

Full wwPDB X-ray Structure Validation Report (i)

May 14, 2020 – 11:08 am BST

PDB ID	:	1SS8
Title	:	GroEL
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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 A user guide is available at https://www.wwpdb.org/validation/2017/XrayValidationReportHelp with specific help available everywhere you see the (i) symbol.

The following versions of software and data (see references (1)) were used in the production of this report:

MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.11
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	$7.0.044 \; (Gargrove)$
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.11

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	$egin{array}{c} { m Whole \ archive} \ (\#{ m Entries}) \end{array}$	${f Similar\ resolution}\ (\#{ m Entries},{ m resolution\ range}({ m \AA}))$
R_{free}	130704	$2808 \ (2.70-2.70)$
Clashscore	141614	3122(2.70-2.70)
Ramachandran outliers	138981	3069(2.70-2.70)
Sidechain outliers	138945	3069(2.70-2.70)
RSRZ outliers	127900	2737(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 >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5% The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain		
			6%		
1	A	524	71%	23%	5% •
			9%		
1	В	524	71%	22%	5% •
			6%		
1	C	524	73%	21%	••
	_		6%		
1	D	524	71%	23%	5% •
			4%		
1	E	524	72%	22%	6% •
			13%		
1	F	524	74%	22%	• •



Mol	Chain	Length	Quality of chain		
			6%		
1	G	524	72%	23%	• •



2 Entry composition (i)

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.

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf	Trace		
1	Δ	594	Total	С	Ν	Ο	\mathbf{S}	0	0	0
	A	524	3851	2395	662	774	20	0	0	0
1	В	594	Total	С	Ν	Ο	S	0	0	0
	D	524	3851	2395	662	774	20	0	0	0
1	C	594	Total	С	Ν	Ο	\mathbf{S}	0	0	0
		524	3851	2395	662	774	20	0	0	0
1	а	524	Total	С	Ν	Ο	\mathbf{S}	0	0	0
	D		3851	2395	662	774	20	0	0	0
1	F	594	Total	С	Ν	Ο	\mathbf{S}	0	0	0
		524	3851	2395	662	774	20	0	0	0
1	Б	524	Total	С	Ν	Ο	S	0	0	0
	Г	024	3851	2395	662	774	20	0		0
1	C	594	Total	С	Ν	Ο	S	0	0	0
	G	524	3851	2395	662	774	20	0 0	0	

• Molecule 1 is a protein called groEL protein.

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
А	126	VAL	ALA	SEE REMARK 999	UNP P0A6F5
В	13	GLY	ARG	SEE REMARK 999	UNP P0A6F5
В	126	VAL	ALA	SEE REMARK 999	UNP P0A6F5
С	13	GLY	ARG	SEE REMARK 999	UNP P0A6F5
С	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
Е	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	А	18	Total O 18 18	0	0
2	В	21	Total O 21 21	0	0
2	С	15	Total O 15 15	0	0
2	D	16	Total O 16 16	0	0
2	Е	17	Total O 17 17	0	0
2	F	7	Total O 7 7	0	0
2	G	13	Total O 13 13	0	0



Residue-property plots (i) 3

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



• Molecule 1: groEL protein



• Molecule 1: groEL protein









S463 (7.42) D473 13340 1255 D473 13340 1255 M479 13355 1264 M479 13355 1265 L494 13355 1265 L494 13355 1265 L494 13355 1265 L694 13355 1265 L694 13355 1265 L694 13355 1266 L694 1335 1266 L694 1335 1266 L694 1372 1265 L694 1372 1266 L694 1372 1272 L694 1372 1295 L614 1372 1296 L614 1331 1291 L624 1331 1320



4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants	178.38Å 204.98Å 280.98Å	Depositor
a, b, c, α , β , γ	90.00° 90.00° 90.00°	Depositor
$\mathbf{B}_{\mathrm{ascolution}}(\mathbf{A})$	30.00 - 2.70	Depositor
Resolution (A)	29.96 - 2.70	EDS
% Data completeness	(Not available) (30.00-2.70)	Depositor
(in resolution range)	83.9 (29.96-2.70)	EDS
R_{merge}	(Not available)	Depositor
R _{sym}	(Not available)	Depositor
$< I/\sigma(I) > 1$	$0.59 (at 2.68 \text{\AA})$	Xtriage
Refinement program	REFMAC refmac_5.1.19	Depositor
D D.	0.215 , 0.249	Depositor
Π, Π_{free}	0.209 , 0.241	DCC
R_{free} test set	2966 reflections (2.40%)	wwPDB-VP
Wilson B-factor (Å ²)	38.5	Xtriage
Anisotropy	0.354	Xtriage
Bulk solvent $k_{sol}(e/Å^3), B_{sol}(Å^2)$	0.34 , 45.3	EDS
L-test for twinning ²	$ < L >=0.47, < L^2>=0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	27064	wwPDB-VP
Average B, all atoms $(Å^2)$	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.

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



 $^{^1 {\}rm Intensities}$ estimated from amplitudes.

5 Model quality (i)

5.1 Standard geometry (i)

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	B	ond lengths	Bond angles		
	Unam	RMSZ	# Z > 5	RMSZ	# Z > 5	
1	А	1.24	28/3879~(0.7%)	1.11	22/5237~(0.4%)	
1	В	1.28	33/3879~(0.9%)	1.15	27/5237~(0.5%)	
1	С	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	Е	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(A)	Ideal(Å)
1	Ε	129	GLU	CD-OE2	15.67	1.42	1.25
1	Ε	129	GLU	CD-OE1	15.50	1.42	1.25
1	Ε	156	GLU	CD-OE2	11.11	1.37	1.25
1	Ε	76	GLU	CD-OE1	11.03	1.37	1.25
1	В	473	ASP	CB-CG	11.01	1.74	1.51
1	А	44	PHE	CD1-CE1	10.82	1.60	1.39
1	В	44	PHE	CD2-CE2	9.93	1.59	1.39
1	В	76	GLU	CD-OE1	9.68	1.36	1.25
1	С	44	PHE	CD1-CE1	9.37	1.57	1.39
1	Е	44	PHE	CD1-CE1	9.32	1.57	1.39
1	Е	118	ARG	NE-CZ	9.16	1.45	1.33
1	Е	44	PHE	CD2-CE2	9.12	1.57	1.39
1	F	44	PHE	CD1-CE1	9.06	1.57	1.39
1	А	114	MET	SD-CE	9.03	2.28	1.77
1	В	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	В	118	ARG	NE-CZ	8.63	1.44	1.33
1	А	44	PHE	CD2-CE2	8.49	1.56	1.39
1	Ε	44	PHE	CE2-CZ	8.45	1.53	1.37
1	В	44	PHE	CD1-CE1	8.43	1.56	1.39



Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	А	432	GLN	CG-CD	8.38	1.70	1.51
1	G	76	GLU	CD-OE1	8.32	1.34	1.25
1	А	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	В	10	ASN	CB-CG	8.10	1.69	1.51
1	С	445	ARG	CG-CD	8.08	1.72	1.51
1	А	434	GLU	CD-OE2	8.06	1.34	1.25
1	Е	10	ASN	CB-CG	8.03	1.69	1.51
1	F	76	GLU	CD-OE2	8.03	1.34	1.25
1	С	44	PHE	CD2-CE2	7.93	1.55	1.39
1	С	76	GLU	CD-OE1	7.92	1.34	1.25
1	С	118	ARG	NE-CZ	7.91	1.43	1.33
1	С	76	GLU	CD-OE2	7.90	1.34	1.25
1	А	44	PHE	CE2-CZ	7.87	1.52	1.37
1	Е	129	GLU	CG-CD	7.84	1.63	1.51
1	А	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	С	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	С	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	А	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	В	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	С	59	GLU	CD-OE1	6.92	1.33	1.25
1	A	76	GLU	CD-OE1	6.86	1.33	1.25
1	В	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



Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	В	466	ALA	CA-CB	-6.67	1.38	1.52
1	Е	434	GLU	CD-OE1	6.67	1.32	1.25
1	Е	44	PHE	CG-CD2	6.64	1.48	1.38
1	G	118	ARG	NE-CZ	6.62	1.41	1.33
1	Е	44	PHE	CE1-CZ	6.60	1.49	1.37
1	В	490	ASP	CB-CG	-6.58	1.38	1.51
1	В	44	PHE	CG-CD2	6.56	1.48	1.38
1	В	44	PHE	CB-CG	6.53	1.62	1.51
1	С	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	С	514	MET	CG-SD	6.49	1.98	1.81
1	А	44	PHE	CB-CG	6.48	1.62	1.51
1	D	156	GLU	CD-OE2	6.47	1.32	1.25
1	Е	156	GLU	CD-OE1	6.41	1.32	1.25
1	С	434	GLU	CD-OE1	6.41	1.32	1.25
1	С	58	ARG	CZ-NH1	6.40	1.41	1.33
1	С	42	LYS	CD-CE	6.38	1.67	1.51
1	D	44	PHE	CD2-CE2	6.37	1.51	1.39
1	Е	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	В	76	GLU	CD-OE2	6.31	1.32	1.25
1	В	69	MET	SD-CE	-6.30	1.42	1.77
1	А	118	ARG	CZ-NH2	6.29	1.41	1.33
1	С	284	ARG	CG-CD	6.28	1.67	1.51
1	С	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	С	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



Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	Е	118	ARG	CZ-NH1	5.91	1.40	1.33
1	D	485	TYR	CE1-CZ	5.90	1.46	1.38
1	А	284	ARG	NE-CZ	5.90	1.40	1.33
1	Е	114	MET	CG-SD	5.88	1.96	1.81
1	А	434	GLU	CG-CD	5.88	1.60	1.51
1	Е	118	ARG	CZ-NH2	5.85	1.40	1.33
1	В	411	VAL	CB-CG2	-5.83	1.40	1.52
1	С	434	GLU	CD-OE2	5.82	1.32	1.25
1	А	118	ARG	CZ-NH1	5.81	1.40	1.33
1	G	18	ARG	CZ-NH2	5.80	1.40	1.33
1	В	118	ARG	CZ-NH2	5.80	1.40	1.33
1	А	18	ARG	CZ-NH2	5.79	1.40	1.33
1	F	18	ARG	CG-CD	5.78	1.66	1.51
1	В	44	PHE	CA-CB	5.78	1.66	1.53
1	D	44	PHE	CG-CD2	5.77	1.47	1.38
1	А	484	GLU	CD-OE1	5.75	1.31	1.25
1	G	44	PHE	CG-CD2	5.73	1.47	1.38
1	В	82	ASN	CG-OD1	5.73	1.36	1.24
1	В	44	PHE	CG-CD1	5.72	1.47	1.38
1	F	118	ARG	NE-CZ	5.72	1.40	1.33
1	В	164	GLU	CD-OE1	5.70	1.31	1.25
1	G	518	GLU	CD-OE2	-5.70	1.19	1.25
1	Ε	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	В	284	ARG	CG-CD	5.65	1.66	1.51
1	Ε	484	GLU	CD-OE1	5.53	1.31	1.25
1	В	445	ARG	CG-CD	5.51	1.65	1.51
1	В	156	GLU	CD-OE2	5.49	1.31	1.25
1	С	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	В	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	С	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	С	44	PHE	CG-CD2	5.40	1.46	1.38
$\mid 1$	F	129	GLU	CD-OE2	5.39	1.31	1.25



Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	76	GLU	CD-OE2	5.39	1.31	1.25
1	В	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	Е	58	ARG	NE-CZ	5.36	1.40	1.33
1	D	514	MET	CG-SD	5.35	1.95	1.81
1	Е	118	ARG	CG-CD	5.35	1.65	1.51
1	С	491	MET	SD-CE	5.34	2.07	1.77
1	Е	71	ALA	CA-CB	-5.34	1.41	1.52
1	В	58	ARG	CZ-NH2	5.33	1.40	1.33
1	D	432	GLN	CB-CG	5.33	1.67	1.52
1	В	129	GLU	CD-OE2	5.32	1.31	1.25
1	С	58	ARG	NE-CZ	5.31	1.40	1.33
1	Е	18	ARG	CG-CD	5.30	1.65	1.51
1	А	58	ARG	CZ-NH1	5.29	1.40	1.33
1	Ε	128	VAL	CB-CG2	-5.29	1.41	1.52
1	D	44	PHE	CG-CD1	5.25	1.46	1.38
1	С	69	MET	SD-CE	-5.25	1.48	1.77
1	С	18	ARG	NE-CZ	5.24	1.39	1.33
1	С	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	В	422	VAL	CB-CG2	-5.20	1.42	1.52
1	D	18	ARG	CZ-NH1	5.17	1.39	1.33
1	В	490	ASP	CA-CB	-5.17	1.42	1.53
1	Е	105	LYS	CE-NZ	5.16	1.61	1.49
1	А	463	SER	CB-OG	-5.15	1.35	1.42
1	Ε	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	Е	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	С	129	GLU	CD-OE1	5.08	1.31	1.25
1	A	92	ALA	CA-CB	-5.05	1.41	1.52
1	В	172	GLU	$\overline{\text{CD-OE2}}$	5.05	1.31	1.25



Mol	Chain	\mathbf{Res}	Type	Atoms	Z	$\operatorname{Observed}(\operatorname{\AA})$	Ideal(Å)
1	G	284	ARG	CG-CD	5.04	1.64	1.51
1	А	156	GLU	CD-OE2	5.04	1.31	1.25
1	D	44	PHE	CA-CB	5.04	1.65	1.53
1	В	44	PHE	CA-C	5.04	1.66	1.52
1	Е	18	ARG	CZ-NH1	5.04	1.39	1.33
1	В	489	ILE	CG1-CD1	5.03	1.85	1.50
1	С	432	GLN	CG-CD	5.02	1.62	1.51

All (173) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms Z		$\mathbf{Observed}(^{o})$	$Ideal(^{o})$
1	А	421	ARG	NE-CZ-NH1	12.62	126.61	120.30
1	Е	421	ARG	NE-CZ-NH2	-12.43	114.08	120.30
1	Е	452	ARG	NE-CZ-NH1	12.14	126.37	120.30
1	В	491	MET	CG-SD-CE	-11.48	81.84	100.20
1	Е	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	А	421	ARG	NE-CZ-NH2	-11.05	114.77	120.30
1	А	435	ASP	CB-CG-OD2	10.11	127.40	118.30
1	С	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	Е	452	ARG	NE-CZ-NH2	-8.99	115.81	120.30
1	В	490	ASP	CB-CG-OD2	-8.81	110.37	118.30
1	В	25	ASP	CB-CG-OD1	8.76	126.19	118.30
1	С	435	ASP	CB-CG-OD2	8.75	126.18	118.30
1	С	167	ASP	CB-CG-OD2	8.47	125.92	118.30
1	Е	491	MET	CG-SD-CE	-8.36	86.83	100.20
1	С	421	ARG	NE-CZ-NH1	8.31	124.46	120.30
1	С	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	Е	167	ASP	CB-CG-OD2	8.01	125.50	118.30
1	Е	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	С	328	ASP	CB-CG-OD2	7.81	125.33	118.30
1	Е	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



Mol	Chain	Res	Type	${f e} \hspace{0.5 cm} {f Atoms} \hspace{0.5 cm} {f Z} \hspace{0.5 cm} {f Observed}(^{\scriptscriptstyle O})$		$Observed(^{o})$	$Ideal(^{o})$
1	С	283	ASP	CB-CG-OD2	7.67	125.20	118.30
1	С	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	В	421	ARG	NE-CZ-NH2	-7.55	116.53	120.30
1	В	490	ASP	CB-CA-C	-7.50	95.41	110.40
1	А	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	Е	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	С	41	ASP	CB-CG-OD2	7.20	124.78	118.30
1	Е	523	ASP	CB-CG-OD2	7.17	124.75	118.30
1	В	121	ASP	CB-CG-OD2	7.15	124.73	118.30
1	В	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	А	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	В	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	А	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	А	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	С	140	ASP	CB-CG-OD2	6.64	124.28	118.30
1	В	316	ASP	CB-CG-OD2	6.63	124.27	118.30
1	С	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	С	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	Е	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



Mol	Chain	Res	Type	Atoms	$\mathbf{Z} = \mathbf{Observed}(^{o})$		$Ideal(^{o})$
1	С	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	В	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	С	316	ASP	CB-CG-OD2	6.41	124.07	118.30
1	Е	185	ASP	CB-CG-OD2	6.40	124.06	118.30
1	А	495	ASP	CB-CG-OD1	-6.34	112.59	118.30
1	А	328	ASP	CB-CG-OD2	6.33	124.00	118.30
1	А	140	ASP	CB-CG-OD2	6.33	124.00	118.30
1	В	334	ASP	CB-CG-OD2	6.32	123.99	118.30
1	В	36	ARG	NE-CZ-NH2	-6.28	117.16	120.30
1	В	328	ASP	CB-CG-OD2	6.27	123.95	118.30
1	В	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	Е	188	ASP	CB-CG-OD2	6.24	123.92	118.30
1	А	495	ASP	CB-CG-OD2	6.24	123.92	118.30
1	Е	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	В	58	ARG	NE-CZ-NH2	-6.20	117.20	120.30
1	Е	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	А	452	ARG	NE-CZ-NH1	6.18	123.39	120.30
1	С	196	ASP	CB-CG-OD2	6.17	123.86	118.30
1	А	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	Е	52	ASP	CB-CG-OD2	6.12	123.80	118.30
1	С	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	Ε	328	ASP	CB-CG-OD2	6.09	123.78	118.30
1	Е	510	VAL	CB-CA-C	-6.08	99.86	111.40
1	Е	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	В	283	ASP	CB-CG-OD2	6.01	123.71	118.30
1	Ε	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	С	334	ASP	CB-CG-OD2	5.97	123.67	118.30



Mol	Chain	Res	Type	Atoms Z Observed		$Observed(^{o})$	$Ideal(^{o})$
1	D	510	VAL	CB-CA-C	-5.93	100.14	111.40
1	А	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	В	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	В	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	Е	140	ASP	CB-CG-OD2	5.76	123.48	118.30
1	А	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	С	523	ASP	CB-CG-OD2	5.69	123.42	118.30
1	Е	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	А	87	ASP	CB-CG-OD1	5.57	123.31	118.30
1	В	361	ASP	CB-CG-OD2	5.56	123.30	118.30
1	В	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	Ε	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	Е	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	В	291	ASP	CB-CG-OD2	5.46	123.22	118.30
1	В	196	ASP	CB-CG-OD2	5.46	123.22	118.30
1	С	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	С	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	В	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	С	80	LYS	CD-CE-NZ	-5.34	99.42	111.70
1	Е	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



Mol	Chain	Res	Type	Atoms Z		$Observed(^{o})$	$Ideal(^{o})$
1	G	87	ASP	CB-CG-OD1 5.28		123.06	118.30
1	С	155	ASP	CB-CG-OD2	5.28	123.05	118.30
1	С	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	В	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	Е	125	THR	OG1-CB-CG2	-5.14	98.18	110.00
1	Е	473	ASP	CB-CG-OD2	5.13	122.92	118.30
1	С	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	В	432	GLN	CA-CB-CG	5.05	124.51	113.40
1	С	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 (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	А	3851	0	3970	77	0
1	В	3851	0	3970	83	0
1	С	3851	0	3970	77	1
1	D	3851	0	3970	77	0
1	Е	3851	0	3970	77	0
1	F	3851	0	3970	69	0
1	G	3851	0	3970	76	1
2	А	18	0	0	1	0
2	В	21	0	0	4	0
2	С	15	0	0	0	0
2	D	16	0	0	0	0
2	Ē	17	0	0	0	0
2	F	7	0	0	1	0



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	Clash
Atom-1		distance (Å)	overlap (Å)
1:B:489:ILE:CD1	1:B:489:ILE:CG1	1.85	1.52
1:B:473:ASP:CB	1:B:473:ASP:CG	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



		Interatomic	Clash
Atom-1	Atom-2	distance $(Å)$	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:A:149:THR:HG22	1:A:159:GLY:HA3	1.64	0.78
1:E:145:ALA:O	1:E:149:THR:HG23	1.82	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



		Interatomic	Clash
Atom-1	Atom-2	distance (Å)	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:D:77:VAL:HG21	1:D:510:VAL:HG13	1.71	0.72
1:F:145:ALA:O	1:F:149:THR:HG23	1.90	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:B:431:GLY:H	1:B:437:ASN:HD21	1.38	0.70
1:E:431:GLY:H	1:E:437:ASN:ND2	1.90	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:F:42:LYS:HE2	1:F:48:THR:HG23	1.75	0.66
1:G:349:ILE:HA	1:G:352:GLN:HG3	1.77	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



		Interatomic	Clash
Atom-1	Atom-2	distance (\AA)	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:B:431:GLY:H	1:B:437:ASN:ND2	1.95	0.65
1:E:142:LYS:CD	1:E:142:LYS:H	2.08	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:B:224:ASP:O	1:B:225:LYS:HB3	1.99	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: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:A:349:ILE:HA	1:A:352:GLN:HG3	1.82	0.62
1:E:68:ASN:HD21	1:E:72:GLN:HE21	1.47	0.62
1:C:229:ASN:OD1	1:D:269:GLY:O	2.18	0.62
1:E:321:LYS:HG3	1:E:334:ASP:HB3	1.81	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: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:C:77:VAL:HG21	1:C:510:VAL:HG13	1.82	0.61
1:D:142:LYS:H	1:D:142:LYS:CD	2.11	0.61
1:F:224:ASP:O	1:F:225:LYS:HB3	2.01	0.61



		Interatomic	Clash
Atom-1	Atom-2	distance (Å)	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:142:LYS:H	1:C:142:LYS:CD	2.13	0.60
1:C:491:MET:CE	1:C:491:MET:CG	2.79	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:A:224:ASP:O	1:A:225:LYS:HB3	2.03	0.59
1:D:42:LYS:CE	1:D:48:THR:CG2	2.81	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:A:66:PHE:HA	1:A:69:MET:HE3	1.85	0.58
1:C:421:ARG:CD	1:C:474:GLY:O	2.50	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:B:7:LYS:HE3	1:B:15:LYS:HE3	1.86	0.57
1:C:284:ARG:O	1:C:288:MET:HG3	2.03	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:E:42:LYS:HE3	1:E:48:THR:CG2	2.35	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



		Interatomic	Clash
Atom-1	Atom-2	distance $(Å)$	overlap (Å)
1:D:179:ASP:OD1	1:D:393:LYS:HE3	2.05	0.56
1:C:326:ASN:HD22	1:C:329:THR:HB	1.70	0.56
1:G:421:ARG:CD	1:G:474:GLY:O	2.53	0.56
1:E:319:GLN:HB3	1:E:336:VAL:HG21	1.86	0.56
1:A:321:LYS:HG3	1:A:334:ASP:HB3	1.87	0.56
1:C:42:LYS:CE	1:C:48:THR:CG2	2.84	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:A:230:ILE:HD12	1:A:261:THR:HG21	1.88	0.55
1:B:27:VAL:HG13	1:B:90:THR:HG23	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:218:PRO:HD2	1:F:320:ALA:O	2.08	0.53
1:F:325:ILE:HG22	1:F:330:THR:OG1	2.08	0.53
1:G:319:GLN:HB3	1:G:336:VAL:HG21	1.91	0.53
1:C:448:GLU:O	1:C:452:ARG:HG3	2.08	0.53
1:D:494:LEU:HD12	1:D:494:LEU:C	2.28	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:A:142:LYS:H	1:A:142:LYS:CD	2.18	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:G:224:ASP:O	1:G:225:LYS:HB3	2.08	0.53



		Interatomic	Clash
Atom-1	Atom-2	distance $(Å)$	overlan (Å)
1·A·257·GLU·HG3	1·B·269·GLV·HA3	1.91	0.53
1.B.118.ABG.HH22	1:C:34:LYS:HE2	1.74	0.55
1.C.69.MET.CE	$1 \cdot C \cdot 522 \cdot THB \cdot HB$	2.39	0.53
$1 \cdot B \cdot 230 \cdot ILE \cdot HD12$	$1 \cdot B \cdot 261 \cdot THB \cdot HG21$	1.89	0.50
1:A:179:ASP:OD1	$1 \cdot A \cdot 393 \cdot LYS \cdot HE3$	2.09	0.52
1.F.42.LVS.HE3	1.F.48.THB.HG21	1.00	0.52
1.E.326.ASN.HB3	1.1.40.1110.11021 1.E.328.ASP.H	1.31	0.52
1.A.218.PRO.HD2	1.A.320.ALA.O	2 10	0.52
1:A:27:VAL:CG1	$1 \cdot A \cdot 90 \cdot THB \cdot HG23$	2.10	0.52
$1 \cdot F \cdot 42 \cdot LVS \cdot HE3$	1:F:48:THB:CG2	2.30	0.52
1.G.448.GLU.HB3	1.G·452·ABG·HD2	1.03	0.52
1.0.140.010.1100 1.D.325.11 E.HG22	1.0.492	2 10	0.52
1.E.448.GLU.OE1	1.E.452.ABG:NH1	2.10	0.52
1.B.172.GLU.CA	1.R.172.GLU.OE1	2.42	0.52
$\frac{1.6.349 \cdot \text{ILE} \cdot \text{CG2}}{1.6.349 \cdot \text{ILE} \cdot \text{CG2}}$	1.G.369.VAL:HG13	2.50	0.51
1.C.218.PRO.HD2	$\frac{1.0.309.111019}{1.0.320.41.4.0}$	2.40	0.51
$1 \cdot \text{F} \cdot 124 \cdot \text{VAL} \cdot \text{HG13}$	1.E.504.LEU.HD13	1.02	0.51
1.R.162.ILE.HD12	1.B·400·LEU·HΔ	1.92	0.51
$\frac{1.0.102.1101.11012}{1.4.62.11012}$	1.400.1100.11X $1.400.11X$	1.92	0.51
1.A.02.DD0.R	1.G.336.VAL:HG21	1.90	0.51
$1 \cdot \Delta \cdot 69 \cdot MET \cdot HE1$	$1 \cdot \Delta \cdot 522 \cdot \text{THB} \cdot \text{HB}$	1.99	0.51
1.C.358.SEB.HB3	$1:C:361:\Delta SP:OD1$	2 10	0.51
1.E.918.PBO.HD9	1.0.301.ASI .0D1	2.10	0.51
$1 \cdot E \cdot 326 \cdot \Delta SN \cdot HB3$	$1 \cdot \text{E} \cdot 328 \cdot \Delta \text{SP} \cdot \text{H}$	1.76	0.51
1.R.319.GLN.HB3	1.1.320.AST.M	2.41	0.51
1.E.494.LEU.O	1.E.330.VIII.002	2.41	0.50
1:C·263·VAL:O	1.1.494.DD0.HD12	2.11	0.50
1.C.73.MET.HG3	1.D.47.PBO.HG2	1.93	0.50
1.D.27.VAL.CG1	1.D.90.THB.HG23	2.40	0.50
1:E:42:LYS:CE	1.E.48.THB.CG2	2.10	0.50
1.D.180.GLV.HA3	1.D.381.VAL:O	2.00	0.50
1.F.431.GLV·H	$1 \cdot F \cdot 437 \cdot A SN \cdot HD 21$	1.57	0.50
1.F.478.TYB.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.G.448.GLU.OE1	1.G.452.ABG.NH1	2.40	0.50
$1 \cdot C \cdot 230 \cdot ILE \cdot HD12$	$1 \cdot C \cdot 261 \cdot THR \cdot HG21$	1.92	0.50
1.D.172.GLU.OE1	1.D.172.GLU.HA	2.11	0.50
1:E:288:MET·CE	1:E:288:MET:CG	2.11	0.50
1:B:82:ASN:HB2	1:B:89:THB: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



		Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlan (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:B:479:ASN:HD22	1:B:491:MET:CE	2.25	0.49
1:D:266:THR:CG2	1:D:273:VAL:H	2.25	0.49
1:D:519:CYS:HB3	1:E:38:VAL:HG22	1.92	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:B:218:PRO:HD2	1:B:320:ALA:O	2.12	0.49
1:B:73:MET:HG3	1:C:47:PRO:HG2	1.94	0.49
1:D:66:PHE:HA	1:D:69:MET:HE3	1.94	0.49
1:D:68:ASN:ND2	1:D:72:GLN:HE21	2.11	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: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:G:62:LEU:N	1:G:68:ASN:HD22	2.06	0.48
1:B:321:LYS:HG3	1:B:334:ASP:HB3	1.96	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: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:452:ARG:NH2	1:G:463:SER:CB	2.76	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:C:348:GLN:O	1:C:351:GLN:HB2	2.14	0.48
1:D:452:ARG:NH2	1:D:463:SER:CB	2.74	0.48
1:F:262:LEU:O	1:F:266:THR:HG23	2.14	0.48
1:D:351:GLN:HE21	1:D:351:GLN:HB3	1.48	0.48
1:D:448:GLU:OE1	1:D:452:ARG:NH1	2.42	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:A:254:VAL:HG12	1:A:259:LEU:HB2	1.97	0.47
1:E:42:LYS:HE3	1:E:48:THR:HG21	1.96	0.47
1:A:27:VAL:HG13	1:A:90:THR:HG23	1.96	0.47
1:E:280:GLY:HA2	1:E:284:ARG:HH21	1.79	0.47
1:F:263:VAL:O	1:F:267:MET:HB2	2.14	0.47



	<i>io us puye</i>	Interatomic	Clash
Atom-1	Atom-2	distance $(Å)$	overlan(Å)
1·A·325·ILE·HG22	1·A·330·THR·HA	1.95	
1:B:16:MET:SD	1:B:514:MET:HG3	$\frac{1.58}{2.54}$	0.47
1.C.42.LYS.CE	1:C:48:THB:HG21	2.01	0.47
1.D.452.ABG.HH21	$1 \cdot D \cdot 463 \cdot SEB \cdot HB3$	1 79	0.47
1:D:42:LYS:HE3	1:D:48:THB:CG2	2 44	0.47
1·B·41·ASP·O	1.B.42.LVS.HD3	2.11	0.47
1:C:266:THR:CG2	1:C:273:VAL:H	$\frac{2.10}{2.26}$	0.47
1:E:325:ILE:HG22	1:E:330:THB:HA	1.97	0.47
1:A:348:GLN:O	1:A:351:GLN:HB2	2.15	0.47
1:B:273:VAL:HG12	1:B:274:ALA:N	2.30	0.47
1.E.448.GLU.OE1	1.E.452.ABG.NH1	2.35	0.47
1:G:514:MET:HE2	1:G:514:MET:HB2	1.60	0.47
1:C:478:TYB:C	1:C:488:MET:HE1	2.35	0.47
1:D:448:GLU:O	1:D:452:ARG:HG3	2.15	0.47
1:D:27:VAL:HG13	1:D:90:THB:HG23	1.97	0.47
1:E:41:ASP:0	1:E:42:LYS:HD3	2.15	0.47
1:G:348:GLN:O	1:G:351:GLN:HB2	2.14	0.47
1:B:466:ALA:O	1:B:470:LYS:HG3	2.16	0.46
1:D:348:GLN:O	1:D:351:GLN:HB2	2.15	0.46
1:A:326:ASN:HB3	1:A:328:ASP:H	1.80	0.46
1:B:42:LYS:CE	1:B:48:THR:HG23	2.45	0.46
1:D:273:VAL:HG12	1:D:274:ALA:N	2.31	0.46
1:E:349:ILE:CG2	1:E:369:VAL:HG13	2.46	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:F:166:MET:HG2	1:F:171:LYS:HA	1.98	0.46
1:G:305:ILE:O	1:G:305:ILE:HG22	2.15	0.46
1:D:284:ARG:O	1:D:288:MET:HG3	2.15	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:F:452:ARG:HH22	1:F:463:SER:HB3	1.77	0.46
1:B:490:ASP:CB	2:B:536:HOH:O	2.64	0.46
1:B:263:VAL:O	1:B:267:MET:HB2	2.16	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:F:421:ARG:CD	1:F:474:GLY:O	2.59	0.45
1:A:41:ASP:O	1:A:42:LYS:HD3	2.17	0.45
1:D:178:GLU:HG2	1:D:322:ARG:CZ	2.46	0.45
1:E:217:SER:N	1:E:218:PRO:CD	2.78	0.45



		Interatomic	Clash
Atom-1	Atom-2	distance $(Å)$	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:525:PRO:O	2:A:537:HOH:O	2.21	0.45
1:A:68:ASN:O	1:A:72:GLN:HG2	2.16	0.45
1:D:234:LEU:N	1:D:235:PRO:HD2	2.32	0.45
1:F:519:CYS:HB3	1:G:38:VAL:HG22	1.97	0.45
1:B:305:ILE:HG22	1:B:305:ILE:O	2.17	0.45
1:D:68:ASN:O	1:D:72:GLN:HG2	2.16	0.45
1:C:65:LYS:H	1:C:65:LYS:HG2	1.67	0.45
1:G:42:LYS:CE	1:G:48:THR:HG23	2.44	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:E:273:VAL:HG12	1:E:274:ALA:N	2.32	0.44
1:G:494:LEU:HD12	1:G:494:LEU:O	2.17	0.44
1:B:351:GLN:HB3	1:B:351:GLN:HE21	1.36	0.44
1:B:42:LYS:CE	1:B:48:THR:CG2	2.95	0.44
1:C:41:ASP:O	1:C:42:LYS:HD3	2.17	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:G:449:ALA:HB3	1:G:450:PRO:HD3	1.98	0.44
1:C:217:SER:N	1:C:218:PRO:HD3	2.33	0.44
1:E:364:LYS:HA	1:E:364:LYS:HD3	1.70	0.44
1:F:28:LYS:HB2	1:F:453:GLN:HG2	2.00	0.44
1:A:305:ILE:O	1:A:305:ILE:HG22	2.18	0.43
1:B:68:ASN:ND2	1:B:72:GLN:HE21	2.15	0.43
1:C:364:LYS:HA	1:C:364:LYS:HD3	1.86	0.43
1:G:263:VAL:O	1:G:267:MET:HB2	2.18	0.43
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:B:42:LYS:HE2	1:B:48:THR:CG2	2.46	0.43



		Interatomic	Clash
Atom-1	Atom-2	distance $(Å)$	overlap (Å)
1:D:42:LYS:CE	1:D:48:THR:HG21	2.47	0.43
1:G:326:ASN:HB3	1:G:328:ASP:H	1.83	0.43
1:A:162:ILE:HD12	1:A:400:LEU:HA	$\frac{2.00}{2.00}$	0.43
1:A:172:GLU:CA	1:A:172:GLU:OE1	2.66	0.43
1:D:479:ASN:HD22	1:D:491:MET:CE	2.31	0.43
1:E:421:ARG:CD	1:E:474:GLY:O	2.65	0.43
1:G:86:GLY:O	1:G:87:ASP:HB2	2.17	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:A:262:LEU:O	1:A:266:THR:HG23	2.18	0.43
1:G:452:ARG:HH21	1:G:463:SER:HB3	1.82	0.43
1:C:288:MET:CE	1:C:288:MET:CG	2.93	0.43
1:E:228:SER:O	1:E:257:GLU:HB3	2.18	0.43
1:E:325:ILE:HD13	1:E:325:ILE:HG23	1.74	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:B:96:ALA:O	1:B:100:ILE:HD12	2.19	0.42
1:E:266:THR:CG2	1:E:273:VAL:H	2.31	0.42
1:F:319:GLN:HB3	1:F:336:VAL:CG2	2.48	0.42
1:G:180:GLY:HA3	1:G:381:VAL:O	2.18	0.42
1:A:214:GLU:HG3	1:A:324:VAL:HG22	2.01	0.42
1:B:68:ASN:HD21	1:B:72:GLN:HE21	1.67	0.42
1:C:325:ILE:HG22	1:C:330:THR:HA	2.01	0.42
1:E:73:MET:HG3	1:F:47:PRO:HG2	2.00	0.42
1:G:217:SER:N	1:G:218:PRO:CD	2.82	0.42
1:B:186:GLU:HB2	1:B:380:LYS:HG3	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: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:F:217:SER:N	1:F:218:PRO:HD3	2.34	0.42
1:G:171:LYS:HB3	1:G:407:VAL:HG21	2.02	0.42
1:G:502:SER:O	1:G:503:ALA:C	2.55	0.42
1:A:263:VAL:O	1:A:267:MET:HB2	2.19	0.42

	lous page	Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
1:A:452:ARG:HH22	1:A:463:SER:HB3	1.80	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:A:270:ILE:HG22	1:A:271:VAL:HG23	2.01	0.42
1:C:221:LEU:HD12	1:C:222:LEU:N	2.35	0.42
1:A:234:LEU:N	1:A:235:PRO:HD2	2.35	0.42
1:E:418:ALA:O	1:E:422:VAL:HG13	2.19	0.42
1:G:273:VAL:HG12	1:G:274:ALA:N	2.34	0.42
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:E:254:VAL:HG12	1:E:259:LEU:HB2	2.02	0.41
1:E:325:ILE:HG21	1:E:325:ILE:HD12	1.78	0.41
1:E:348:GLN:O	1:E:351:GLN:HB2	2.20	0.41
1:F:273:VAL:HG12	1:F:274:ALA:N	2.35	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:E:205:ILE:HA	1:E:213:VAL:HG22	2.02	0.41
1:E:258:ALA:O	1:E:262:LEU:HG	2.20	0.41
1:E:228:SER:HB3	1:F:272:LYS:NZ	2.34	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:B:325:ILE:HG22	1:B:330:THR:HA	2.02	0.41
1:B:364:LYS:HA	1:B:364:LYS:HD3	1.86	0.41
1:C:228:SER:O	1:C:257:GLU:HB3	2.20	0.41
1:D:266:THR:HG21	1:D:273:VAL:H	1.85	0.41
1:D:325:ILE:HG22	1:D:330:THR:HA	2.01	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:C:266:THR:HG21	1:C:273:VAL:H	1.85	0.41
1:C:325:ILE:HG22	1:C:330:THR:OG1	2.20	0.41
1:F:77:VAL:HG21	1:F:510:VAL:HG13	2.02	0.41
1:G:221:LEU:HD12	1:G:222:LEU:N	2.34	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: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:G:325:ILE:HG22	1:G:330:THR:OG1	2.20	0.41
1:A:8:PHE:HA	1:A:518:GLU:O	2.21	0.41
1:E:351:GLN:HE21	1:E:351:GLN:HB3	1.43	0.41
1:B:284:ARG:O	1:B:288:MET:HG3	2.20	0.41

	A +	Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
1:C:265:ASN:HA	1:C:265:ASN:HD22	1.68	0.41
1:C:68:ASN:ND2	1:C:72:GLN:HE21	2.19	0.41
1:E:305:ILE:HG22	1:E:305:ILE:O	2.20	0.41
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:G:104:LEU:HA	1:G:104:LEU:HD23	1.87	0.41
1:G:82:ASN:HB2	1:G:89:THR:OG1	2.21	0.41
1:B:448:GLU:HB3	1:B:452:ARG:HD2	2.02	0.41
1:C:205:ILE:HA	1:C:213:VAL:HG22	2.03	0.41
1:G:172:GLU:OE1	1:G:172:GLU:CA	2.69	0.41
1:C:42:LYS:HE3	1:C:48:THR:HG21	2.01	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:A:519:CYS:HB3	1:B:38:VAL:HG22	2.04	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: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: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:C:258:ALA:O	1:C:262:LEU:HG	2.21	0.40
1:E:510:VAL:O	1:E:511:ALA:C	2.59	0.40
1:F:452:ARG:NH2	1:F:463:SER:CB	2.80	0.40
1:G:358:SER:HB3	1:G:361:ASP:OD1	2.21	0.40
1:G:479:ASN:HD22	1:G:491:MET:CE	2.34	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:D:65:LYS:HB3	1:D:65:LYS:HE2	1.84	0.40
1:E:184:GLN:HA	1:E:184:GLN:OE1	2.21	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

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 (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	Perce	entiles
1	А	522/524~(100%)	507~(97%)	12 (2%)	3~(1%)	25	50
1	В	522/524~(100%)	505~(97%)	15~(3%)	2 (0%)	34	60
1	С	522/524~(100%)	506~(97%)	13~(2%)	3~(1%)	25	50
1	D	522/524~(100%)	507~(97%)	13~(2%)	2 (0%)	34	60
1	Ε	522/524~(100%)	504 (97%)	17~(3%)	1 (0%)	47	73
1	F	522/524~(100%)	506~(97%)	14 (3%)	2 (0%)	34	60
1	G	522/524~(100%)	504 (97%)	15~(3%)	3~(1%)	25	50
All	All	3654/3668~(100%)	3539~(97%)	99~(3%)	16(0%)	34	60

All (16) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	А	256	GLY
1	В	256	GLY
1	С	256	GLY
1	D	256	GLY
1	Е	256	GLY
1	F	256	GLY
1	G	256	GLY
1	А	225	LYS
1	D	257	GLU
1	F	225	LYS
1	G	257	GLU
1	В	225	LYS
1	С	225	LYS
1	А	205	ILE
1	G	205	ILE
1	С	205	ILE

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Perce	entiles
1	А	404/404~(100%)	351~(87%)	53~(13%)	4	10
1	В	404/404~(100%)	347~(86%)	57~(14%)	3	8
1	С	404/404~(100%)	356~(88%)	48 (12%)	5	12
1	D	404/404~(100%)	350~(87%)	54~(13%)	4	9
1	Ε	404/404~(100%)	354~(88%)	50~(12%)	4	11
1	F	404/404~(100%)	$350 \ (87\%)$	54 (13%)	4	9
1	G	404/404~(100%)	351~(87%)	53~(13%)	4	10
All	All	2828/2828~(100%)	2459 (87%)	369~(13%)	4	10

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

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

Mol	Chain	Res	Type
1	А	201	SER
1	А	209	GLU
1	А	216	GLU
1	А	225	LYS
1	А	230	ILE
1	А	265	ASN
1	А	284	ARG
1	А	295	LEU
1	А	303	GLU
1	А	304	GLU
1	А	317	LEU
1	А	322	ARG
1	А	325	ILE
1	А	328	ASP
1	А	329	THR
1	A	331	THR
1	А	339	GLU
1	А	343	GLN
1	А	345	ARG
1	А	348	GLN
1	А	350	ARG
1	А	351	GLN
1	А	352	GLN
1	А	355	GLU
1	А	358	SER
1	А	363	GLU
1	А	364	LYS
1	А	380	LYS
1	А	404	ARG
1	A	411	VAL
1	A	421	ARG
1	A	$50\overline{4}$	LEU
1	A	510	VAL
1	В	14	VAL
1	В	27	VAL
1	В	43	SER
1	В	48	THR
1	В	55	SER
1	В	58	ARG
1	В	64	ASP
1	В	76	GLU
1	В	82	ASN

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

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

Mol	Chain	Res	Type
1	С	348	GLN
1	С	350	ARG
1	С	351	GLN
1	С	352	GLN
1	С	355	GLU
1	С	364	LYS
1	С	380	LYS
1	С	404	ARG
1	С	411	VAL
1	С	421	ARG
1	С	504	LEU
1	С	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

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	Е	27	VAL
1	Е	43	SER
1	Е	48	THR
1	Е	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

Mol	Chain	Res	Type
1	Е	190	VAL
1	Е	201	SER
1	Е	209	GLU
1	Е	216	GLU
1	Е	225	LYS
1	Е	230	ILE
1	Е	265	ASN
1	Е	284	ARG
1	Е	295	LEU
1	Е	303	GLU
1	Е	304	GLU
1	Е	317	LEU
1	Е	322	ARG
1	Е	325	ILE
1	Е	329	THR
1	Е	331	THR
1	Е	339	GLU
1	Е	343	GLN
1	Е	348	GLN
1	Е	350	ARG
1	Е	351	GLN
1	Е	352	GLN
1	Е	355	GLU
1	Е	358	SER
1	Е	364	LYS
1	Е	372	LEU
1	Е	380	LYS
1	Е	404	ARG
1	Е	411	VAL
1	E	421	ARG
1	E	504	LEU
1	Е	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

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

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

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	А	10	ASN
1	А	68	ASN
1	А	265	ASN
1	А	351	GLN
1	А	437	ASN
1	В	68	ASN
1	В	265	ASN
1	В	326	ASN
1	В	351	GLN
1	В	437	ASN
1	С	68	ASN
1	С	265	ASN
1	С	351	GLN
1	С	437	ASN
1	D	10	ASN
1	D	68	ASN
1	D	265	ASN
1	D	351	GLN
1	D	437	ASN
1	Е	68	ASN
1	Е	265	ASN
1	Е	351	GLN
1	Е	437	ASN
1	Е	453	GLN
1	F	68	ASN

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Mol	Chain	\mathbf{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		

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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 (i)

6.1 Protein, DNA and RNA chains (i)

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

Mol	Chain	Analysed	<RSRZ $>$	#RSRZ>2	$OWAB(Å^2)$	Q < 0.9
1	А	524/524~(100%)	0.06	33 (6%) 20 19	2, 2, 4, 6	0
1	В	524/524~(100%)	0.17	46 (8%) 10 8	2, 2, 4, 6	0
1	С	524/524~(100%)	0.08	32 (6%) 21 20	2, 2, 4, 6	0
1	D	524/524~(100%)	0.07	32 (6%) 21 20	2, 2, 4, 6	0
1	Е	524/524~(100%)	-0.14	20 (3%) 40 39	2, 2, 4, 6	0
1	F	524/524~(100%)	0.41	66 (12%) <mark>3</mark> 3	2, 2, 4, 6	0
1	G	524/524~(100%)	0.01	30 (5%) 23 22	2, 2, 4, 6	0
All	All	3668/3668~(100%)	0.09	259 (7%) 16 14	2, 2, 4, 6	0

All (259) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	F	270	ILE	8.0
1	С	203	TYR	7.9
1	А	305	ILE	7.4
1	G	268	ARG	6.9
1	G	44	PHE	6.6
1	F	203	TYR	6.5
1	F	268	ARG	6.4
1	G	305	ILE	6.2
1	F	340	ALA	6.0
1	А	44	PHE	5.8
1	F	305	ILE	5.7
1	А	268	ARG	5.7
1	F	242	LYS	5.6
1	F	243	ALA	5.5
1	С	268	ARG	5.3
1	F	264	VAL	5.3
1	D	44	PHE	5.3

Continued from previous page...MolChainResTypeRSRZ

1	G	203	TYR	5.3
1	G	270	ILE	5.2
1	F	271	VAL	5.2
1	С	44	PHE	5.1
1	G	264	VAL	5.0
1	D	268	ARG	5.0
1	В	44	PHE	4.8
1	D	264	VAL	4.8
1	Е	354	GLU	4.7
1	В	305	ILE	4.7
1	G	202	PRO	4.6
1	С	305	ILE	4.6
1	D	305	ILE	4.6
1	F	44	PHE	4.6
1	Е	44	PHE	4.6
1	В	354	GLU	4.6
1	F	267	MET	4.5
1	G	387	VAL	4.5
1	F	356	ALA	4.4
1	G	267	MET	4.4
1	А	270	ILE	4.4
1	В	203	TYR	4.3
1	С	208	PRO	4.3
1	F	231	ARG	4.2
1	А	353	ILE	4.2
1	F	259	LEU	4.2
1	Е	203	TYR	4.2
1	С	234	LEU	4.1
1	С	387	VAL	4.1
1	В	353	ILE	4.1
1	A	357	THR	4.1
1	В	351	GLN	4.1
1	A	356	ALA	4.1
1	С	231	ARG	4.0
1	C	267	MET	3.9
1	F	260	ALA	3.9
1	F	349	ILE	3.8
1	С	306	GLY	3.8
1	F	299	THR	3.8
1	F	211	GLY	3.8
1	В	268	ARG	3.8
1	F	261	THR	3.8

Mol	Chain	Res	Type	RSRZ
1	F	265	ASN	3.8
1	F	307	MET	3.8
1	А	231	ARG	3.7
1	В	211	GLY	3.7
1	А	203	TYR	3.7
1	F	350	ARG	3.7
1	С	269	GLY	3.7
1	А	202	PRO	3.6
1	D	263	VAL	3.6
1	F	304	GLU	3.6
1	В	356	ALA	3.6
1	F	201	SER	3.6
1	В	209	GLU	3.5
1	Е	305	ILE	3.5
1	F	360	TYR	3.5
1	D	203	TYR	3.5
1	Е	351	GLN	3.5
1	Е	270	ILE	3.5
1	D	208	PRO	3.5
1	F	311	LYS	3.5
1	В	264	VAL	3.5
1	А	304	GLU	3.5
1	F	313	THR	3.4
1	F	233	MET	3.4
1	G	307	MET	3.4
1	A	354	GLU	3.4
1	Е	387	VAL	3.4
1	F	263	VAL	3.4
1	F	238	GLU	3.4
1	F	306	GLY	3.4
1	D	304	GLU	3.3
1	Е	356	ALA	3.3
1	F	354	GLU	3.3
1	G	327	LYS	3.3
1	С	242	LYS	3.3
1	А	266	THR	3.3
1	D	311	LYS	3.3
1	D	270	ILE	3.2
1	В	387	VAL	3.2
1	G	205	ILE	3.2
1	F	312	ALA	3.2
1	D	202	PRO	3.2

Mol	Chain	Res	Type	RSRZ
1	В	304	GLU	3.2
1	Е	209	GLU	3.2
1	F	208	PRO	3.2
1	F	351	GLN	3.2
1	F	273	VAL	3.2
1	Е	268	ARG	3.1
1	В	267	MET	3.1
1	F	387	VAL	3.1
1	D	267	MET	3.1
1	D	353	ILE	3.1
1	А	363	GLU	3.1
1	F	219	PHE	3.0
1	G	210	THR	3.0
1	В	312	ALA	3.0
1	A	361	ASP	3.0
1	С	209	GLU	3.0
1	В	359	ASP	3.0
1	D	242	LYS	3.0
1	G	234	LEU	3.0
1	D	356	ALA	3.0
1	G	199	TYR	3.0
1	В	233	MET	2.9
1	D	360	TYR	2.9
1	F	362	ARG	2.9
1	D	209	GLU	2.9
1	В	349	ILE	2.9
1	D	231	ARG	2.9
1	G	351	GLN	2.9
1	F	266	THR	2.9
1	G	271	VAL	2.9
1	C	270	ILE	2.9
1	F	315	GLU	2.9
1	F	342	ILE	2.9
1	F	209	GLU	2.8
1	A	271	VAL	2.8
1	C	263	VAL	2.8
1	D	387	VAL	2.8
1	G	391	GLU	2.8
1	G	306	GLY	2.8
1	A	209	GLU	2.8
1	D	391	GLU	2.8
1	С	233	MET	2.8

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 Mol
 Chain
 Res
 Type
 RSRZ
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1	В	360	TYR	2.8
1	А	256	GLY	2.8
1	F	235	PRO	2.7
1	F	339	GLU	2.7
1	А	311	LYS	2.7
1	F	391	GLU	2.7
1	D	211	GLY	2.7
1	F	257	GLU	2.7
1	В	243	ALA	2.7
1	F	202	PRO	2.7
1	В	242	LYS	2.7
1	А	358	SER	2.7
1	В	366	GLN	2.7
1	С	388	GLU	2.7
1	F	310	GLU	2.7
1	С	304	GLU	2.7
1	С	391	GLU	2.7
1	С	351	GLN	2.6
1	С	229	ASN	2.6
1	В	355	GLU	2.6
1	F	300	VAL	2.6
1	А	234	LEU	2.6
1	Ε	256	GLY	2.6
1	В	239	ALA	2.6
1	D	395	ARG	2.6
1	D	234	LEU	2.6
1	С	302	SER	2.6
1	С	210	THR	2.6
1	А	306	GLY	2.6
1	В	340	ALA	2.6
1	A	211	GLY	2.6
1	В	205	ILE	2.5
1	А	172	GLU	2.5
1	A	201	SER	2.5
1	F	363	GLU	2.5
1	В	269	GLY	2.5
1	F	301	ILE	2.5
1	F	338	GLU	2.5
1	A	265	ASN	2.5
1	В	313	THR	2.5
1	С	238	GLU	2.5
1	F	244	GLY	2.4

Mol	Chain	Res	Type	RSRZ
1	G	356	ALA	2.4
1	В	347	ALA	2.4
1	В	391	GLU	2.4
1	G	354	GLU	2.4
1	В	357	THR	2.4
1	F	223	ALA	2.4
1	F	384	ALA	2.4
1	С	327	LYS	2.4
1	F	272	LYS	2.4
1	F	358	SER	2.4
1	G	242	LYS	2.4
1	G	304	GLU	2.4
1	G	388	GLU	2.4
1	F	343	GLN	2.4
1	В	362	ARG	2.4
1	В	210	THR	2.4
1	В	358	SER	2.4
1	D	269	GLY	2.4
1	Е	311	LYS	2.4
1	E	243	ALA	2.3
1	G	238	GLU	2.3
1	А	267	MET	2.3
1	В	302	SER	2.3
1	В	208	PRO	2.3
1	Е	359	ASP	2.3
1	С	350	ARG	2.3
1	Е	208	PRO	2.3
1	E	267	MET	2.3
1	E	306	GLY	2.3
1	E	242	LYS	2.3
1	F	229	ASN	2.3
1	D	355	GLU	2.3
1	В	271	VAL	2.3
1	G	355	GLU	2.2
1	В	327	LYS	2.2
1	В	263	VAL	2.2
1	F	345	ARG	2.2
1	F	347	ALA	2.2
1	G	363	GLU	2.2
1	A	387	VAL	2.2
1	G	362	ARG	2.2
1	В	311	LYS	2.2

Mol	Chain	Res	Type	RSRZ
1	D	306	GLY	2.2
1	Е	355	GLU	2.2
1	G	313	THR	2.2
1	С	236	VAL	2.2
1	С	264	VAL	2.2
1	В	257	GLU	2.2
1	D	260	ALA	2.2
1	F	302	SER	2.1
1	F	303	GLU	2.1
1	Е	353	ILE	2.1
1	F	249	ILE	2.1
1	F	365	LEU	2.1
1	В	261	THR	2.1
1	А	303	GLU	2.1
1	А	259	LEU	2.1
1	С	205	ILE	2.1
1	D	256	GLY	2.1
1	А	352	GLN	2.1
1	С	384	ALA	2.1
1	В	270	ILE	2.1
1	С	307	MET	2.1
1	В	259	LEU	2.1
1	В	84	ALA	2.1
1	А	208	PRO	2.1
1	D	205	ILE	2.1
1	D	243	ALA	2.1
1	В	339	GLU	2.1
1	С	257	GLU	2.1
1	D	354	GLU	2.1
1	G	209	GLU	2.1
1	А	272	LYS	2.0
1	D	188	ASP	2.0

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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.

