257:GLU:HG3	1:C:269:GLY:HA3	1.86	0.57
1:B:145:ALA:O	1:B:149:THR:CG2	2.52	0.56
1:C:448:GLU:OE1	1:C:452:ARG:NH1	2.34	0.56
1:A:42:LYS:CE	1:A:48:THR:CG2	2.84	0.56
1:E:145:ALA:O	1:E:149:THR:HG22	2.04	0.56
1:E:42:LYS:HE3	1:E:48:THR:CG2	2.35	0.56

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:179:ASP:OD1	1:D:393:LYS:HE3	2.05	0.56
1:G:421:ARG:CD	1:G:474:GLY:O	2.53	0.56
1:C:326:ASN:HD22	1:C:329:THR:HB	1.70	0.56
1:E:319:GLN:HB3	1:E:336:VAL:HG21	1.86	0.56
1:C:42:LYS:CE	1:C:48:THR:CG2	2.84	0.56
1:A:321:LYS:HG3	1:A:334:ASP:HB3	1.87	0.56
1:B:68:ASN:O	1:B:72:GLN:HG2	2.05	0.56
1:G:431:GLY:H	1:G:437:ASN:ND2	2.02	0.56
1:A:47:PRO:HG2	1:G:73:MET:HG3	1.86	0.55
1:A:288:MET:CE	1:A:288:MET:CG	2.83	0.55
1:F:491:MET:CG	1:F:491:MET:CE	2.84	0.55
1:A:431:GLY:H	1:A:437:ASN:ND2	2.04	0.55
1:E:27:VAL:CG1	1:E:90:THR:HG23	2.37	0.55
1:B:27:VAL:HG13	1:B:90:THR:HG23	1.88	0.55
1:A:230:ILE:HD12	1:A:261:THR:HG21	1.88	0.55
1:D:326:ASN:HB3	1:D:328:ASP:H	1.72	0.55
1:E:224:ASP:O	1:E:225:LYS:HB3	2.07	0.55
1:B:172:GLU:HA	1:B:172:GLU:OE1	2.07	0.54
1:G:124:VAL:HG13	1:G:504:LEU:HD13	1.88	0.54
1:A:166:MET:HG2	1:A:171:LYS:HA	1.89	0.54
1:F:326:ASN:HD22	1:F:329:THR:HB	1.72	0.54
1:F:230:ILE:HD12	1:F:261:THR:HG21	1.89	0.54
1:D:326:ASN:HD22	1:D:329:THR:HB	1.72	0.54
1:E:124:VAL:HG13	1:E:504:LEU:HD13	1.88	0.54
1:E:230:ILE:HD12	1:E:261:THR:HG21	1.90	0.54
1:A:325:ILE:HG22	1:A:330:THR:OG1	2.08	0.54
1:D:218:PRO:HD2	1:D:320:ALA:O	2.07	0.54
1:C:494:LEU:C	1:C:494:LEU:HD12	2.28	0.54
1:E:358:SER:HB3	1:E:361:ASP:OD1	2.08	0.54
1:F:68:ASN:O	1:F:72:GLN:HG2	2.07	0.54
1:F:325:ILE:HG22	1:F:330:THR:OG1	2.08	0.53
1:F:218:PRO:HD2	1:F:320:ALA:O	2.08	0.53
1:G:319:GLN:HB3	1:G:336:VAL:HG21	1.91	0.53
1:D:494:LEU:C	1:D:494:LEU:HD12	2.28	0.53
1:C:448:GLU:O	1:C:452:ARG:HG3	2.08	0.53
1:D:73:MET:HG3	1:E:47:PRO:HG2	1.90	0.53
1:A:494:LEU:HD12	1:A:494:LEU:O	2.08	0.53
1:C:479:ASN:HD22	1:C:491:MET:CE	2.21	0.53
1:G:145:ALA:O	1:G:149:THR:CG2	2.55	0.53
1:A:142:LYS:H	1:A:142:LYS:CD	2.18	0.53
1:G:224:ASP:O	1:G:225:LYS:HB3	2.08	0.53

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:257:GLU:HG3	1:B:269:GLY:HA3	1.91	0.53
1:B:118:ARG:HH22	1:C:34:LYS:HE2	1.74	0.53
1:C:69:MET:CE	1:C:522:THR:HB	2.39	0.53
1:B:230:ILE:HD12	1:B:261:THR:HG21	1.89	0.52
1:A:179:ASP:OD1	1:A:393:LYS:HE3	2.09	0.52
1:F:42:LYS:HE3	1:F:48:THR:HG21	1.91	0.52
1:E:326:ASN:HB3	1:E:328:ASP:H	1.74	0.52
1:F:42:LYS:HE3	1:F:48:THR:CG2	2.39	0.52
1:G:448:GLU:HB3	1:G:452:ARG:HD2	1.91	0.52
1:A:27:VAL:CG1	1:A:90:THR:HG23	2.39	0.52
1:A:218:PRO:HD2	1:A:320:ALA:O	2.10	0.52
1:D:325:ILE:HG22	1:D:330:THR:OG1	2.10	0.52
1:F:448:GLU:OE1	1:F:452:ARG:NH1	2.42	0.52
1:B:172:GLU:CA	1:B:172:GLU:OE1	2.58	0.51
1:G:349:ILE:CG2	1:G:369:VAL:HG13	2.40	0.51
1:C:218:PRO:HD2	1:C:320:ALA:O	2.10	0.51
1:F:124:VAL:HG13	1:F:504:LEU:HD13	1.92	0.51
1:B:162:ILE:HD12	1:B:400:LEU:HA	1.92	0.51
1:A:62:LEU:N	1:A:68:ASN:HD22	1.96	0.51
1:C:319:GLN:HB3	1:C:336:VAL:HG21	1.93	0.51
1:A:69:MET:HE1	1:A:522:THR:HB	1.92	0.51
1:F:326:ASN:HB3	1:F:328:ASP:H	1.76	0.51
1:E:218:PRO:HD2	1:E:320:ALA:O	2.11	0.51
1:C:358:SER:HB3	1:C:361:ASP:OD1	2.10	0.51
1:B:319:GLN:HB3	1:B:336:VAL:CG2	2.41	0.50
1:F:494:LEU:O	1:F:494:LEU:HD12	2.11	0.50
1:C:263:VAL:O	1:C:267:MET:HB2	2.12	0.50
1:C:73:MET:HG3	1:D:47:PRO:HG2	1.93	0.50
1:F:42:LYS:CE	1:F:48:THR:CG2	2.89	0.50
1:D:27:VAL:CG1	1:D:90:THR:HG23	2.40	0.50
1:D:180:GLY:HA3	1:D:381:VAL:O	2.12	0.50
1:G:448:GLU:OE1	1:G:452:ARG:NH1	2.40	0.50
1:F:431:GLY:H	1:F:437:ASN:HD21	1.57	0.50
1:F:478:TYR:C	1:F:488:MET:HE1	2.32	0.50
1:G:321:LYS:HG3	1:G:334:ASP:HB3	1.93	0.50
1:E:288:MET:CE	1:E:288:MET:CG	2.89	0.50
1:C:230:ILE:HD12	1:C:261:THR:HG21	1.92	0.50
1:D:172:GLU:OE1	1:D:172:GLU:HA	2.11	0.50
1:B:82:ASN:HB2	1:B:89:THR:OG1	2.12	0.50
1:D:69:MET:HE1	1:D:522:THR:HB	1.94	0.50
1:D:224:ASP:O	1:D:225:LYS:HB3	2.11	0.49

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:421:ARG:HD2	1:B:474:GLY:O	2.12	0.49
1:E:16:MET:SD	1:E:514:MET:HG3	2.52	0.49
1:D:519:CYS:HB3	1:E:38:VAL:HG22	1.92	0.49
1:D:266:THR:CG2	1:D:273:VAL:H	2.25	0.49
1:B:479:ASN:HD22	1:B:491:MET:CE	2.25	0.49
1:G:142:LYS:N	1:G:142:LYS:CD	2.62	0.49
1:G:179:ASP:OD1	1:G:393:LYS:HE3	2.13	0.49
1:G:230:ILE:HD12	1:G:261:THR:HG21	1.93	0.49
1:D:16:MET:SD	1:D:514:MET:HG3	2.53	0.49
1:B:124:VAL:HG13	1:B:504:LEU:HD13	1.95	0.49
1:F:358:SER:HB3	1:F:361:ASP:OD1	2.13	0.49
1:D:68:ASN:ND2	1:D:72:GLN:HE21	2.11	0.49
1:D:66:PHE:HA	1:D:69:MET:HE3	1.94	0.49
1:B:73:MET:HG3	1:C:47:PRO:HG2	1.94	0.49
1:B:218:PRO:HD2	1:B:320:ALA:O	2.12	0.49
1:B:77:VAL:HG21	1:B:510:VAL:HG13	1.94	0.49
1:B:473:ASP:CA	1:B:473:ASP:CG	2.74	0.48
1:G:351:GLN:HB3	1:G:351:GLN:HE21	1.40	0.48
1:G:62:LEU:N	1:G:68:ASN:HD22	2.06	0.48
1:B:247:LEU:HD21	1:B:249:ILE:HD11	1.95	0.48
1:D:478:TYR:C	1:D:488:MET:HE1	2.32	0.48
1:D:77:VAL:CG2	1:D:510:VAL:HG13	2.42	0.48
1:F:305:ILE:HG22	1:F:305:ILE:O	2.14	0.48
1:B:321:LYS:HG3	1:B:334:ASP:HB3	1.96	0.48
1:G:452:ARG:NH2	1:G:463:SER:CB	2.76	0.48
1:A:443:ALA:O	1:A:447:MET:HG3	2.13	0.48
1:C:65:LYS:HB3	1:C:65:LYS:HE2	1.60	0.48
1:G:284:ARG:O	1:G:288:MET:HG3	2.12	0.48
1:C:66:PHE:HA	1:C:69:MET:HE3	1.96	0.48
1:D:452:ARG:NH2	1:D:463:SER:CB	2.74	0.48
1:C:348:GLN:O	1:C:351:GLN:HB2	2.14	0.48
1:F:262:LEU:O	1:F:266:THR:HG23	2.14	0.48
1:D:448:GLU:OE1	1:D:452:ARG:NH1	2.42	0.48
1:D:351:GLN:HE21	1:D:351:GLN:HB3	1.48	0.48
1:G:218:PRO:HD2	1:G:320:ALA:O	2.14	0.48
1:E:284:ARG:O	1:E:288:MET:HG3	2.14	0.47
1:E:42:LYS:HE3	1:E:48:THR:HG21	1.96	0.47
1:A:254:VAL:HG12	1:A:259:LEU:HB2	1.97	0.47
1:E:280:GLY:HA2	1:E:284:ARG:HH21	1.79	0.47
1:A:27:VAL:HG13	1:A:90:THR:HG23	1.96	0.47
1:F:263:VAL:O	1:F:267:MET:HB2	2.14	0.47

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:325:ILE:HG22	1:A:330:THR:HA	1.95	0.47
1:E:325:ILE:HG22	1:E:330:THR:HA	1.97	0.47
1:C:42:LYS:CE	1:C:48:THR:HG21	2.44	0.47
1:D:42:LYS:HE3	1:D:48:THR:CG2	2.44	0.47
1:D:452:ARG:HH21	1:D:463:SER:HB3	1.79	0.47
1:B:41:ASP:O	1:B:42:LYS:HD3	2.15	0.47
1:B:16:MET:SD	1:B:514:MET:HG3	2.54	0.47
1:C:266:THR:CG2	1:C:273:VAL:H	2.26	0.47
1:A:348:GLN:O	1:A:351:GLN:HB2	2.15	0.47
1:E:448:GLU:OE1	1:E:452:ARG:NH1	2.35	0.47
1:B:273:VAL:HG12	1:B:274:ALA:N	2.30	0.47
1:G:514:MET:HE2	1:G:514:MET:HB2	1.60	0.47
1:D:448:GLU:O	1:D:452:ARG:HG3	2.15	0.47
1:E:41:ASP:O	1:E:42:LYS:HD3	2.15	0.47
1:D:27:VAL:HG13	1:D:90:THR:HG23	1.97	0.47
1:G:348:GLN:O	1:G:351:GLN:HB2	2.14	0.47
1:C:478:TYR:C	1:C:488:MET:HE1	2.35	0.47
1:D:348:GLN:O	1:D:351:GLN:HB2	2.15	0.46
1:B:466:ALA:O	1:B:470:LYS:HG3	2.16	0.46
1:B:42:LYS:CE	1:B:48:THR:HG23	2.45	0.46
1:E:349:ILE:CG2	1:E:369:VAL:HG13	2.46	0.46
1:A:326:ASN:HB3	1:A:328:ASP:H	1.80	0.46
1:D:273:VAL:HG12	1:D:274:ALA:N	2.31	0.46
1:C:326:ASN:HB3	1:C:328:ASP:H	1.81	0.46
1:E:86:GLY:O	1:E:87:ASP:HB2	2.14	0.46
1:D:205:ILE:HA	1:D:213:VAL:HG22	1.96	0.46
1:D:68:ASN:HD21	1:D:72:GLN:HE21	1.63	0.46
1:G:305:ILE:O	1:G:305:ILE:HG22	2.15	0.46
1:F:166:MET:HG2	1:F:171:LYS:HA	1.98	0.46
1:D:284:ARG:O	1:D:288:MET:HG3	2.15	0.46
1:F:452:ARG:HH22	1:F:463:SER:HB3	1.77	0.46
1:A:358:SER:HB3	1:A:361:ASP:OD1	2.16	0.46
1:B:34:LYS:O	1:B:457:ASN:HB3	2.16	0.46
1:B:490:ASP:CB	2:B:536:HOH:O	2.64	0.46
1:F:421:ARG:CD	1:F:474:GLY:O	2.59	0.45
1:B:326:ASN:HB3	1:B:328:ASP:H	1.82	0.45
1:E:224:ASP:HB3	1:E:302:SER:HB3	1.98	0.45
1:B:263:VAL:O	1:B:267:MET:HB2	2.16	0.45
1:A:41:ASP:O	1:A:42:LYS:HD3	2.17	0.45
1:E:217:SER:N	1:E:218:PRO:CD	2.78	0.45
1:D:178:GLU:HG2	1:D:322:ARG:CZ	2.46	0.45

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:62:LEU:N	1:C:68:ASN:HD22	1.99	0.45
1:D:230:ILE:HD12	1:D:261:THR:HG21	1.97	0.45
1:A:68:ASN:O	1:A:72:GLN:HG2	2.16	0.45
1:A:525:PRO:O	2:A:537:HOH:O	2.21	0.45
1:F:519:CYS:HB3	1:G:38:VAL:HG22	1.97	0.45
1:D:234:LEU:N	1:D:235:PRO:HD2	2.32	0.45
1:D:68:ASN:O	1:D:72:GLN:HG2	2.16	0.45
1:B:305:ILE:HG22	1:B:305:ILE:O	2.17	0.45
1:G:42:LYS:CE	1:G:48:THR:HG23	2.44	0.45
1:C:65:LYS:H	1:C:65:LYS:HG2	1.67	0.45
1:G:288:MET:CG	1:G:288:MET:CE	2.94	0.45
1:E:68:ASN:O	1:E:72:GLN:HG2	2.16	0.45
1:F:87:ASP:OD1	1:F:88:GLY:N	2.46	0.45
1:B:490:ASP:HB3	2:B:536:HOH:O	2.16	0.45
1:A:205:ILE:HA	1:A:213:VAL:HG22	1.99	0.44
1:A:319:GLN:HB3	1:A:336:VAL:CG2	2.43	0.44
1:C:305:ILE:HG22	1:C:305:ILE:O	2.17	0.44
1:D:228:SER:O	1:D:257:GLU:HB3	2.16	0.44
1:F:96:ALA:O	1:F:97:GLN:C	2.55	0.44
1:A:364:LYS:HD3	1:A:364:LYS:HA	1.81	0.44
1:A:478:TYR:C	1:A:488:MET:HE3	2.38	0.44
1:A:479:ASN:HD22	1:A:491:MET:CE	2.31	0.44
1:D:237:LEU:HD23	1:D:237:LEU:HA	1.86	0.44
1:G:494:LEU:HD12	1:G:494:LEU:O	2.17	0.44
1:E:273:VAL:HG12	1:E:274:ALA:N	2.32	0.44
1:B:42:LYS:CE	1:B:48:THR:CG2	2.95	0.44
1:B:351:GLN:HB3	1:B:351:GLN:HE21	1.36	0.44
1:C:41:ASP:O	1:C:42:LYS:HD3	2.17	0.44
1:G:449:ALA:HB3	1:G:450:PRO:HD3	1.98	0.44
1:D:403:THR:O	1:D:407:VAL:HG13	2.18	0.44
1:F:364:LYS:HD3	1:F:364:LYS:HA	1.86	0.44
1:C:217:SER:N	1:C:218:PRO:HD3	2.33	0.44
1:F:28:LYS:HB2	1:F:453:GLN:HG2	2.00	0.44
1:E:364:LYS:HA	1:E:364:LYS:HD3	1.70	0.44
1:B:68:ASN:ND2	1:B:72:GLN:HE21	2.15	0.43
1:G:263:VAL:O	1:G:267:MET:HB2	2.18	0.43
1:A:305:ILE:O	1:A:305:ILE:HG22	2.18	0.43
1:C:364:LYS:HA	1:C:364:LYS:HD3	1.86	0.43
1:D:42:LYS:CE	1:D:48:THR:HG21	2.47	0.43
1:B:42:LYS:HE2	1:B:48:THR:CG2	2.46	0.43
1:G:326:ASN:HB3	1:G:328:ASP:H	1.83	0.43

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:69:MET:CE	1:A:522:THR:HB	2.47	0.43
1:B:266:THR:CG2	1:B:273:VAL:H	2.31	0.43
1:E:421:ARG:CD	1:E:474:GLY:O	2.65	0.43
1:A:162:ILE:HD12	1:A:400:LEU:HA	2.00	0.43
1:D:479:ASN:HD22	1:D:491:MET:CE	2.31	0.43
1:G:86:GLY:O	1:G:87:ASP:HB2	2.17	0.43
1:A:172:GLU:CA	1:A:172:GLU:OE1	2.66	0.43
1:B:494:LEU:C	1:B:494:LEU:CD1	2.86	0.43
1:D:524:LEU:O	1:D:525:PRO:C	2.57	0.43
1:A:73:MET:HG3	1:B:47:PRO:HG2	1.99	0.43
1:D:263:VAL:O	1:D:267:MET:HB2	2.18	0.43
1:A:42:LYS:HE3	1:A:48:THR:HG21	2.00	0.43
1:G:234:LEU:N	1:G:235:PRO:HD2	2.34	0.43
1:G:452:ARG:HH21	1:G:463:SER:HB3	1.82	0.43
1:A:262:LEU:O	1:A:266:THR:HG23	2.18	0.43
1:C:288:MET:CE	1:C:288:MET:CG	2.93	0.43
1:E:325:ILE:HG23	1:E:325:ILE:HD13	1.74	0.43
1:E:228:SER:O	1:E:257:GLU:HB3	2.18	0.43
1:B:171:LYS:HB3	1:B:407:VAL:HG21	2.01	0.43
1:B:479:ASN:ND2	1:B:493:ILE:HD11	2.34	0.43
1:F:171:LYS:HB3	1:F:407:VAL:HG21	2.01	0.43
1:A:511:ALA:O	1:A:515:ILE:HD12	2.19	0.42
1:F:319:GLN:HB3	1:F:336:VAL:CG2	2.48	0.42
1:E:266:THR:CG2	1:E:273:VAL:H	2.31	0.42
1:G:180:GLY:HA3	1:G:381:VAL:O	2.18	0.42
1:B:96:ALA:O	1:B:100:ILE:HD12	2.19	0.42
1:C:325:ILE:HG22	1:C:330:THR:HA	2.01	0.42
1:B:68:ASN:HD21	1:B:72:GLN:HE21	1.67	0.42
1:G:217:SER:N	1:G:218:PRO:CD	2.82	0.42
1:E:73:MET:HG3	1:F:47:PRO:HG2	2.00	0.42
1:A:214:GLU:HG3	1:A:324:VAL:HG22	2.01	0.42
1:D:41:ASP:O	1:D:42:LYS:HD3	2.18	0.42
1:E:452:ARG:HH22	1:E:463:SER:HB3	1.83	0.42
1:G:262:LEU:O	1:G:266:THR:HG23	2.19	0.42
1:B:186:GLU:HB2	1:B:380:LYS:HG3	2.01	0.42
1:G:171:LYS:HB3	1:G:407:VAL:HG21	2.02	0.42
1:F:217:SER:N	1:F:218:PRO:HD3	2.34	0.42
1:C:217:SER:N	1:C:218:PRO:CD	2.83	0.42
1:D:449:ALA:N	1:D:450:PRO:CD	2.83	0.42
1:G:502:SER:O	1:G:503:ALA:C	2.55	0.42
1:A:452:ARG:HH22	1:A:463:SER:HB3	1.80	0.42

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:263:VAL:O	1:A:267:MET:HB2	2.19	0.42
1:F:514:MET:HE2	1:F:514:MET:HB2	1.58	0.42
1:A:494:LEU:HD12	1:A:494:LEU:C	2.40	0.42
1:C:162:ILE:HD12	1:C:400:LEU:HA	2.02	0.42
1:C:221:LEU:HD12	1:C:222:LEU:N	2.35	0.42
1:A:270:ILE:HG22	1:A:271:VAL:HG23	2.01	0.42
1:G:273:VAL:HG12	1:G:274:ALA:N	2.34	0.42
1:E:418:ALA:O	1:E:422:VAL:HG13	2.19	0.42
1:A:234:LEU:N	1:A:235:PRO:HD2	2.35	0.42
1:E:325:ILE:HG21	1:E:325:ILE:HD12	1.78	0.41
1:B:62:LEU:N	1:B:68:ASN:HD22	2.09	0.41
1:C:69:MET:HE2	1:C:522:THR:HB	2.02	0.41
1:F:494:LEU:C	1:F:494:LEU:HD12	2.41	0.41
1:G:217:SER:N	1:G:218:PRO:HD3	2.34	0.41
1:F:273:VAL:HG12	1:F:274:ALA:N	2.35	0.41
1:E:348:GLN:O	1:E:351:GLN:HB2	2.20	0.41
1:E:254:VAL:HG12	1:E:259:LEU:HB2	2.02	0.41
1:E:205:ILE:HA	1:E:213:VAL:HG22	2.02	0.41
1:F:62:LEU:N	1:F:68:ASN:HD22	2.06	0.41
1:G:69:MET:CE	1:G:522:THR:HB	2.50	0.41
1:E:228:SER:HB3	1:F:272:LYS:NZ	2.34	0.41
1:E:258:ALA:O	1:E:262:LEU:HG	2.20	0.41
1:D:325:ILE:HG22	1:D:330:THR:HA	2.01	0.41
1:B:325:ILE:HG22	1:B:330:THR:HA	2.02	0.41
1:G:228:SER:O	1:G:257:GLU:HB3	2.20	0.41
1:G:349:ILE:HG21	1:G:369:VAL:HG13	2.02	0.41
1:D:266:THR:HG21	1:D:273:VAL:H	1.85	0.41
1:C:228:SER:O	1:C:257:GLU:HB3	2.20	0.41
1:B:364:LYS:HA	1:B:364:LYS:HD3	1.86	0.41
1:C:325:ILE:HG22	1:C:330:THR:OG1	2.20	0.41
1:C:266:THR:HG21	1:C:273:VAL:H	1.85	0.41
1:G:221:LEU:HD12	1:G:222:LEU:N	2.34	0.41
1:F:77:VAL:HG21	1:F:510:VAL:HG13	2.02	0.41
1:A:112:ASN:HA	1:A:113:PRO:HD3	1.95	0.41
1:G:172:GLU:HA	1:G:172:GLU:OE1	2.20	0.41
1:G:325:ILE:HG22	1:G:330:THR:OG1	2.20	0.41
1:A:217:SER:N	1:A:218:PRO:CD	2.84	0.41
1:D:304:GLU:HG3	1:D:304:GLU:H	1.75	0.41
1:E:351:GLN:HE21	1:E:351:GLN:HB3	1.43	0.41
1:A:8:PHE:HA	1:A:518:GLU:O	2.21	0.41
1:C:68:ASN:ND2	1:C:72:GLN:HE21	2.19	0.41

*Continued on next page...*



*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:68:ASN:HD21	1:E:72:GLN:NE2	2.17	0.41
1:E:7:LYS:HE3	1:E:15:LYS:HE3	2.03	0.41
1:B:284:ARG:O	1:B:288:MET:HG3	2.20	0.41
1:G:82:ASN:HB2	1:G:89:THR:OG1	2.21	0.41
1:E:305:ILE:HG22	1:E:305:ILE:O	2.20	0.41
1:G:104:LEU:HA	1:G:104:LEU:HD23	1.87	0.41
1:C:265:ASN:HA	1:C:265:ASN:HD22	1.68	0.41
1:C:205:ILE:HA	1:C:213:VAL:HG22	2.03	0.41
1:C:42:LYS:HE3	1:C:48:THR:HG21	2.01	0.41
1:B:448:GLU:HB3	1:B:452:ARG:HD2	2.02	0.41
1:G:172:GLU:OE1	1:G:172:GLU:CA	2.69	0.41
1:E:237:LEU:HD23	1:E:237:LEU:HA	1.88	0.41
1:G:122:LYS:NZ	2:G:528:HOH:O	2.44	0.41
1:B:489:ILE:CD1	1:B:489:ILE:HA	2.52	0.40
1:E:77:VAL:CG2	1:E:510:VAL:HG13	2.50	0.40
1:F:217:SER:N	1:F:218:PRO:CD	2.84	0.40
1:C:68:ASN:O	1:C:72:GLN:HG2	2.20	0.40
1:F:77:VAL:O	1:F:80:LYS:HB2	2.22	0.40
1:A:519:CYS:HB3	1:B:38:VAL:HG22	2.04	0.40
1:C:69:MET:HE1	1:C:522:THR:HB	2.03	0.40
1:C:66:PHE:O	1:C:67:GLU:C	2.60	0.40
1:A:172:GLU:OE1	1:A:172:GLU:HA	2.21	0.40
1:B:231:ARG:NH1	1:C:241:ALA:HB1	2.35	0.40
1:F:452:ARG:NH2	1:F:463:SER:CB	2.80	0.40
1:E:510:VAL:O	1:E:511:ALA:C	2.59	0.40
1:G:358:SER:HB3	1:G:361:ASP:OD1	2.21	0.40
1:C:258:ALA:O	1:C:262:LEU:HG	2.21	0.40
1:G:479:ASN:HD22	1:G:491:MET:CE	2.34	0.40
1:F:205:ILE:HA	1:F:213:VAL:HG22	2.03	0.40
1:F:68:ASN:HD21	1:F:72:GLN:NE2	2.17	0.40
1:B:455:VAL:HG13	1:B:460:GLU:HB2	2.04	0.40
1:C:169:VAL:HG13	1:C:173:GLY:HA3	2.03	0.40
1:E:184:GLN:HA	1:E:184:GLN:OE1	2.21	0.40
1:D:65:LYS:HB3	1:D:65:LYS:HE2	1.84	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:C:354:GLU:OE1	1:G:350:ARG:NH1[5_455]	2.05	0.15

## 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	522/524 (100%)	507 (97%)	12 (2%)	3 (1%)	30	59
1	B	522/524 (100%)	505 (97%)	15 (3%)	2 (0%)	39	69
1	C	522/524 (100%)	506 (97%)	13 (2%)	3 (1%)	30	59
1	D	522/524 (100%)	507 (97%)	13 (2%)	2 (0%)	39	69
1	E	522/524 (100%)	504 (97%)	17 (3%)	1 (0%)	52	80
1	F	522/524 (100%)	506 (97%)	14 (3%)	2 (0%)	39	69
1	G	522/524 (100%)	504 (97%)	15 (3%)	3 (1%)	30	59
All	All	3654/3668 (100%)	3539 (97%)	99 (3%)	16 (0%)	39	69

All (16) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	256	GLY
1	B	256	GLY
1	C	256	GLY
1	D	256	GLY
1	E	256	GLY
1	F	256	GLY
1	G	256	GLY
1	A	225	LYS
1	D	257	GLU
1	F	225	LYS
1	G	257	GLU
1	B	225	LYS
1	C	225	LYS
1	A	205	ILE
1	G	205	ILE
1	C	205	ILE

### 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	404/404 (100%)	351 (87%)	53 (13%)	5	12
1	B	404/404 (100%)	347 (86%)	57 (14%)	4	10
1	C	404/404 (100%)	356 (88%)	48 (12%)	6	15
1	D	404/404 (100%)	350 (87%)	54 (13%)	5	11
1	E	404/404 (100%)	354 (88%)	50 (12%)	6	13
1	F	404/404 (100%)	350 (87%)	54 (13%)	5	11
1	G	404/404 (100%)	351 (87%)	53 (13%)	5	12
All	All	2828/2828 (100%)	2459 (87%)	369 (13%)	5	12

All (369) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	43	SER
1	A	48	THR
1	A	65	LYS
1	A	76	GLU
1	A	105	LYS
1	A	116	LEU
1	A	118	ARG
1	A	138	CYS
1	A	141	SER
1	A	142	LYS
1	A	149	THR
1	A	151	SER
1	A	153	ASN
1	A	156	GLU
1	A	168	LYS
1	A	169	VAL
1	A	172	GLU
1	A	174	VAL
1	A	186	GLU
1	A	190	VAL

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	A	201	SER
1	A	209	GLU
1	A	216	GLU
1	A	225	LYS
1	A	230	ILE
1	A	265	ASN
1	A	284	ARG
1	A	295	LEU
1	A	303	GLU
1	A	304	GLU
1	A	317	LEU
1	A	322	ARG
1	A	325	ILE
1	A	328	ASP
1	A	329	THR
1	A	331	THR
1	A	339	GLU
1	A	343	GLN
1	A	345	ARG
1	A	348	GLN
1	A	350	ARG
1	A	351	GLN
1	A	352	GLN
1	A	355	GLU
1	A	358	SER
1	A	363	GLU
1	A	364	LYS
1	A	380	LYS
1	A	404	ARG
1	A	411	VAL
1	A	421	ARG
1	A	504	LEU
1	A	510	VAL
1	B	14	VAL
1	B	27	VAL
1	B	43	SER
1	B	48	THR
1	B	55	SER
1	B	58	ARG
1	B	64	ASP
1	B	76	GLU
1	B	82	ASN

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	B	105	LYS
1	B	116	LEU
1	B	118	ARG
1	B	141	SER
1	B	142	LYS
1	B	149	THR
1	B	151	SER
1	B	153	ASN
1	B	156	GLU
1	B	168	LYS
1	B	169	VAL
1	B	172	GLU
1	B	174	VAL
1	B	176	THR
1	B	186	GLU
1	B	190	VAL
1	B	201	SER
1	B	209	GLU
1	B	216	GLU
1	B	225	LYS
1	B	230	ILE
1	B	284	ARG
1	B	295	LEU
1	B	303	GLU
1	B	317	LEU
1	B	322	ARG
1	B	325	ILE
1	B	328	ASP
1	B	329	THR
1	B	331	THR
1	B	343	GLN
1	B	345	ARG
1	B	348	GLN
1	B	350	ARG
1	B	351	GLN
1	B	352	GLN
1	B	355	GLU
1	B	358	SER
1	B	363	GLU
1	B	364	LYS
1	B	380	LYS
1	B	387	VAL

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	B	404	ARG
1	B	411	VAL
1	B	421	ARG
1	B	422	VAL
1	B	504	LEU
1	B	510	VAL
1	C	43	SER
1	C	48	THR
1	C	65	LYS
1	C	76	GLU
1	C	105	LYS
1	C	116	LEU
1	C	118	ARG
1	C	141	SER
1	C	142	LYS
1	C	149	THR
1	C	153	ASN
1	C	156	GLU
1	C	168	LYS
1	C	169	VAL
1	C	172	GLU
1	C	174	VAL
1	C	186	GLU
1	C	190	VAL
1	C	201	SER
1	C	209	GLU
1	C	216	GLU
1	C	225	LYS
1	C	230	ILE
1	C	265	ASN
1	C	284	ARG
1	C	295	LEU
1	C	303	GLU
1	C	304	GLU
1	C	317	LEU
1	C	322	ARG
1	C	325	ILE
1	C	328	ASP
1	C	329	THR
1	C	331	THR
1	C	343	GLN
1	C	345	ARG

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	C	348	GLN
1	C	350	ARG
1	C	351	GLN
1	C	352	GLN
1	C	355	GLU
1	C	364	LYS
1	C	380	LYS
1	C	404	ARG
1	C	411	VAL
1	C	421	ARG
1	C	504	LEU
1	C	510	VAL
1	D	43	SER
1	D	48	THR
1	D	65	LYS
1	D	76	GLU
1	D	82	ASN
1	D	105	LYS
1	D	116	LEU
1	D	118	ARG
1	D	132	LYS
1	D	141	SER
1	D	142	LYS
1	D	149	THR
1	D	151	SER
1	D	153	ASN
1	D	156	GLU
1	D	168	LYS
1	D	169	VAL
1	D	172	GLU
1	D	174	VAL
1	D	186	GLU
1	D	190	VAL
1	D	201	SER
1	D	209	GLU
1	D	216	GLU
1	D	225	LYS
1	D	230	ILE
1	D	265	ASN
1	D	284	ARG
1	D	295	LEU
1	D	303	GLU

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	D	304	GLU
1	D	322	ARG
1	D	325	ILE
1	D	328	ASP
1	D	329	THR
1	D	331	THR
1	D	339	GLU
1	D	343	GLN
1	D	345	ARG
1	D	348	GLN
1	D	350	ARG
1	D	351	GLN
1	D	352	GLN
1	D	355	GLU
1	D	358	SER
1	D	363	GLU
1	D	364	LYS
1	D	372	LEU
1	D	380	LYS
1	D	404	ARG
1	D	411	VAL
1	D	421	ARG
1	D	504	LEU
1	D	510	VAL
1	E	27	VAL
1	E	43	SER
1	E	48	THR
1	E	76	GLU
1	E	105	LYS
1	E	116	LEU
1	E	118	ARG
1	E	141	SER
1	E	142	LYS
1	E	149	THR
1	E	151	SER
1	E	153	ASN
1	E	156	GLU
1	E	168	LYS
1	E	169	VAL
1	E	172	GLU
1	E	174	VAL
1	E	186	GLU

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type
1	E	190	VAL
1	E	201	SER
1	E	209	GLU
1	E	216	GLU
1	E	225	LYS
1	E	230	ILE
1	E	265	ASN
1	E	284	ARG
1	E	295	LEU
1	E	303	GLU
1	E	304	GLU
1	E	317	LEU
1	E	322	ARG
1	E	325	ILE
1	E	329	THR
1	E	331	THR
1	E	339	GLU
1	E	343	GLN
1	E	348	GLN
1	E	350	ARG
1	E	351	GLN
1	E	352	GLN
1	E	355	GLU
1	E	358	SER
1	E	364	LYS
1	E	372	LEU
1	E	380	LYS
1	E	404	ARG
1	E	411	VAL
1	E	421	ARG
1	E	504	LEU
1	E	510	VAL
1	F	14	VAL
1	F	34	LYS
1	F	43	SER
1	F	55	SER
1	F	65	LYS
1	F	76	GLU
1	F	105	LYS
1	F	116	LEU
1	F	118	ARG
1	F	141	SER

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	F	142	LYS
1	F	149	THR
1	F	151	SER
1	F	153	ASN
1	F	156	GLU
1	F	168	LYS
1	F	169	VAL
1	F	172	GLU
1	F	174	VAL
1	F	186	GLU
1	F	190	VAL
1	F	201	SER
1	F	209	GLU
1	F	216	GLU
1	F	225	LYS
1	F	230	ILE
1	F	265	ASN
1	F	284	ARG
1	F	295	LEU
1	F	303	GLU
1	F	317	LEU
1	F	322	ARG
1	F	325	ILE
1	F	328	ASP
1	F	329	THR
1	F	331	THR
1	F	339	GLU
1	F	343	GLN
1	F	345	ARG
1	F	348	GLN
1	F	350	ARG
1	F	351	GLN
1	F	352	GLN
1	F	355	GLU
1	F	358	SER
1	F	363	GLU
1	F	364	LYS
1	F	372	LEU
1	F	380	LYS
1	F	404	ARG
1	F	411	VAL
1	F	421	ARG

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	F	504	LEU
1	F	510	VAL
1	G	27	VAL
1	G	42	LYS
1	G	43	SER
1	G	48	THR
1	G	76	GLU
1	G	82	ASN
1	G	105	LYS
1	G	116	LEU
1	G	141	SER
1	G	142	LYS
1	G	149	THR
1	G	151	SER
1	G	153	ASN
1	G	156	GLU
1	G	168	LYS
1	G	169	VAL
1	G	172	GLU
1	G	174	VAL
1	G	186	GLU
1	G	190	VAL
1	G	201	SER
1	G	209	GLU
1	G	216	GLU
1	G	225	LYS
1	G	230	ILE
1	G	265	ASN
1	G	284	ARG
1	G	295	LEU
1	G	304	GLU
1	G	317	LEU
1	G	322	ARG
1	G	325	ILE
1	G	328	ASP
1	G	329	THR
1	G	331	THR
1	G	339	GLU
1	G	343	GLN
1	G	345	ARG
1	G	348	GLN
1	G	350	ARG

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	G	351	GLN
1	G	352	GLN
1	G	355	GLU
1	G	358	SER
1	G	363	GLU
1	G	364	LYS
1	G	372	LEU
1	G	380	LYS
1	G	404	ARG
1	G	411	VAL
1	G	421	ARG
1	G	504	LEU
1	G	510	VAL

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (34) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	10	ASN
1	A	68	ASN
1	A	265	ASN
1	A	351	GLN
1	A	437	ASN
1	B	68	ASN
1	B	265	ASN
1	B	326	ASN
1	B	351	GLN
1	B	437	ASN
1	C	68	ASN
1	C	265	ASN
1	C	351	GLN
1	C	437	ASN
1	D	10	ASN
1	D	68	ASN
1	D	265	ASN
1	D	351	GLN
1	D	437	ASN
1	E	68	ASN
1	E	265	ASN
1	E	351	GLN
1	E	437	ASN
1	E	453	GLN
1	F	68	ASN

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	F	265	ASN
1	F	351	GLN
1	F	437	ASN
1	F	453	GLN
1	G	68	ASN
1	G	265	ASN
1	G	351	GLN
1	G	437	ASN
1	G	453	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](#)

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](#)

There are no ligands in this entry.

## 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 ⓘ

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	524/524 (100%)	0.10	34 (6%)	22 20	2, 2, 4, 6	0
1	B	524/524 (100%)	0.20	47 (8%)	12 9	2, 2, 4, 6	0
1	C	524/524 (100%)	0.12	32 (6%)	25 23	2, 2, 4, 6	0
1	D	524/524 (100%)	0.11	33 (6%)	23 22	2, 2, 4, 6	0
1	E	524/524 (100%)	-0.11	22 (4%)	40 39	2, 2, 4, 6	0
1	F	524/524 (100%)	0.45	73 (13%)	4 3	2, 2, 4, 6	0
1	G	524/524 (100%)	0.04	31 (5%)	26 24	2, 2, 4, 6	0
All	All	3668/3668 (100%)	0.13	272 (7%)	17 15	2, 2, 4, 6	0

All (272) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	F	270	ILE	8.1
1	C	203	TYR	8.1
1	A	305	ILE	7.4
1	G	268	ARG	7.0
1	G	44	PHE	6.7
1	F	203	TYR	6.5
1	F	268	ARG	6.5
1	G	305	ILE	6.2
1	F	340	ALA	6.2
1	A	44	PHE	5.8
1	A	268	ARG	5.8
1	F	242	LYS	5.8
1	F	305	ILE	5.8
1	F	243	ALA	5.6
1	F	264	VAL	5.4
1	C	268	ARG	5.4
1	D	44	PHE	5.3

*Continued on next page...*

*Continued from previous page...*

<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
1	G	270	ILE	5.3
1	G	203	TYR	5.3
1	F	271	VAL	5.2
1	C	44	PHE	5.2
1	D	268	ARG	5.1
1	G	264	VAL	5.0
1	B	44	PHE	4.9
1	D	264	VAL	4.9
1	E	354	GLU	4.9
1	F	267	MET	4.8
1	B	354	GLU	4.7
1	G	202	PRO	4.7
1	C	305	ILE	4.7
1	D	305	ILE	4.7
1	F	44	PHE	4.6
1	E	44	PHE	4.6
1	G	387	VAL	4.6
1	B	305	ILE	4.6
1	F	356	ALA	4.6
1	G	267	MET	4.5
1	A	270	ILE	4.5
1	C	208	PRO	4.4
1	B	203	TYR	4.4
1	F	231	ARG	4.3
1	C	234	LEU	4.2
1	F	259	LEU	4.2
1	A	353	ILE	4.2
1	B	351	GLN	4.2
1	E	203	TYR	4.2
1	B	353	ILE	4.2
1	A	357	THR	4.2
1	C	387	VAL	4.2
1	C	231	ARG	4.1
1	A	356	ALA	4.1
1	C	267	MET	4.1
1	F	260	ALA	4.0
1	F	307	MET	3.9
1	F	299	THR	3.9
1	C	306	GLY	3.9
1	F	265	ASN	3.9
1	F	349	ILE	3.9
1	F	211	GLY	3.8

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
1	B	268	ARG	3.8
1	B	211	GLY	3.7
1	A	231	ARG	3.7
1	C	269	GLY	3.7
1	F	350	ARG	3.7
1	F	261	THR	3.7
1	A	203	TYR	3.7
1	B	209	GLU	3.7
1	F	201	SER	3.7
1	F	304	GLU	3.7
1	E	351	GLN	3.6
1	D	203	TYR	3.6
1	B	356	ALA	3.6
1	F	311	LYS	3.6
1	A	202	PRO	3.6
1	F	313	THR	3.6
1	D	263	VAL	3.6
1	G	307	MET	3.6
1	E	305	ILE	3.6
1	F	360	TYR	3.6
1	D	208	PRO	3.5
1	A	304	GLU	3.5
1	F	238	GLU	3.5
1	B	264	VAL	3.5
1	A	354	GLU	3.5
1	F	233	MET	3.5
1	F	354	GLU	3.5
1	E	387	VAL	3.5
1	E	270	ILE	3.4
1	G	327	LYS	3.4
1	D	304	GLU	3.4
1	A	266	THR	3.4
1	F	263	VAL	3.4
1	D	311	LYS	3.4
1	F	306	GLY	3.4
1	E	356	ALA	3.4
1	B	267	MET	3.3
1	C	242	LYS	3.3
1	E	209	GLU	3.3
1	B	304	GLU	3.3
1	B	387	VAL	3.3
1	F	208	PRO	3.3

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
1	F	312	ALA	3.3
1	G	205	ILE	3.3
1	D	202	PRO	3.2
1	F	351	GLN	3.2
1	D	270	ILE	3.2
1	D	267	MET	3.2
1	D	353	ILE	3.2
1	E	268	ARG	3.2
1	F	273	VAL	3.1
1	A	361	ASP	3.1
1	B	359	ASP	3.1
1	F	219	PHE	3.1
1	C	209	GLU	3.1
1	G	234	LEU	3.1
1	A	363	GLU	3.1
1	G	210	THR	3.1
1	D	360	TYR	3.1
1	F	387	VAL	3.1
1	B	233	MET	3.0
1	B	312	ALA	3.0
1	F	315	GLU	3.0
1	G	199	TYR	3.0
1	D	209	GLU	3.0
1	D	242	LYS	3.0
1	D	356	ALA	3.0
1	B	349	ILE	3.0
1	G	351	GLN	3.0
1	F	362	ARG	3.0
1	D	231	ARG	3.0
1	C	233	MET	3.0
1	F	209	GLU	3.0
1	C	270	ILE	3.0
1	F	266	THR	2.9
1	D	391	GLU	2.9
1	A	209	GLU	2.9
1	G	271	VAL	2.9
1	G	391	GLU	2.9
1	B	360	TYR	2.9
1	D	211	GLY	2.9
1	F	342	ILE	2.9
1	F	391	GLU	2.9
1	A	271	VAL	2.9

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
1	A	256	GLY	2.9
1	G	306	GLY	2.9
1	A	311	LYS	2.9
1	B	243	ALA	2.8
1	C	263	VAL	2.8
1	D	387	VAL	2.8
1	F	235	PRO	2.8
1	F	257	GLU	2.8
1	A	358	SER	2.8
1	F	202	PRO	2.8
1	F	339	GLU	2.8
1	B	242	LYS	2.7
1	C	391	GLU	2.7
1	B	366	GLN	2.7
1	C	304	GLU	2.7
1	E	256	GLY	2.7
1	C	229	ASN	2.7
1	F	310	GLU	2.7
1	C	351	GLN	2.7
1	A	172	GLU	2.7
1	C	388	GLU	2.7
1	D	395	ARG	2.7
1	F	300	VAL	2.7
1	C	210	THR	2.7
1	B	355	GLU	2.7
1	B	340	ALA	2.7
1	C	302	SER	2.7
1	A	306	GLY	2.6
1	A	234	LEU	2.6
1	B	239	ALA	2.6
1	C	238	GLU	2.6
1	B	205	ILE	2.6
1	A	201	SER	2.6
1	D	234	LEU	2.6
1	F	223	ALA	2.6
1	A	211	GLY	2.6
1	B	391	GLU	2.5
1	F	244	GLY	2.5
1	F	338	GLU	2.5
1	F	363	GLU	2.5
1	A	265	ASN	2.5
1	B	347	ALA	2.5

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
1	F	301	ILE	2.5
1	G	356	ALA	2.5
1	B	313	THR	2.5
1	B	357	THR	2.5
1	G	304	GLU	2.5
1	G	354	GLU	2.5
1	G	388	GLU	2.5
1	E	243	ALA	2.5
1	F	384	ALA	2.5
1	G	238	GLU	2.5
1	B	362	ARG	2.4
1	B	269	GLY	2.4
1	B	302	SER	2.4
1	C	327	LYS	2.4
1	F	343	GLN	2.4
1	E	359	ASP	2.4
1	A	267	MET	2.4
1	D	355	GLU	2.4
1	E	242	LYS	2.4
1	E	311	LYS	2.4
1	F	272	LYS	2.4
1	F	358	SER	2.4
1	E	306	GLY	2.4
1	F	229	ASN	2.4
1	E	267	MET	2.4
1	G	242	LYS	2.4
1	E	208	PRO	2.4
1	D	269	GLY	2.4
1	B	358	SER	2.4
1	C	350	ARG	2.3
1	B	210	THR	2.3
1	B	208	PRO	2.3
1	B	327	LYS	2.3
1	A	387	VAL	2.3
1	G	363	GLU	2.3
1	G	362	ARG	2.3
1	E	355	GLU	2.3
1	F	345	ARG	2.3
1	B	311	LYS	2.3
1	D	260	ALA	2.3
1	F	347	ALA	2.3
1	B	271	VAL	2.3

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
1	E	353	ILE	2.3
1	B	257	GLU	2.2
1	G	355	GLU	2.2
1	A	303	GLU	2.2
1	C	236	VAL	2.2
1	D	256	GLY	2.2
1	D	306	GLY	2.2
1	C	307	MET	2.2
1	A	352	GLN	2.2
1	B	263	VAL	2.2
1	F	302	SER	2.2
1	F	249	ILE	2.2
1	F	303	GLU	2.2
1	B	261	THR	2.2
1	G	313	THR	2.2
1	C	205	ILE	2.2
1	C	257	GLU	2.2
1	C	264	VAL	2.2
1	A	259	LEU	2.1
1	B	270	ILE	2.1
1	C	384	ALA	2.1
1	D	354	GLU	2.1
1	D	188	ASP	2.1
1	B	259	LEU	2.1
1	F	365	LEU	2.1
1	B	84	ALA	2.1
1	D	243	ALA	2.1
1	B	339	GLU	2.1
1	G	209	GLU	2.1
1	A	272	LYS	2.1
1	D	205	ILE	2.1
1	F	355	GLU	2.1
1	A	208	PRO	2.1
1	E	327	LYS	2.1
1	F	239	ALA	2.1
1	F	327	LYS	2.0
1	F	294	THR	2.0
1	A	205	ILE	2.0
1	F	250	ILE	2.0
1	B	286	LYS	2.0
1	F	297	GLY	2.0
1	G	311	LYS	2.0

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
1	D	265	ASN	2.0
1	E	362	ARG	2.0
1	F	331	THR	2.0

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

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

## 6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 6.4 Ligands [i](#)

There are no ligands in this entry.

## 6.5 Other polymers [i](#)

There are no such residues in this entry.