



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 04:55 AM UTC

PDB ID : 9F82 / pdb_00009f82
Title : Arbitrium receptor from ATCC13952 phage in complex with GVVRGA peptide
Authors : Gallego del Sol, F.; Marina, A.
Deposited on : 2024-05-06
Resolution : 3.10 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 ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity	:	4-5-2 with Phenix2.0
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

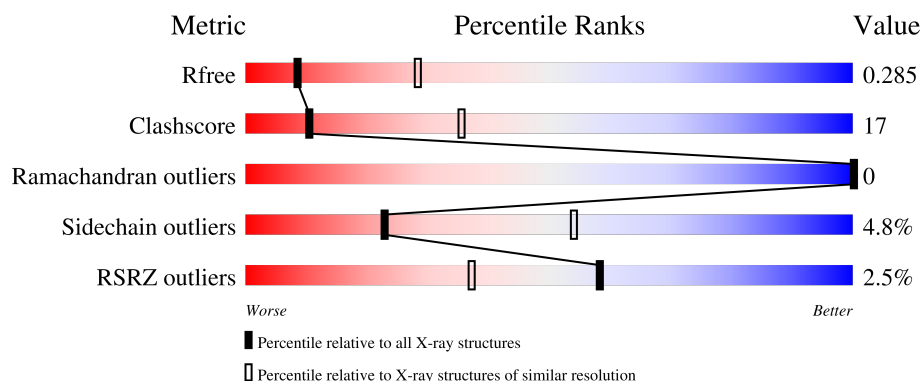
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

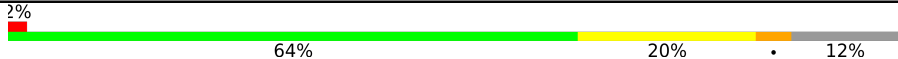
The reported resolution of this entry is 3.10 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	1456 (3.10-3.10)
Clashscore	190562	1539 (3.10-3.10)
Ramachandran outliers	187476	1467 (3.10-3.10)
Sidechain outliers	187428	1467 (3.10-3.10)
RSRZ outliers	180081	1456 (3.10-3.10)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of 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 $\leq 5\%$. 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	386	
1	C	386	
1	E	386	
1	G	386	
2	B	6	

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Mol	Chain	Length	Quality of chain
2	D	6	17% 67% 17% 17%
2	F	6	17% 50% 17% 33%
2	K	6	17% 50% 50%

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 11488 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 Arbitrium receptor from ATCC13952 phage.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	341	Total	C	N	O	S	0	0	0
			2827	1822	457	539	9			
1	C	341	Total	C	N	O	S	0	0	0
			2827	1822	457	539	9			
1	E	341	Total	C	N	O	S	0	0	0
			2827	1822	457	539	9			
1	G	341	Total	C	N	O	S	0	0	0
			2827	1822	457	539	9			

- Molecule 2 is a protein called GLY-VAL-VAL-ARG-GLY-ALA.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	B	6	Total	C	N	O	0	0	0
			39	23	9	7			
2	D	6	Total	C	N	O	0	0	0
			39	23	9	7			
2	F	6	Total	C	N	O	0	0	0
			39	23	9	7			
2	K	6	Total	C	N	O	0	0	0
			39	23	9	7			

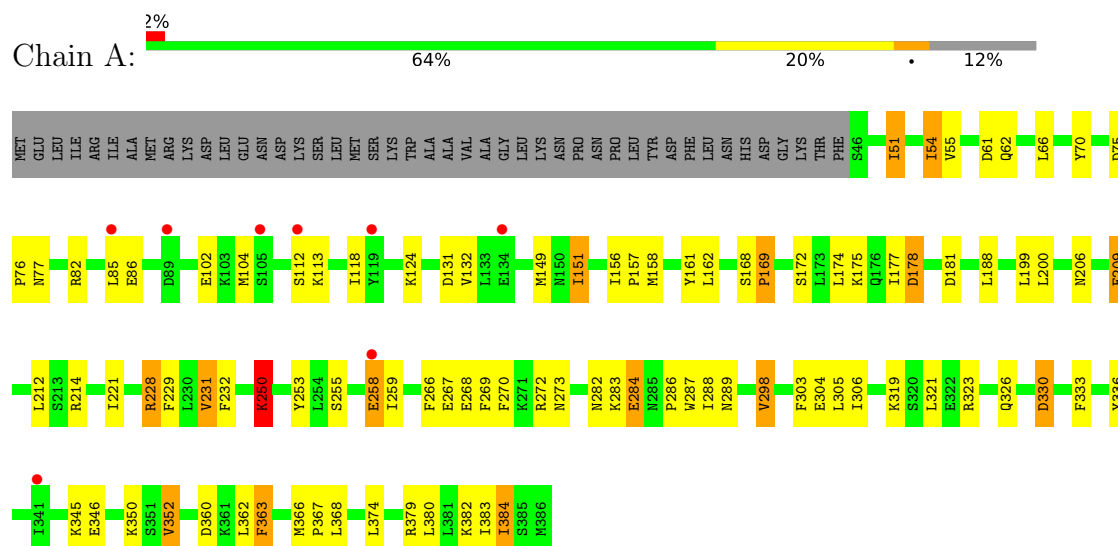
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	5	Total	O	0	0
			5	5		
3	C	3	Total	O	0	0
			3	3		
3	E	6	Total	O	0	0
			6	6		
3	G	10	Total	O	0	0
			10	10		

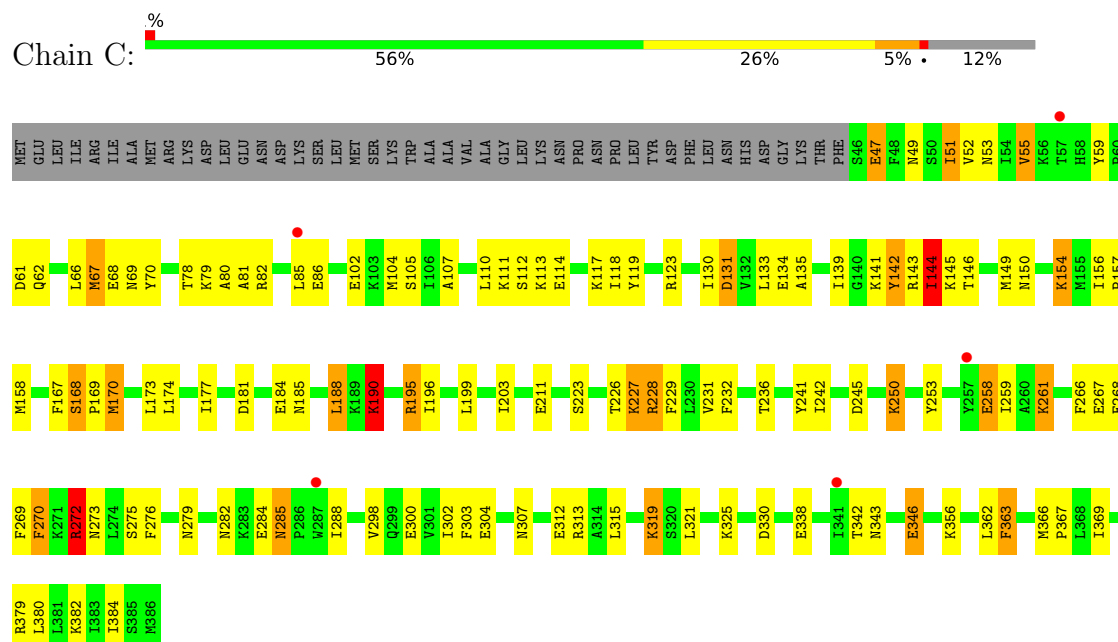
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA, DNA and oligosaccharide 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.

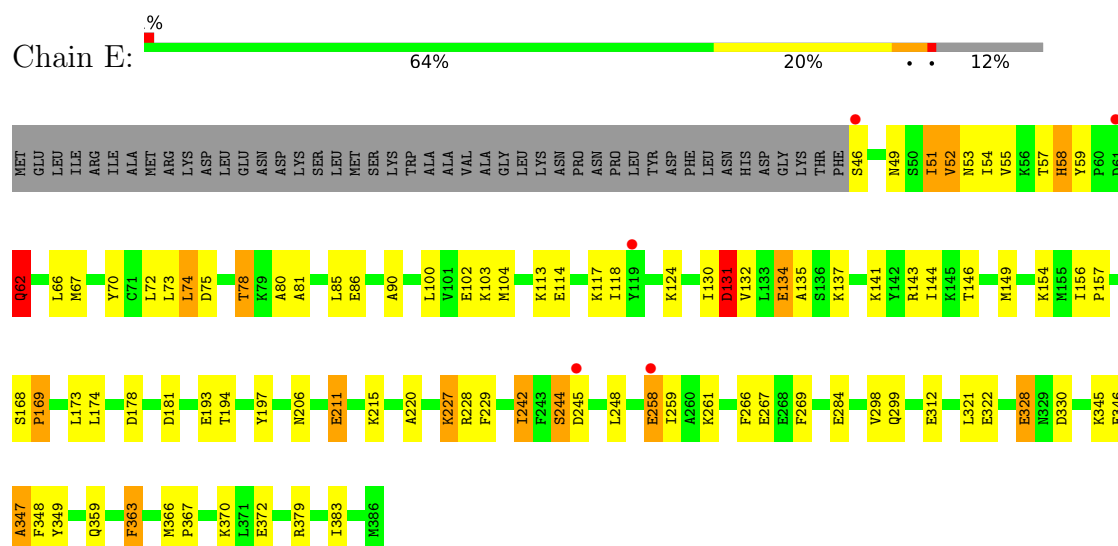
- Molecule 1: Arbitrium receptor from ATCC13952 phage



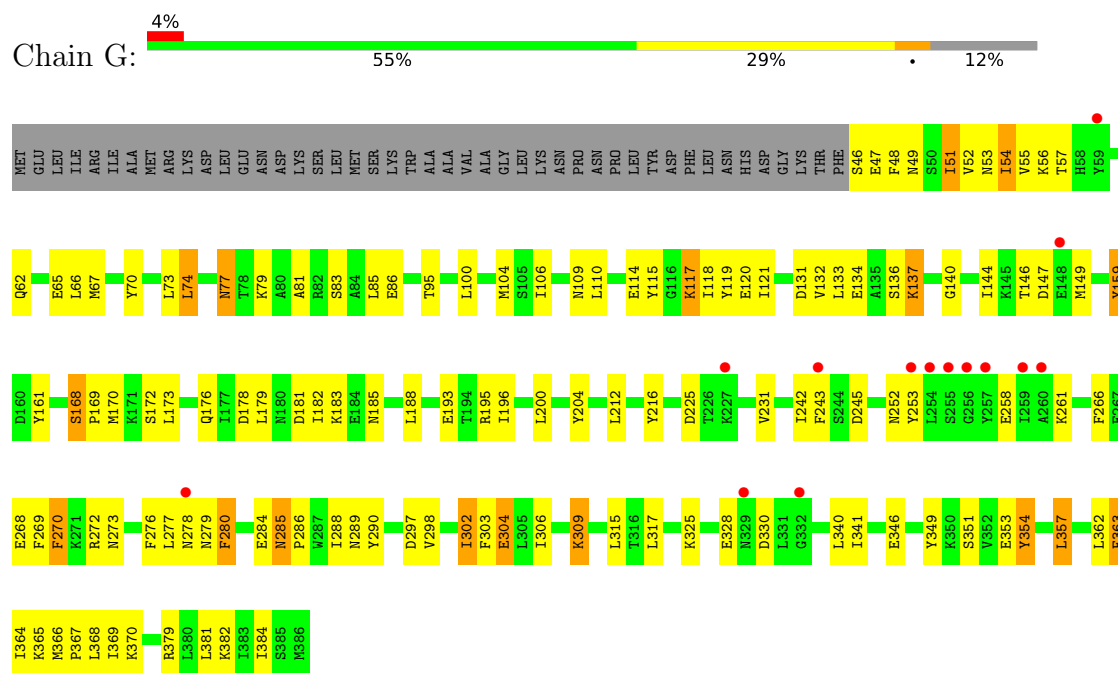
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- Molecule 1: Arbitrium receptor from ATCC13952 phage



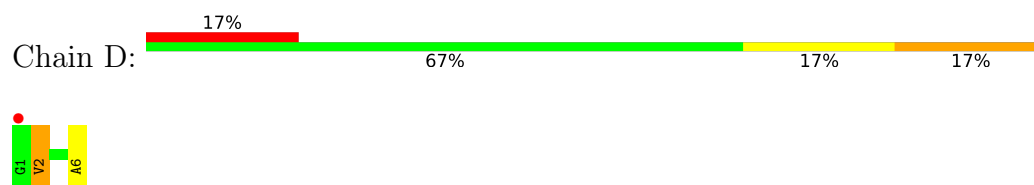
- Molecule 1: Arbitrium receptor from ATCC13952 phage



- Molecule 2: GLY-VAL-VAL-ARG-GLY-ALA



- Molecule 2: GLY-VAL-VAL-ARG-GLY-ALA



- Molecule 2: GLY-VAL-VAL-ARG-GLY-ALA

Chain F: 



- Molecule 2: GLY-VAL-VAL-ARG-GLY-ALA

Chain K: 



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	67.34Å 82.96Å 146.86Å 90.00° 90.88° 90.00°	Depositor
Resolution (Å)	146.84 – 3.10 146.84 – 3.10	Depositor EDS
% Data completeness (in resolution range)	99.7 (146.84-3.10) 99.6 (146.84-3.10)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.22 (at 3.07Å)	Xtriage
Refinement program	REFMAC 5.8.0425	Depositor
R, R_{free}	0.228 , 0.277 0.237 , 0.285	Depositor DCC
R_{free} test set	1523 reflections (5.15%)	wwPDB-VP
Wilson B-factor (Å ²)	75.0	Xtriage
Anisotropy	0.604	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.25 , 32.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	0.027 for h,-k,-l	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	11488	wwPDB-VP
Average B, all atoms (Å ²)	80.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 31.67 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 1.0654e-03. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

¹ Intensities estimated from amplitudes.

² Theoretical 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.

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	0.90	0/2881	1.50	23/3872 (0.6%)
1	C	0.87	0/2881	1.59	54/3872 (1.4%)
1	E	0.77	0/2881	1.54	32/3872 (0.8%)
1	G	0.77	0/2881	1.57	41/3872 (1.1%)
2	B	1.21	0/38	1.75	1/48 (2.1%)
2	D	1.05	0/38	2.38	1/48 (2.1%)
2	F	1.15	0/38	1.80	1/48 (2.1%)
2	K	1.11	0/38	1.80	0/48
All	All	0.83	0/11676	1.56	153/15680 (1.0%)

There are no bond length outliers.

All (153) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	G	170	MET	N-CA-C	12.36	124.29	111.07
1	E	58	HIS	CA-CB-CG	-10.54	103.25	113.80
1	G	51	ILE	CB-CA-C	-10.45	98.59	111.97
1	G	121	ILE	N-CA-C	-10.28	100.76	110.42
1	G	121	ILE	N-CA-CB	9.76	121.68	110.65
1	C	170	MET	N-CA-C	9.04	121.13	111.28
1	C	146	THR	N-CA-C	8.73	123.20	110.28
1	E	143	ARG	N-CA-C	8.72	123.34	107.99
1	E	131	ASP	CA-CB-CG	8.64	121.24	112.60
1	C	346	GLU	CB-CG-CD	8.63	127.27	112.60
1	E	372	GLU	CB-CG-CD	8.51	127.06	112.60
1	A	284	GLU	CB-CG-CD	8.50	127.05	112.60
1	C	266	PHE	CA-CB-CG	8.26	122.06	113.80
1	C	181	ASP	CA-CB-CG	8.06	120.66	112.60
1	E	144	ILE	N-CA-CB	8.00	121.14	111.31
1	G	225	ASP	CA-CB-CG	7.95	120.55	112.60
1	A	178	ASP	CA-CB-CG	7.93	120.53	112.60
2	D	2	VAL	N-CA-CB	7.92	123.54	110.86
1	G	330	ASP	CA-CB-CG	7.64	120.24	112.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	285	ASN	CA-C-N	7.54	129.54	120.94
1	C	285	ASN	C-N-CA	7.54	129.54	120.94
1	A	266	PHE	CA-CB-CG	7.50	121.30	113.80
1	C	190	LYS	N-CA-C	7.49	119.53	111.36
1	E	244	SER	N-CA-C	7.46	119.20	111.14
1	A	61	ASP	CB-CA-C	7.43	122.54	111.17
1	E	269	PHE	CB-CA-C	-7.39	98.29	110.85
1	E	328	GLU	CB-CG-CD	-7.39	100.04	112.60
1	C	67	MET	N-CA-C	7.34	119.36	111.36
2	F	4	ARG	CB-CG-CD	7.34	128.17	111.30
1	G	168	SER	CA-C-N	7.22	126.93	119.56
1	G	168	SER	C-N-CA	7.22	126.93	119.56
1	C	61	ASP	CB-CA-C	7.08	122.00	111.17
1	E	266	PHE	CA-CB-CG	7.08	120.88	113.80
1	E	62	GLN	N-CA-C	7.07	121.00	111.24
1	C	269	PHE	CA-CB-CG	7.06	120.86	113.80
1	C	250	LYS	CA-CB-CG	-7.01	100.08	114.10
1	A	330	ASP	CA-CB-CG	6.99	119.59	112.60
1	G	119	TYR	N-CA-C	6.95	119.75	111.33
1	A	181	ASP	CB-CA-C	6.94	123.47	110.63
1	G	258	GLU	CB-CG-CD	6.92	124.37	112.60
1	E	284	GLU	CB-CG-CD	6.84	124.22	112.60
1	A	258	GLU	CB-CG-CD	6.80	124.16	112.60
1	E	181	ASP	CA-CB-CG	6.78	119.38	112.60
1	G	95	THR	CA-CB-OG1	-6.77	99.45	109.60
1	C	185	ASN	CA-CB-CG	6.72	119.32	112.60
1	C	146	THR	N-CA-CB	-6.69	100.13	109.97
1	C	211	GLU	N-CA-CB	6.69	119.95	110.12
1	G	243	PHE	N-CA-C	-6.65	104.81	113.12
1	C	167	PHE	N-CA-C	-6.64	105.15	113.18
1	E	178	ASP	CA-CB-CG	6.62	119.22	112.60
1	A	267	GLU	CB-CG-CD	6.61	123.84	112.60
1	A	269	PHE	CA-CB-CG	6.57	120.37	113.80
1	C	304	GLU	N-CA-CB	6.55	119.51	110.01
2	B	2	VAL	N-CA-CB	6.54	120.44	111.41
1	G	302	ILE	N-CA-C	6.51	117.26	110.62
1	C	312	GLU	N-CA-CB	6.50	119.50	110.07
1	E	78	THR	CA-CB-OG1	-6.50	99.85	109.60
1	G	176	GLN	CB-CA-C	-6.49	103.24	111.22
1	A	209	GLU	CB-CG-CD	6.46	123.58	112.60
1	C	141	LYS	N-CA-C	6.45	117.97	111.07
1	G	147	ASP	CA-CB-CG	6.44	119.04	112.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	258	GLU	CB-CG-CD	6.42	123.51	112.60
1	C	62	GLN	N-CA-CB	-6.39	100.66	111.27
1	E	131	ASP	N-CA-CB	-6.37	101.34	110.44
1	C	144	ILE	N-CA-C	6.34	117.94	109.37
1	C	184	GLU	CB-CG-CD	6.29	123.29	112.60
1	E	86	GLU	N-CA-CB	6.25	119.13	110.07
1	G	269	PHE	CB-CA-C	-6.24	100.25	110.85
1	G	266	PHE	CA-CB-CG	6.22	120.02	113.80
1	C	330	ASP	CA-CB-CG	6.22	118.82	112.60
1	C	267	GLU	CB-CG-CD	6.20	123.14	112.60
1	G	268	GLU	CB-CG-CD	6.19	123.12	112.60
1	A	298	VAL	N-CA-CB	6.18	117.78	110.55
1	C	270	PHE	CA-CB-CG	-6.18	107.62	113.80
1	E	52	VAL	N-CA-CB	6.16	117.76	110.55
1	G	178	ASP	CA-CB-CG	6.15	118.75	112.60
1	A	319	LYS	CB-CG-CD	6.11	125.35	111.30
1	C	228	ARG	CG-CD-NE	-6.10	98.58	112.00
1	G	181	ASP	CA-CB-CG	6.09	118.69	112.60
1	G	56	LYS	CB-CA-C	-6.00	101.21	110.81
1	E	267	GLU	CB-CG-CD	6.00	122.80	112.60
1	A	363	PHE	CA-CB-CG	-5.96	107.84	113.80
1	C	47	GLU	N-CA-C	5.96	117.57	111.14
1	A	352	VAL	CB-CA-C	-5.87	104.21	112.14
1	G	309	LYS	CB-CG-CD	5.87	124.81	111.30
1	E	330	ASP	CA-CB-CG	5.87	118.47	112.60
1	G	298	VAL	N-CA-CB	5.84	117.38	110.55
1	G	304	GLU	N-CA-C	-5.83	104.83	111.07
1	E	242	ILE	N-CA-C	5.83	116.56	110.62
1	E	347	ALA	N-CA-C	-5.80	103.94	111.02
1	C	319	LYS	CB-CG-CD	5.80	124.63	111.30
1	E	169	PRO	N-CA-C	5.79	121.37	113.84
1	C	272	ARG	CG-CD-NE	5.78	124.72	112.00
1	G	363	PHE	CA-CB-CG	-5.77	108.03	113.80
1	A	250	LYS	CA-CB-CG	-5.76	102.59	114.10
1	G	325	LYS	CA-CB-CG	5.75	125.60	114.10
1	A	62	GLN	N-CA-CB	-5.75	100.17	111.60
1	C	302	ILE	N-CA-C	5.74	116.48	110.62
1	G	276	PHE	CA-CB-CG	-5.73	108.07	113.80
1	A	102	GLU	CB-CA-C	-5.72	101.82	110.92
1	E	347	ALA	N-CA-CB	5.71	118.50	109.82
1	E	86	GLU	N-CA-C	-5.69	104.99	111.14
1	C	227	LYS	CG-CD-CE	5.67	124.33	111.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	G	77	ASN	CB-CA-C	5.67	122.15	110.31
1	G	285	ASN	CA-C-O	5.66	124.01	119.59
1	G	286	PRO	N-CA-C	5.66	121.19	113.84
1	G	56	LYS	N-CA-CB	5.62	118.31	109.94
1	G	280	PHE	CA-CB-CG	-5.60	108.20	113.80
1	E	345	LYS	N-CA-C	5.60	118.31	111.82
1	C	80	ALA	N-CA-C	5.59	118.10	111.33
1	C	102	GLU	N-CA-CB	5.58	118.10	110.01
1	G	270	PHE	CA-CB-CG	-5.55	108.25	113.80
1	C	363	PHE	CA-CB-CG	-5.49	108.31	113.80
1	E	359	GLN	N-CA-CB	5.49	120.42	112.13
1	C	80	ALA	N-CA-CB	-5.47	101.85	110.06
1	C	342	THR	N-CA-C	-5.44	106.77	113.41
1	C	261	LYS	N-CA-C	-5.44	101.99	110.10
1	C	139	ILE	CA-C-N	5.39	125.96	119.98
1	C	139	ILE	C-N-CA	5.39	125.96	119.98
1	G	140	GLY	CA-C-N	5.38	127.44	120.44
1	G	140	GLY	C-N-CA	5.38	127.44	120.44
1	C	143	ARG	N-CA-C	-5.38	99.75	108.52
1	C	245	ASP	CA-CB-CG	5.38	117.97	112.60
1	C	55	VAL	N-CA-CB	5.37	116.47	110.51
1	C	188	LEU	N-CA-CB	5.36	118.59	110.28
1	G	245	ASP	CA-CB-CG	5.36	117.96	112.60
1	E	363	PHE	CA-CB-CG	-5.36	108.44	113.80
1	G	357	LEU	N-CA-CB	5.36	117.78	110.01
1	E	74	LEU	N-CA-CB	-5.33	101.40	109.92
1	G	159	TYR	N-CA-CB	5.33	117.95	110.12
1	A	228	ARG	CG-CD-NE	-5.31	100.32	112.00
1	C	279	ASN	N-CA-CB	5.28	117.66	110.01
1	C	236	THR	CA-CB-OG1	-5.26	101.70	109.60
1	A	214	ARG	NH1-CZ-NH2	5.25	126.13	119.30
1	C	338	GLU	CA-C-N	5.25	125.92	119.99
1	C	338	GLU	C-N-CA	5.25	125.92	119.99
1	C	195	ARG	N-CA-CB	5.23	117.73	109.94
1	C	226	THR	CA-CB-OG1	-5.23	101.76	109.60
1	A	283	LYS	CG-CD-CE	5.22	123.31	111.30
1	E	102	GLU	CB-CA-C	-5.18	102.68	110.92
1	C	167	PHE	CB-CA-C	5.16	120.22	109.95
1	A	169	PRO	N-CA-C	5.13	120.27	113.86
1	G	252	ASN	CA-CB-CG	-5.09	107.50	112.60
1	E	312	GLU	N-CA-CB	5.09	117.44	110.07
1	A	124	LYS	CG-CD-CE	5.07	122.97	111.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	346	GLU	CB-CA-C	5.07	118.92	110.81
1	C	313	ARG	N-CA-CB	5.05	117.64	110.16
1	E	73	LEU	N-CA-CB	5.05	117.91	110.33
1	A	131	ASP	CA-CB-CG	5.03	117.63	112.60
1	C	59	TYR	CA-C-O	-5.02	116.25	121.07
1	C	81	ALA	N-CA-C	-5.02	105.81	111.28
1	G	285	ASN	N-CA-CB	5.00	120.70	110.50
1	G	382	LYS	N-CA-CB	5.00	117.26	110.01

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	2827	0	2846	77	3
1	C	2827	0	2843	118	0
1	E	2827	0	2845	84	5
1	G	2827	0	2846	135	2
2	B	39	0	44	9	0
2	D	39	0	44	4	0
2	F	39	0	44	3	0
2	K	39	0	44	7	0
3	A	5	0	0	0	0
3	C	3	0	0	1	0
3	E	6	0	0	1	0
3	G	10	0	0	3	0
All	All	11488	0	11556	390	5

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 17.

All (390) 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:G:279:ASN:HB3	1:G:303:PHE:CD2	1.34	1.62
1:G:51:ILE:HD13	1:G:70:TYR:CE2	1.28	1.59
1:G:51:ILE:CD1	1:G:70:TYR:CZ	1.79	1.58
1:G:51:ILE:CD1	1:G:70:TYR:CE2	1.82	1.51
1:G:279:ASN:CB	1:G:303:PHE:HD2	1.46	1.28
1:G:279:ASN:CB	1:G:303:PHE:CD2	2.13	1.28
1:E:130:ILE:CB	1:E:134:GLU:OE1	1.83	1.26
1:E:130:ILE:CG2	1:E:134:GLU:OE1	1.92	1.18
1:G:51:ILE:CD1	1:G:70:TYR:OH	1.91	1.17
1:G:51:ILE:HD12	1:G:70:TYR:CE2	1.74	1.16
1:E:130:ILE:HB	1:E:134:GLU:OE1	1.36	1.15
1:C:170:MET:HE3	1:C:203:ILE:HG12	1.27	1.14
1:G:279:ASN:HB3	1:G:303:PHE:CE2	1.84	1.11
1:G:51:ILE:HD11	1:G:70:TYR:CZ	1.69	1.08
1:G:51:ILE:HD12	1:G:70:TYR:CZ	1.72	1.06
1:G:279:ASN:C	1:G:303:PHE:HE2	1.64	1.05
1:E:168:SER:OG	1:E:169:PRO:HD3	1.56	1.04
1:E:130:ILE:HB	1:E:134:GLU:CD	1.83	1.04
1:G:51:ILE:HD12	1:G:70:TYR:OH	1.50	1.02
1:C:170:MET:HE3	1:C:203:ILE:CG1	1.92	0.99
1:C:276:PHE:N	1:C:300:GLU:OE2	1.96	0.98
1:C:133:LEU:HD12	1:C:134:GLU:N	1.80	0.96
1:G:279:ASN:C	1:G:303:PHE:CE2	2.41	0.96
1:E:130:ILE:HG21	1:E:134:GLU:OE1	1.66	0.96
1:G:51:ILE:CD1	1:G:70:TYR:HE2	1.80	0.94
1:C:52:VAL:HG22	1:C:67:MET:CE	1.98	0.94
1:G:46:SER:HB2	1:G:49:ASN:HB3	1.50	0.92
1:A:255:SER:O	1:A:258:GLU:HG2	1.70	0.92
1:G:133:LEU:HD12	1:G:133:LEU:H	1.35	0.92
1:G:204:TYR:CZ	1:G:212:LEU:HD21	2.05	0.91
1:G:279:ASN:CB	1:G:303:PHE:CE2	2.47	0.91
1:A:250:LYS:HD2	1:C:258:GLU:OE1	1.68	0.90
1:G:51:ILE:HD13	1:G:70:TYR:CD2	2.06	0.90
1:E:85:LEU:HD11	1:E:100:LEU:HB3	1.50	0.90
1:E:85:LEU:CD1	1:E:100:LEU:HB3	2.01	0.89
1:C:52:VAL:HG22	1:C:67:MET:HE1	1.53	0.89
1:E:55:VAL:HG11	1:E:67:MET:HE2	1.55	0.88
1:G:280:PHE:N	1:G:303:PHE:HE2	1.69	0.88
1:C:144:ILE:HG21	1:C:150:ASN:HB2	1.55	0.88
1:C:232:PHE:HD2	2:D:6:ALA:C	1.84	0.85
1:C:105:SER:HB3	1:C:117:LYS:HE2	1.55	0.84
1:C:285:ASN:HB3	1:C:288:ILE:HD11	1.58	0.84

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:51:ILE:HD13	1:G:70:TYR:CZ	1.77	0.82
1:E:194:THR:CG2	1:E:229:PHE:CD2	2.62	0.82
1:E:227:LYS:NZ	1:E:227:LYS:HB3	1.95	0.82
1:G:204:TYR:CE2	1:G:212:LEU:HD21	2.14	0.82
1:G:81:ALA:O	1:G:104:MET:HE1	1.78	0.82
1:G:159:TYR:CE1	2:K:6:ALA:C	2.58	0.82
1:G:168:SER:HB2	1:G:169:PRO:HD3	1.61	0.82
1:C:52:VAL:CG2	1:C:67:MET:HE1	2.11	0.81
1:A:206:ASN:OD1	2:B:4:ARG:NH1	2.13	0.81
1:C:276:PHE:CA	1:C:300:GLU:OE2	2.29	0.81
1:G:51:ILE:HD11	1:G:70:TYR:OH	1.65	0.80
1:A:268:GLU:OE2	1:A:272:ARG:NH2	2.14	0.80
1:A:258:GLU:OE1	1:C:250:LYS:NZ	2.13	0.79
1:C:157:PRO:HG2	1:C:173:LEU:HD21	1.65	0.78
1:G:54:ILE:HG22	1:G:55:VAL:N	1.98	0.77
1:E:194:THR:HG21	1:E:229:PHE:CD2	2.19	0.77
1:C:82:ARG:HG3	1:C:104:MET:CE	2.15	0.77
1:C:232:PHE:CD2	2:D:6:ALA:C	2.63	0.76
1:E:130:ILE:CD1	1:E:134:GLU:OE1	2.33	0.75
1:G:159:TYR:HE1	2:K:6:ALA:OXT	1.72	0.73
1:E:54:ILE:O	1:E:58:HIS:HD2	1.72	0.73
1:E:228:ARG:HD2	1:E:228:ARG:O	1.88	0.73
1:A:258:GLU:OE1	1:C:250:LYS:HD3	1.88	0.72
1:C:52:VAL:HA	1:C:67:MET:HE1	1.70	0.72
1:G:279:ASN:HB2	1:G:303:PHE:CD2	2.21	0.72
1:C:130:ILE:HD12	1:C:131:ASP:O	1.89	0.71
1:G:285:ASN:OD1	1:G:288:ILE:HD11	1.90	0.71
1:G:51:ILE:HG22	1:G:67:MET:HE1	1.72	0.71
1:A:360:ASP:OD2	2:B:4:ARG:NH2	2.23	0.71
1:E:194:THR:HG21	1:E:229:PHE:HD2	1.53	0.71
1:G:159:TYR:CE1	2:K:6:ALA:OXT	2.43	0.71
1:G:55:VAL:HG13	1:G:66:LEU:HD12	1.73	0.71
1:G:118:ILE:HB	1:G:149:MET:HE2	1.72	0.71
1:C:298:VAL:HG11	1:C:321:LEU:HD21	1.72	0.70
1:E:194:THR:HG22	1:E:229:PHE:CD2	2.26	0.70
1:A:232:PHE:CD2	2:B:6:ALA:O	2.45	0.70
1:A:288:ILE:HD12	1:A:304:GLU:OE2	1.92	0.70
1:G:159:TYR:HE1	2:K:6:ALA:C	1.99	0.70
1:C:282:ASN:OD1	1:C:307:ASN:CG	2.34	0.70
1:C:346:GLU:OE1	1:E:379:ARG:NH2	2.25	0.70
1:G:52:VAL:HG12	1:G:67:MET:CE	2.21	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:154:LYS:HB3	1:C:177:ILE:HD11	1.73	0.69
1:C:158:MET:CG	1:C:173:LEU:HD23	2.22	0.69
1:E:168:SER:OG	1:E:169:PRO:CD	2.39	0.69
1:A:282:ASN:C	1:A:282:ASN:HD22	2.00	0.69
1:C:105:SER:HB3	1:C:117:LYS:CE	2.22	0.69
1:G:366:MET:HB2	1:G:367:PRO:HD3	1.74	0.69
1:A:286:PRO:HB2	1:C:261:LYS:HB3	1.74	0.68
1:A:172:SER:HB2	1:G:172:SER:HB2	1.75	0.68
1:G:280:PHE:N	1:G:303:PHE:CE2	2.60	0.68
1:C:133:LEU:HD12	1:C:134:GLU:CA	2.23	0.68
1:C:170:MET:CE	1:C:203:ILE:HG12	2.17	0.67
1:C:52:VAL:HG22	1:C:67:MET:HE3	1.74	0.67
1:C:47:GLU:HG2	1:C:51:ILE:HD13	1.76	0.67
1:E:55:VAL:HG11	1:E:67:MET:CE	2.24	0.67
1:E:228:ARG:HD2	1:E:228:ARG:C	2.19	0.67
1:E:228:ARG:NE	1:E:229:PHE:CD1	2.63	0.66
1:C:170:MET:CE	1:C:203:ILE:CG1	2.71	0.66
1:C:343:ASN:OD1	1:C:343:ASN:O	2.12	0.66
1:G:351:SER:OG	1:G:367:PRO:HG3	1.96	0.66
1:A:55:VAL:HG13	1:A:66:LEU:HD12	1.77	0.65
1:E:174:LEU:O	1:E:174:LEU:HD23	1.96	0.65
1:G:46:SER:HB2	1:G:49:ASN:HD22	1.62	0.65
1:G:159:TYR:CD1	2:K:6:ALA:O	2.49	0.65
1:C:144:ILE:HG21	1:C:150:ASN:CB	2.26	0.65
1:A:323:ARG:O	1:A:323:ARG:HG2	1.95	0.65
1:C:133:LEU:CD1	1:C:134:GLU:N	2.59	0.65
1:E:62:GLN:O	1:E:66:LEU:HD13	1.97	0.64
1:C:82:ARG:CG	1:C:104:MET:CE	2.75	0.64
1:G:280:PHE:HA	1:G:303:PHE:CZ	2.32	0.64
1:C:276:PHE:HA	1:C:300:GLU:OE2	1.96	0.64
1:G:81:ALA:C	1:G:104:MET:HE1	2.22	0.63
1:C:315:LEU:C	1:C:315:LEU:HD23	2.23	0.63
1:E:227:LYS:HB3	1:E:227:LYS:HZ3	1.63	0.63
1:C:52:VAL:HA	1:C:67:MET:CE	2.29	0.63
1:E:46:SER:OG	1:E:80:ALA:HB2	1.98	0.63
1:E:137:LYS:O	1:E:141:LYS:HG2	1.99	0.63
1:G:51:ILE:HD12	1:G:70:TYR:HE2	1.46	0.63
1:A:380:LEU:CD1	1:G:349:TYR:CE1	2.82	0.63
1:C:158:MET:HG2	1:C:173:LEU:HD23	1.80	0.63
1:C:315:LEU:HD21	1:C:319:LYS:CE	2.29	0.62
1:E:118:ILE:HB	1:E:149:MET:HE2	1.81	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:288:ILE:CD1	1:A:304:GLU:OE2	2.48	0.62
1:E:366:MET:HB2	1:E:367:PRO:CD	2.30	0.61
1:A:174:LEU:O	1:A:177:ILE:HG13	2.01	0.61
1:C:144:ILE:CG2	1:C:150:ASN:HB2	2.28	0.61
1:C:315:LEU:HD21	1:C:319:LYS:HE2	1.82	0.61
1:G:62:GLN:HG3	1:G:65:GLU:HB2	1.82	0.61
2:F:3:VAL:HG12	2:F:4:ARG:H	1.66	0.60
1:E:130:ILE:HD12	1:E:134:GLU:OE1	2.02	0.60
1:E:130:ILE:CG1	1:E:134:GLU:OE1	2.48	0.60
1:E:227:LYS:HB3	1:E:227:LYS:HZ2	1.66	0.60
1:G:200:LEU:HD23	1:G:216:TYR:CE2	2.36	0.60
1:E:74:LEU:HD21	1:E:81:ALA:N	2.16	0.60
1:C:131:ASP:HB2	1:C:133:LEU:HG	1.84	0.60
1:A:151:ILE:HD11	1:A:178:ASP:O	2.02	0.59
1:E:53:ASN:O	1:E:57:THR:HG22	2.01	0.59
1:A:363:PHE:CE2	2:B:2:VAL:HG11	2.36	0.59
1:A:76:PRO:O	1:A:104:MET:HE3	2.02	0.59
1:A:380:LEU:HD11	1:G:349:TYR:HE1	1.66	0.59
1:E:174:LEU:HD23	1:E:174:LEU:C	2.28	0.59
1:A:174:LEU:HG	1:A:200:LEU:HD21	1.84	0.58
1:G:204:TYR:CD2	1:G:212:LEU:HG	2.38	0.58
1:E:100:LEU:O	1:E:104:MET:HG2	2.04	0.58
1:G:340:LEU:CD2	1:G:370:LYS:HE3	2.33	0.58
1:C:168:SER:HB2	1:C:169:PRO:HD3	1.86	0.58
1:E:54:ILE:O	1:E:58:HIS:CD2	2.56	0.58
1:C:142:TYR:N	1:C:142:TYR:HD2	2.02	0.57
1:A:336:TYR:CE1	1:A:366:MET:HB3	2.39	0.57
1:E:245:ASP:OD2	1:E:248:LEU:N	2.21	0.57
1:C:82:ARG:NH1	1:C:111:LYS:HE2	2.20	0.57
1:E:51:ILE:HG22	1:E:67:MET:HE1	1.87	0.57
1:G:137:LYS:HE2	1:G:137:LYS:HA	1.86	0.57
1:C:384:ILE:HD13	1:E:383:ILE:HG21	1.86	0.57
1:E:114:GLU:OE1	1:E:146:THR:OG1	2.20	0.57
1:G:54:ILE:CG2	1:G:55:VAL:N	2.68	0.57
1:G:280:PHE:HA	1:G:303:PHE:HZ	1.68	0.56
1:G:354:TYR:HD1	1:G:354:TYR:N	2.03	0.56
1:G:53:ASN:O	1:G:57:THR:HG23	2.05	0.56
1:G:74:LEU:N	1:G:74:LEU:HD13	2.20	0.56
1:C:142:TYR:N	1:C:142:TYR:CD2	2.73	0.56
1:G:183:LYS:HG2	1:G:183:LYS:O	2.05	0.56
1:C:49:ASN:OD1	1:C:53:ASN:OD1	2.23	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:340:LEU:HD21	1:G:370:LYS:HE3	1.86	0.56
1:C:158:MET:HG3	1:C:173:LEU:HD23	1.86	0.56
1:G:159:TYR:CE1	2:K:6:ALA:O	2.58	0.56
1:E:74:LEU:HD11	1:E:80:ALA:HB1	1.86	0.56
1:A:380:LEU:HD21	1:G:381:LEU:HD21	1.88	0.55
1:A:284:GLU:OE1	1:C:227:LYS:NZ	2.34	0.55
1:C:119:TYR:O	1:C:123:ARG:HG2	2.06	0.55
1:G:354:TYR:N	1:G:354:TYR:CD1	2.72	0.55
1:C:142:TYR:HD2	1:C:142:TYR:H	1.54	0.55
1:A:132:VAL:HG11	1:A:161:TYR:CE1	2.42	0.55
1:G:46:SER:HB2	1:G:49:ASN:CB	2.30	0.55
1:A:86:GLU:HB2	1:A:188:LEU:CD1	2.36	0.55
1:C:170:MET:HE3	1:C:203:ILE:HG13	1.85	0.55
1:G:46:SER:HB2	1:G:49:ASN:ND2	2.21	0.55
1:G:185:ASN:CG	1:G:188:LEU:HD13	2.31	0.55
1:C:158:MET:HG3	1:C:173:LEU:CD2	2.37	0.55
1:G:204:TYR:CE2	1:G:212:LEU:CD2	2.86	0.55
1:G:278:ASN:HB3	1:G:285:ASN:HB3	1.87	0.55
1:A:362:LEU:HD23	1:A:363:PHE:CE1	2.42	0.55
1:A:168:SER:HB2	1:A:169:PRO:HD3	1.89	0.54
1:A:232:PHE:HD2	2:B:6:ALA:O	1.89	0.54
1:C:285:ASN:CB	1:C:288:ILE:HD11	2.35	0.54
1:E:52:VAL:HA	1:E:67:MET:HE3	1.89	0.54
1:A:82:ARG:HG3	1:A:104:MET:HE1	1.89	0.54
1:C:86:GLU:HG2	1:C:119:TYR:OH	2.08	0.54
1:C:285:ASN:O	1:C:288:ILE:CD1	2.56	0.54
2:K:3:VAL:O	2:K:4:ARG:HG3	2.07	0.54
1:A:333:PHE:CZ	2:B:2:VAL:HG13	2.42	0.54
1:E:130:ILE:CG2	1:E:134:GLU:CD	2.79	0.54
1:G:204:TYR:CD1	1:G:212:LEU:HD23	2.42	0.54
1:C:51:ILE:HG21	1:C:70:TYR:CE2	2.43	0.53
1:C:177:ILE:HG21	1:C:196:ILE:HD11	1.89	0.53
1:A:380:LEU:HD12	1:G:349:TYR:CE1	2.43	0.53
1:C:366:MET:HB2	1:C:367:PRO:CD	2.38	0.53
1:G:289:ASN:C	1:G:289:ASN:HD22	2.17	0.53
1:G:366:MET:HB2	1:G:367:PRO:CD	2.38	0.53
1:C:86:GLU:HG3	1:C:188:LEU:HG	1.91	0.53
1:C:325:LYS:HA	3:C:402:HOH:O	2.09	0.53
1:G:204:TYR:CZ	1:G:212:LEU:CD2	2.85	0.53
1:A:162:LEU:CD2	2:B:6:ALA:HB2	2.39	0.53
1:A:209:GLU:HB3	1:A:212:LEU:HD13	1.91	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:161:TYR:CE2	1:G:169:PRO:HB2	2.44	0.52
1:C:170:MET:CE	1:C:203:ILE:HG13	2.39	0.52
1:G:353:GLU:O	1:G:357:LEU:HG	2.10	0.52
1:G:46:SER:O	1:G:47:GLU:C	2.53	0.52
1:C:144:ILE:N	1:C:144:ILE:CD1	2.73	0.52
1:E:131:ASP:OD1	1:E:132:VAL:N	2.43	0.52
1:G:117:LYS:O	1:G:120:GLU:HG2	2.11	0.51
1:G:131:ASP:OD2	1:G:133:LEU:HD12	2.10	0.51
1:G:279:ASN:CG	1:G:303:PHE:HD2	2.14	0.51
1:G:86:GLU:OE1	1:G:195:ARG:NH1	2.41	0.51
1:G:185:ASN:OD1	1:G:188:LEU:HD13	2.10	0.51
1:A:118:ILE:HB	1:A:149:MET:HE2	1.93	0.51
1:E:168:SER:HG	1:E:169:PRO:HD3	1.71	0.51
1:E:66:LEU:N	1:E:66:LEU:HD12	2.26	0.51
1:E:52:VAL:HA	1:E:67:MET:CE	2.41	0.51
1:G:131:ASP:OD2	1:G:133:LEU:CD1	2.59	0.51
1:A:305:LEU:O	1:A:306:ILE:C	2.49	0.51
1:E:85:LEU:CD2	1:E:104:MET:HG3	2.41	0.51
1:A:168:SER:N	1:A:169:PRO:HD2	2.26	0.51
1:E:258:GLU:HA	1:E:261:LYS:HD3	1.93	0.51
1:E:49:ASN:HA	1:E:52:VAL:HG22	1.93	0.51
1:G:54:ILE:O	1:G:55:VAL:C	2.53	0.51
1:E:134:GLU:HG2	1:E:135:ALA:N	2.27	0.50
1:G:279:ASN:HB2	1:G:303:PHE:CE2	2.41	0.50
1:G:48:PHE:HA	1:G:51:ILE:HD12	1.93	0.50
1:G:315:LEU:CD2	3:G:406:HOH:O	2.60	0.49
1:C:85:LEU:HD11	1:C:104:MET:SD	2.52	0.49
1:C:105:SER:O	1:C:113:LYS:HG3	2.11	0.49
1:C:379:ARG:HD3	1:E:349:TYR:CD2	2.47	0.49
1:E:227:LYS:HG3	1:E:259:ILE:CG2	2.42	0.49
1:A:253:TYR:CZ	1:A:273:ASN:HB3	2.47	0.49
1:C:78:THR:HG22	1:C:79:LYS:N	2.28	0.49
1:C:82:ARG:NH1	1:C:111:LYS:CE	2.76	0.49
1:G:288:ILE:HD12	1:G:304:GLU:OE2	2.12	0.49
1:C:107:ALA:O	1:C:113:LYS:HE2	2.12	0.49
1:E:55:VAL:CG1	1:E:67:MET:CE	2.91	0.49
1:G:306:ILE:HD11	1:G:341:ILE:HG13	1.95	0.49
1:C:174:LEU:C	1:C:174:LEU:HD13	2.38	0.49
1:A:363:PHE:CZ	2:B:2:VAL:HG11	2.48	0.49
1:C:356:LYS:HE3	1:E:383:ILE:O	2.12	0.49
1:G:118:ILE:HB	1:G:149:MET:CE	2.40	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:90:ALA:O	1:E:228:ARG:HB3	2.13	0.49
1:E:228:ARG:C	1:E:228:ARG:CD	2.85	0.49
1:G:279:ASN:O	1:G:303:PHE:CE2	2.64	0.49
1:C:362:LEU:HD23	1:C:363:PHE:CE1	2.48	0.48
1:G:77:ASN:HB2	1:G:109:ASN:HB2	1.95	0.48
1:C:384:ILE:HD13	1:E:383:ILE:CG2	2.43	0.48
1:C:285:ASN:O	1:C:288:ILE:HD12	2.13	0.48
1:C:303:PHE:HD1	1:C:303:PHE:O	1.96	0.48
1:A:228:ARG:HH21	1:A:229:PHE:HE1	1.58	0.48
1:E:366:MET:HB2	1:E:367:PRO:HD3	1.93	0.48
1:E:70:TYR:O	1:E:74:LEU:HB2	2.14	0.48
1:G:74:LEU:N	1:G:74:LEU:CD1	2.75	0.48
1:A:346:GLU:CD	1:G:379:ARG:HH22	2.22	0.48
1:C:232:PHE:CD2	2:D:6:ALA:N	2.81	0.48
1:C:315:LEU:HD21	1:C:319:LYS:HE3	1.95	0.47
1:A:174:LEU:HD22	1:A:177:ILE:HG12	1.96	0.47
1:C:86:GLU:OE2	1:C:195:ARG:NH1	2.47	0.47
1:A:380:LEU:CD1	1:G:349:TYR:HE1	2.23	0.47
1:A:287:TRP:CE2	1:C:261:LYS:HE3	2.23	0.47
1:C:275:SER:C	1:C:300:GLU:OE2	2.57	0.47
1:C:82:ARG:CD	1:C:112:SER:OG	2.62	0.47
1:A:258:GLU:OE1	1:C:250:LYS:CD	2.60	0.47
1:A:383:ILE:HG21	1:G:384:ILE:HD13	1.97	0.47
1:C:82:ARG:CG	1:C:104:MET:HE2	2.45	0.47
1:G:133:LEU:HD12	1:G:133:LEU:N	2.17	0.47
1:C:118:ILE:HB	1:C:149:MET:HE2	1.97	0.46
1:E:124:LYS:HB3	1:E:130:ILE:HG12	1.96	0.46
1:C:232:PHE:CD2	2:D:6:ALA:OXT	2.68	0.46
1:G:161:TYR:CD2	1:G:169:PRO:HB2	2.49	0.46
1:A:51:ILE:HG21	1:A:70:TYR:CE2	2.50	0.46
1:A:231:VAL:HG13	1:A:270:PHE:HE2	1.81	0.46
1:C:82:ARG:HG2	1:C:104:MET:HE2	1.96	0.46
1:A:174:LEU:O	1:A:177:ILE:CG1	2.64	0.46
1:G:48:PHE:HD2	1:G:70:TYR:CE2	2.33	0.46
1:G:231:VAL:HG13	1:G:270:PHE:HE2	1.81	0.46
1:C:118:ILE:HG21	1:C:149:MET:HE3	1.98	0.46
1:E:51:ILE:HG21	1:E:70:TYR:CE2	2.50	0.46
1:E:85:LEU:HD12	1:E:100:LEU:HD13	1.98	0.46
1:C:366:MET:HB2	1:C:367:PRO:HD3	1.98	0.45
1:E:298:VAL:HG11	1:E:321:LEU:HD21	1.98	0.45
1:A:368:LEU:HD21	1:A:384:ILE:HG22	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:85:LEU:HD21	1:E:104:MET:HG3	1.99	0.45
1:A:286:PRO:HB2	1:C:261:LYS:CB	2.45	0.45
1:C:231:VAL:HG13	1:C:270:PHE:HE2	1.82	0.45
1:A:118:ILE:HB	1:A:149:MET:CE	2.47	0.45
1:A:380:LEU:O	1:A:384:ILE:HD13	2.17	0.45
1:C:82:ARG:HG3	1:C:104:MET:HE3	1.98	0.45
1:E:206:ASN:ND2	3:E:402:HOH:O	2.43	0.45
1:G:46:SER:CB	1:G:49:ASN:HD22	2.30	0.45
1:G:354:TYR:HD1	1:G:354:TYR:H	1.63	0.45
1:C:133:LEU:CG	1:C:134:GLU:N	2.80	0.45
1:E:348:PHE:CZ	1:E:370:LYS:HG2	2.52	0.45
1:A:366:MET:HB2	1:A:367:PRO:CD	2.46	0.45
1:C:158:MET:HE2	1:C:199:LEU:HD22	1.99	0.45
1:E:363:PHE:CE1	2:F:2:VAL:HG21	2.52	0.45
1:G:183:LYS:O	1:G:183:LYS:CG	2.65	0.45
1:A:303:PHE:O	1:A:303:PHE:CD1	2.70	0.44
1:G:315:LEU:HD22	3:G:406:HOH:O	2.18	0.44
1:C:133:LEU:HD12	1:C:133:LEU:C	2.40	0.44
1:G:51:ILE:HG21	1:G:70:TYR:CE2	2.52	0.44
1:G:284:GLU:HA	1:G:284:GLU:OE1	2.18	0.44
1:C:303:PHE:O	1:C:303:PHE:CD1	2.70	0.44
1:E:72:LEU:O	1:E:103:LYS:NZ	2.36	0.44
1:G:364:ILE:O	1:G:368:LEU:HG	2.17	0.44
1:C:369:ILE:HD13	1:C:369:ILE:HA	1.92	0.44
1:E:363:PHE:CZ	2:F:2:VAL:HG21	2.53	0.44
1:G:52:VAL:HG12	1:G:67:MET:HE3	1.99	0.44
1:G:204:TYR:CD2	1:G:212:LEU:CD2	3.00	0.44
1:A:104:MET:HE2	1:A:112:SER:HB3	2.00	0.43
1:A:158:MET:HE3	1:A:199:LEU:HD13	1.98	0.43
1:C:253:TYR:CZ	1:C:273:ASN:HB3	2.53	0.43
1:E:227:LYS:NZ	1:E:227:LYS:CB	2.73	0.43
1:G:272:ARG:NH2	3:G:401:HOH:O	2.50	0.43
1:G:302:ILE:HG12	1:G:317:LEU:HD23	2.00	0.43
1:G:365:LYS:O	1:G:369:ILE:HG13	2.18	0.43
1:C:228:ARG:HH21	1:C:229:PHE:HE1	1.66	0.43
1:G:83:SER:HA	1:G:188:LEU:HD11	2.00	0.43
1:C:110:LEU:O	1:C:114:GLU:HG2	2.18	0.43
1:E:74:LEU:CD2	1:E:81:ALA:N	2.81	0.43
1:A:54:ILE:HD13	1:A:54:ILE:HA	1.84	0.43
1:A:118:ILE:HG21	1:A:149:MET:HE3	2.00	0.43
1:C:190:LYS:HE3	1:C:223:SER:HB2	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:268:GLU:HG2	1:C:272:ARG:HD3	2.01	0.43
1:C:82:ARG:HG2	1:C:104:MET:CE	2.49	0.43
1:E:227:LYS:HD2	1:E:259:ILE:O	2.18	0.43
1:G:204:TYR:CE1	1:G:212:LEU:CD2	3.02	0.43
1:G:362:LEU:HD23	1:G:363:PHE:CE1	2.53	0.43
1:A:231:VAL:HG13	1:A:270:PHE:CE2	2.54	0.43
1:C:144:ILE:HG21	1:C:150:ASN:CA	2.49	0.43
1:E:197:TYR:HB3	1:E:220:ALA:HB2	2.01	0.43
1:G:242:ILE:HG23	1:G:277:LEU:HD12	2.01	0.42
1:G:280:PHE:HA	1:G:303:PHE:CE2	2.53	0.42
1:A:75:ASP:OD1	1:A:77:ASN:N	2.46	0.42
1:A:289:ASN:C	1:A:289:ASN:HD22	2.28	0.42
1:A:379:ARG:NH1	1:G:346:GLU:OE2	2.52	0.42
1:G:114:GLU:OE1	1:G:146:THR:OG1	2.19	0.42
1:G:115:TYR:CE2	1:G:188:LEU:HD21	2.54	0.42
1:A:156:ILE:N	1:A:157:PRO:HD2	2.34	0.42
1:A:250:LYS:NZ	1:C:258:GLU:HG2	2.34	0.42
1:C:145:LYS:HB3	1:C:145:LYS:HE3	1.68	0.42
1:E:49:ASN:ND2	1:E:53:ASN:OD1	2.52	0.42
1:E:346:GLU:O	1:E:347:ALA:C	2.61	0.42
1:G:290:TYR:HH	1:G:304:GLU:CD	2.25	0.42
1:A:258:GLU:CG	1:A:259:ILE:N	2.82	0.42
1:E:85:LEU:CG	1:E:100:LEU:HB3	2.48	0.42
1:G:70:TYR:CE1	1:G:74:LEU:HD11	2.55	0.42
1:G:81:ALA:O	1:G:104:MET:CE	2.59	0.42
1:A:345:LYS:HE2	1:A:374:LEU:HD13	2.01	0.42
1:G:204:TYR:CG	1:G:212:LEU:HD23	2.55	0.42
1:A:258:GLU:OE1	1:C:250:LYS:CE	2.67	0.42
1:A:360:ASP:CG	2:B:4:ARG:HH22	2.25	0.42
1:G:70:TYR:CE1	1:G:74:LEU:HD21	2.55	0.42
1:G:278:ASN:CB	1:G:285:ASN:HB3	2.49	0.42
1:G:285:ASN:OD1	1:G:288:ILE:CD1	2.66	0.41
1:E:74:LEU:HD22	1:E:81:ALA:HA	2.02	0.41
1:G:114:GLU:OE2	1:G:144:ILE:HA	2.20	0.41
1:G:85:LEU:HB2	1:G:104:MET:HE3	2.03	0.41
1:G:100:LEU:O	1:G:104:MET:HG2	2.21	0.41
1:G:253:TYR:CZ	1:G:273:ASN:HB3	2.54	0.41
1:A:82:ARG:HD3	1:A:112:SER:CA	2.51	0.41
1:E:156:ILE:N	1:E:157:PRO:HD2	2.35	0.41
1:G:46:SER:CB	1:G:49:ASN:HB3	2.35	0.41
1:A:298:VAL:HG11	1:A:321:LEU:HD21	2.01	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:282:ASN:OD1	1:C:307:ASN:ND2	2.53	0.41
1:C:55:VAL:HG13	1:C:66:LEU:HD12	2.02	0.41
1:E:75:ASP:O	1:E:78:THR:HG22	2.20	0.41
1:G:179:LEU:HD13	1:G:193:GLU:HG2	2.02	0.41
1:A:326:GLN:HB3	1:A:330:ASP:HB2	2.03	0.41
1:C:156:ILE:N	1:C:157:PRO:HD2	2.35	0.41
1:E:346:GLU:HA	1:E:349:TYR:HB2	2.03	0.41
1:C:113:LYS:O	1:C:117:LYS:HG2	2.21	0.41
1:C:130:ILE:HD11	1:C:135:ALA:HB2	2.03	0.41
1:E:211:GLU:H	1:E:211:GLU:HG2	1.46	0.41
1:A:352:VAL:HG22	1:A:368:LEU:CD1	2.51	0.41
1:E:113:LYS:O	1:E:117:LYS:HG2	2.21	0.41
1:G:231:VAL:HG13	1:G:270:PHE:CE2	2.56	0.41
1:A:345:LYS:O	1:A:346:GLU:C	2.64	0.40
1:C:241:TYR:O	1:C:242:ILE:C	2.65	0.40
1:A:286:PRO:CB	1:C:261:LYS:HB3	2.45	0.40
1:A:346:GLU:OE1	1:G:379:ARG:NH2	2.48	0.40
1:G:161:TYR:CE2	1:G:169:PRO:CB	3.03	0.40
1:C:231:VAL:HG13	1:C:270:PHE:CE2	2.56	0.40
1:C:300:GLU:HA	1:C:300:GLU:OE1	2.22	0.40

All (5) 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:E:59:TYR:CZ	1:G:47:GLU:OE2[1_656]	1.61	0.59
1:E:59:TYR:OH	1:G:47:GLU:OE2[1_656]	1.69	0.51
1:A:350:LYS:NZ	1:E:322:GLU:O[2_646]	1.79	0.41
1:A:323:ARG:NH2	1:E:328:GLU:OE1[2_646]	2.10	0.10
1:A:323:ARG:CZ	1:E:328:GLU:OE1[2_646]	2.14	0.06

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	339/386 (88%)	330 (97%)	9 (3%)	0	100	100
1	C	339/386 (88%)	328 (97%)	11 (3%)	0	100	100
1	E	339/386 (88%)	330 (97%)	9 (3%)	0	100	100
1	G	339/386 (88%)	327 (96%)	12 (4%)	0	100	100
2	B	4/6 (67%)	4 (100%)	0	0	100	100
2	D	4/6 (67%)	4 (100%)	0	0	100	100
2	F	4/6 (67%)	4 (100%)	0	0	100	100
2	K	4/6 (67%)	3 (75%)	1 (25%)	0	100	100
All	All	1372/1568 (88%)	1330 (97%)	42 (3%)	0	100	100

There are no Ramachandran outliers to report.

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	317/356 (89%)	306 (96%)	11 (4%)	32	62
1	C	317/356 (89%)	302 (95%)	15 (5%)	23	55
1	E	317/356 (89%)	304 (96%)	13 (4%)	27	59
1	G	317/356 (89%)	298 (94%)	19 (6%)	17	47
2	B	3/3 (100%)	2 (67%)	1 (33%)	0	0
2	D	3/3 (100%)	2 (67%)	1 (33%)	0	0
2	F	3/3 (100%)	2 (67%)	1 (33%)	0	0
2	K	3/3 (100%)	3 (100%)	0	100	100
All	All	1280/1436 (89%)	1219 (95%)	61 (5%)	23	54

All (61) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	51	ILE
1	A	54	ILE
1	A	85	LEU
1	A	113	LYS
1	A	151	ILE
1	A	175	LYS
1	A	221	ILE
1	A	231	VAL
1	A	250	LYS
1	A	382	LYS
1	A	384	ILE
2	B	2	VAL
1	C	51	ILE
1	C	68	GLU
1	C	69	ASN
1	C	131	ASP
1	C	142	TYR
1	C	144	ILE
1	C	154	LYS
1	C	168	SER
1	C	190	LYS
1	C	258	GLU
1	C	259	ILE
1	C	272	ARG
1	C	284	GLU
1	C	380	LEU
1	C	382	LYS
2	D	2	VAL
1	E	51	ILE
1	E	62	GLN
1	E	131	ASP
1	E	134	GLU
1	E	154	LYS
1	E	173	LEU
1	E	193	GLU
1	E	211	GLU
1	E	215	LYS
1	E	227	LYS
1	E	242	ILE
1	E	244	SER
1	E	299	GLN
2	F	3	VAL
1	G	54	ILE

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Mol	Chain	Res	Type
1	G	73	LEU
1	G	74	LEU
1	G	79	LYS
1	G	106	ILE
1	G	110	LEU
1	G	117	LYS
1	G	132	VAL
1	G	134	GLU
1	G	136	SER
1	G	137	LYS
1	G	173	LEU
1	G	182	ILE
1	G	196	ILE
1	G	261	LYS
1	G	297	ASP
1	G	309	LYS
1	G	328	GLU
1	G	354	TYR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (17) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	91	ASN
1	A	282	ASN
1	A	289	ASN
1	A	299	GLN
1	A	326	GLN
1	A	343	ASN
1	C	150	ASN
1	C	326	GLN
1	C	377	ASN
1	E	58	HIS
1	E	62	GLN
1	E	326	GLN
1	G	49	ASN
1	G	279	ASN
1	G	289	ASN
1	G	299	GLN
1	G	329	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides 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, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q < 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	341/386 (88%)	0.15	8 (2%) 61 39	38, 72, 122, 167	0
1	C	341/386 (88%)	0.11	5 (1%) 72 52	38, 72, 119, 154	0
1	E	341/386 (88%)	0.20	5 (1%) 72 52	36, 77, 117, 153	0
1	G	341/386 (88%)	0.40	14 (4%) 41 23	48, 86, 132, 157	0
2	B	6/6 (100%)	0.43	0 100 100	44, 62, 74, 101	0
2	D	6/6 (100%)	0.89	1 (16%) 4 2	42, 61, 81, 118	0
2	F	6/6 (100%)	0.75	1 (16%) 4 2	47, 51, 71, 73	0
2	K	6/6 (100%)	1.07	1 (16%) 4 2	45, 59, 75, 156	0
All	All	1388/1568 (88%)	0.23	35 (2%) 58 37	36, 77, 123, 167	0

All (35) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	G	256	GLY	6.9
1	G	260	ALA	4.7
1	G	255	SER	4.4
1	E	258	GLU	4.1
1	A	89	ASP	3.9
1	A	105	SER	3.7
1	A	85	LEU	3.6
1	E	46	SER	3.6
2	K	6	ALA	3.4
1	A	119	TYR	3.4
1	G	148	GLU	3.1
1	G	332	GLY	3.1
1	C	341	ILE	3.0
1	G	259	ILE	2.9
1	C	57	THR	2.8
1	C	257	TYR	2.8

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Mol	Chain	Res	Type	RSRZ
1	G	59	TYR	2.8
1	E	245	ASP	2.7
1	C	287	TRP	2.6
1	A	258	GLU	2.5
1	E	119	TYR	2.5
1	G	257	TYR	2.3
1	G	227	LYS	2.3
1	C	85	LEU	2.3
2	D	1	GLY	2.3
1	A	112	SER	2.3
1	G	329	ASN	2.2
1	E	61	ASP	2.2
1	G	278	ASN	2.1
1	A	341	ILE	2.1
1	G	253	TYR	2.1
1	A	134	GLU	2.1
2	F	6	ALA	2.0
1	G	243	PHE	2.0
1	G	254	LEU	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 oligosaccharides 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.