Full wwPDB X-ray Structure Validation Report ⓘ

May 22, 2020 – 12:40 am BST

PDB ID	:	6HP3
Title	:	ARBITRIUM PEPTIDE RECEPTOR FROM SPBETA PHAGE
Authors	:	Marina, A.; Gallego del Sol, F.
Deposited on	:	2018-09-19
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 ⓘ symbol.

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

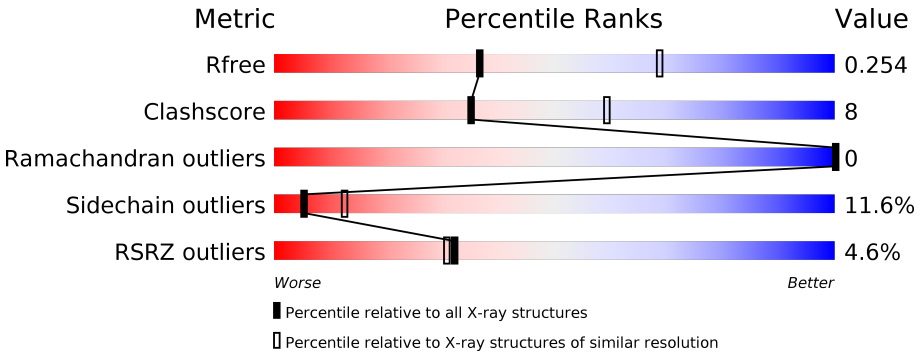
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.11
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, 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	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
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
1	A	386	79% 14% 6%
1	B	386	3% 76% 17% 5%
1	C	386	77% 16% 6%
1	D	386	3% 74% 19% 5%
1	E	386	3% 75% 18% 7%
1	F	386	4% 75% 19% 6%

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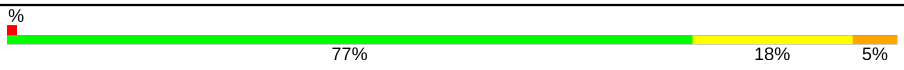
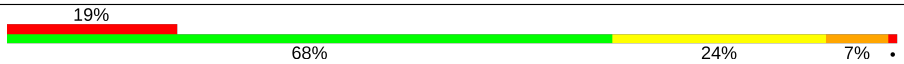
Mol	Chain	Length	Quality of chain
1	G	386	
1	H	386	

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 25680 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 SPBc2 prophage-derived uncharacterized protein YopK.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	386	Total	C	N	O	S	Se	0	0	0
			3183	2031	528	603	6	15			
1	B	386	Total	C	N	O	S	Se	0	0	0
			3183	2031	528	603	6	15			
1	C	386	Total	C	N	O	S	Se	0	0	0
			3183	2031	528	603	6	15			
1	D	386	Total	C	N	O	S	Se	0	0	0
			3183	2031	528	603	6	15			
1	E	386	Total	C	N	O	S	Se	0	1	0
			3188	2035	528	603	6	16			
1	F	386	Total	C	N	O	S	Se	0	0	0
			3183	2031	528	603	6	15			
1	G	386	Total	C	N	O	S	Se	0	0	0
			3183	2031	528	603	6	15			
1	H	386	Total	C	N	O	S	Se	0	0	0
			3183	2031	528	603	6	15			

- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	44	Total	O	0	0
			44	44		
2	B	27	Total	O	0	0
			27	27		
2	C	36	Total	O	0	0
			36	36		
2	D	29	Total	O	0	0
			29	29		
2	E	20	Total	O	0	0
			20	20		
2	F	21	Total	O	0	0
			21	21		

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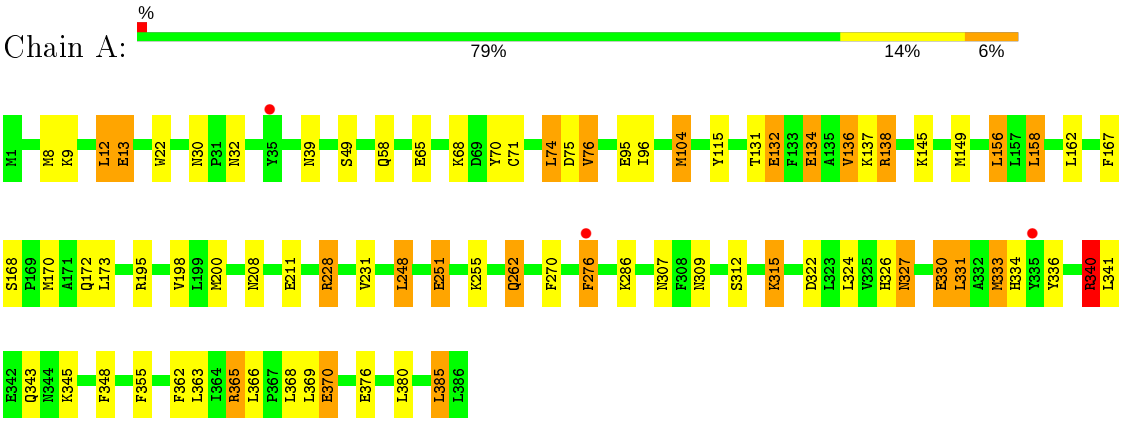
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	G	28	Total O 28 28	0	0
2	H	6	Total O 6 6	0	0

3 Residue-property plots (i)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of 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.

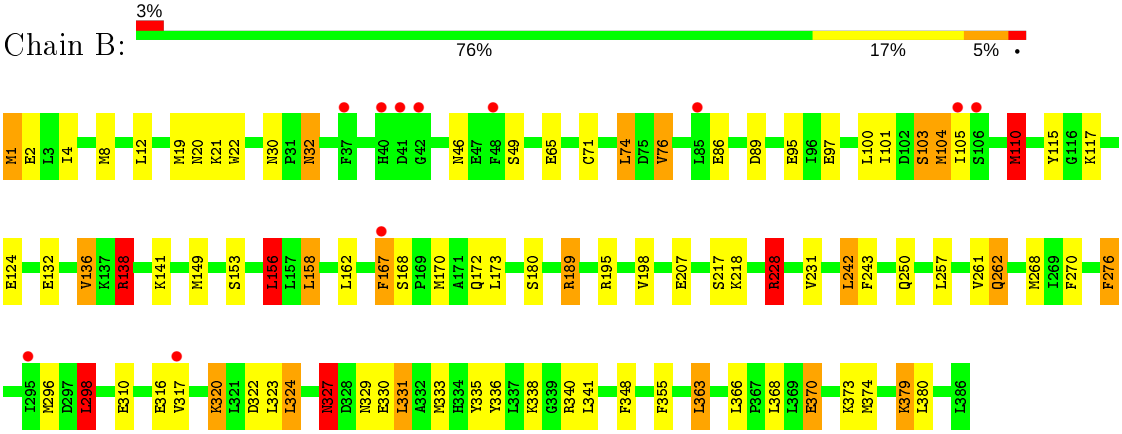
- Molecule 1: SPBc2 prophage-derived uncharacterized protein YopK

Chain A:



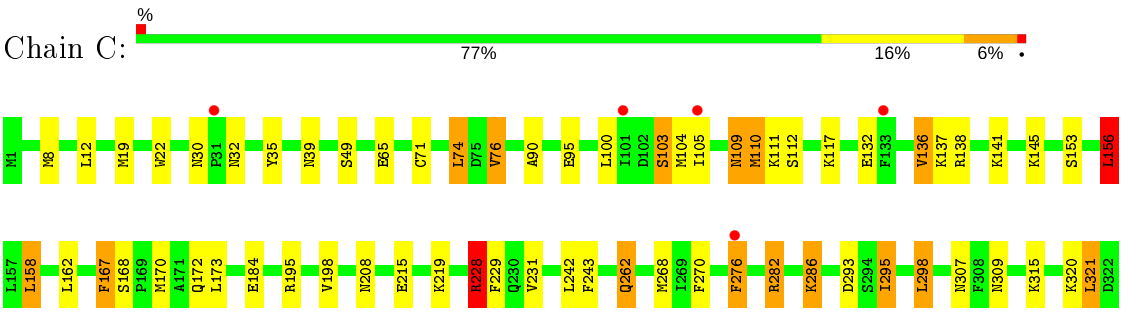
- Molecule 1: SPBc2 prophage-derived uncharacterized protein YopK

Chain B:



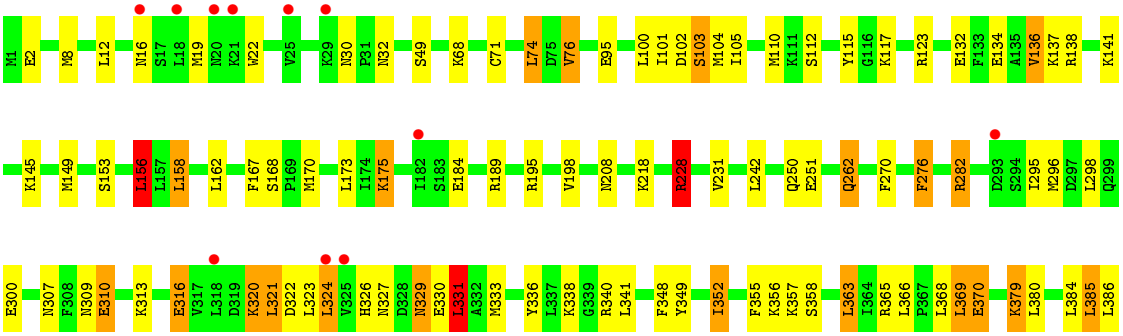
- Molecule 1: SPBc2 prophage-derived uncharacterized protein YopK

Chain C:



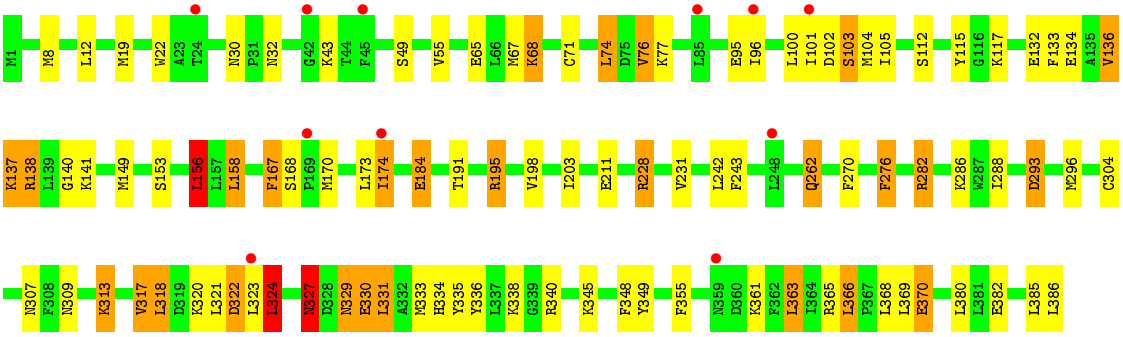
• Molecule 1: SPBc2 prophage-derived uncharacterized protein YopK

Chain D:



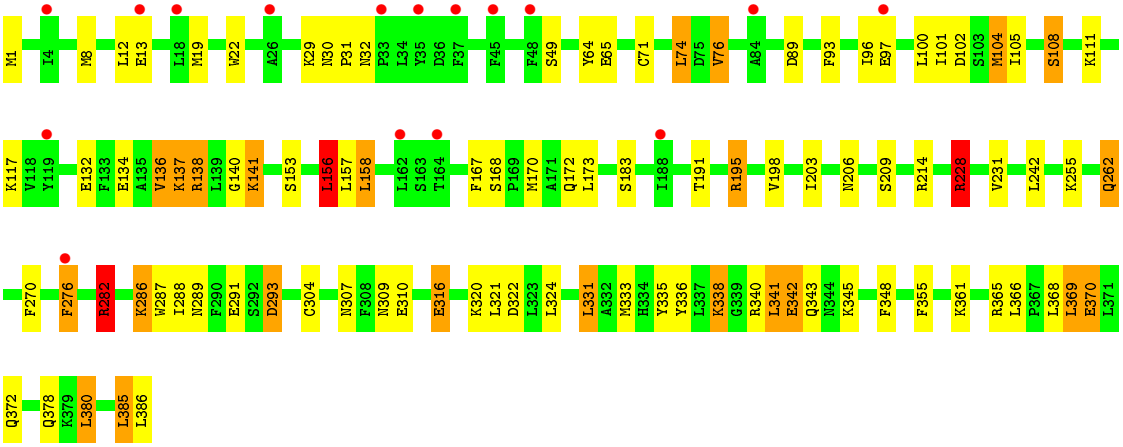
• Molecule 1: SPBc2 prophage-derived uncharacterized protein YopK

Chain E:



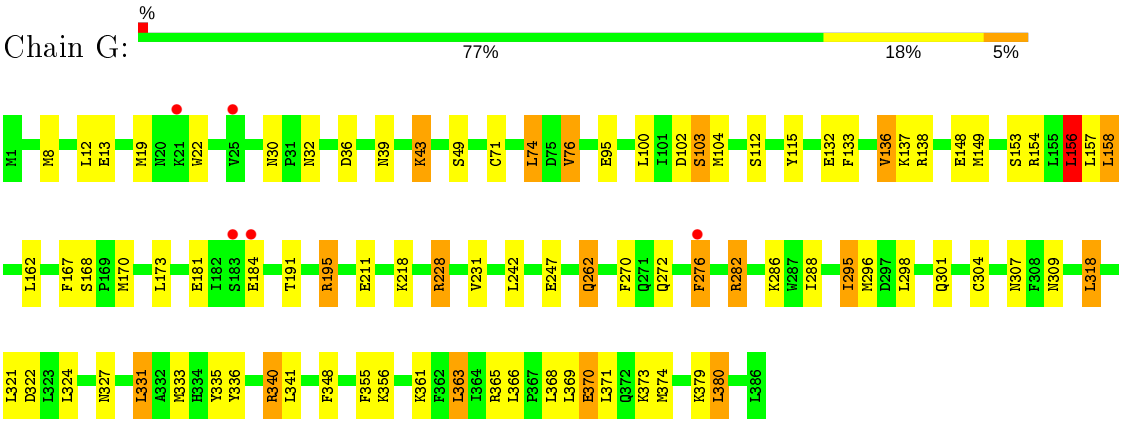
• Molecule 1: SPBc2 prophage-derived uncharacterized protein YopK

Chain F:



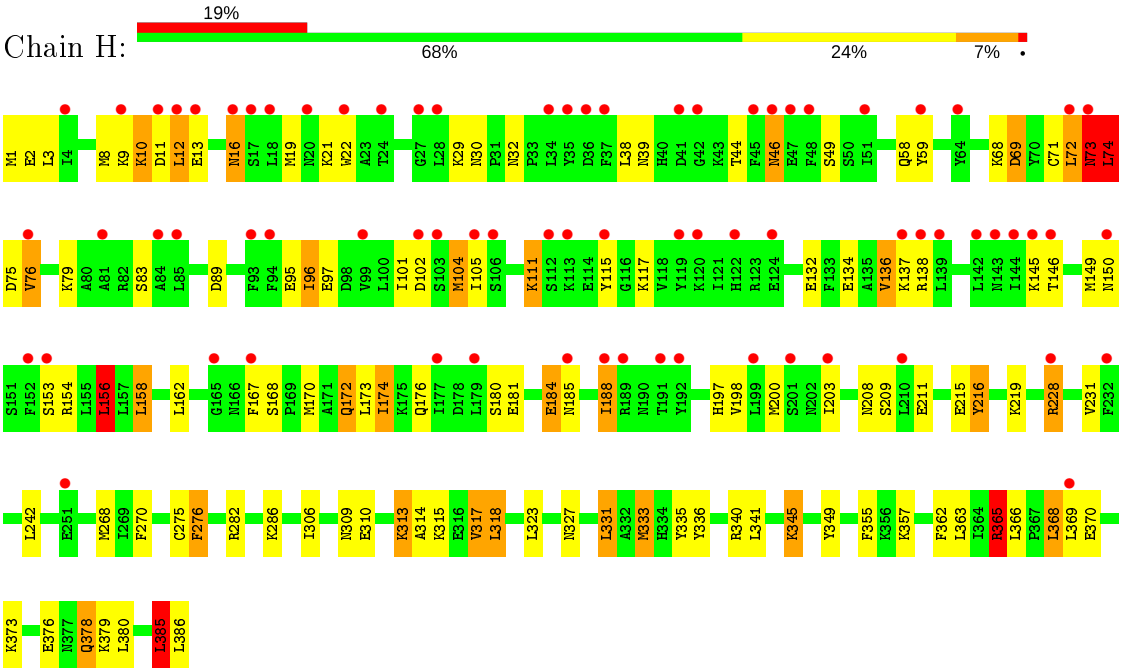
• Molecule 1: SPBc2 prophage-derived uncharacterized protein YopK

Chain G:



• Molecule 1: SPBc2 prophage-derived uncharacterized protein YopK

Chain H:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	78.91Å 251.20Å 95.08Å 90.00° 90.89° 90.00°	Depositor
Resolution (Å)	125.60 – 2.70 95.07 – 2.70	Depositor EDS
% Data completeness (in resolution range)	99.9 (125.60-2.70) 99.9 (95.07-2.70)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.63 (at 2.69Å)	Xtriage
Refinement program	REFMAC 5.8.0158	Depositor
R, R_{free}	0.219 , 0.250 0.226 , 0.254	Depositor DCC
R_{free} test set	4902 reflections (4.85%)	wwPDB-VP
Wilson B-factor (Å^2)	53.1	Xtriage
Anisotropy	0.600	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.33 , 39.3	EDS
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	0.028 for h,-k,-l	Xtriage
F_o,F_c correlation	0.93	EDS
Total number of atoms	25680	wwPDB-VP
Average B, all atoms (Å^2)	65.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.38% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ 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	0.93	6/3226 (0.2%)	1.07	18/4315 (0.4%)
1	B	0.89	5/3226 (0.2%)	1.08	22/4315 (0.5%)
1	C	0.88	2/3226 (0.1%)	1.11	26/4315 (0.6%)
1	D	0.90	4/3226 (0.1%)	1.08	22/4315 (0.5%)
1	E	0.92	4/3234 (0.1%)	1.12	22/4325 (0.5%)
1	F	0.86	3/3226 (0.1%)	1.07	22/4315 (0.5%)
1	G	0.90	2/3226 (0.1%)	1.11	22/4315 (0.5%)
1	H	0.99	8/3226 (0.2%)	1.15	28/4315 (0.6%)
All	All	0.91	34/25816 (0.1%)	1.10	182/34530 (0.5%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	E	0	1
1	H	0	1
All	All	0	2

All (34) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	35	TYR	CG-CD1	8.72	1.50	1.39
1	H	13	GLU	CD-OE2	8.27	1.34	1.25
1	E	276	PHE	CG-CD1	7.69	1.50	1.38
1	H	16	ASN	CG-ND2	7.40	1.51	1.32
1	H	276	PHE	CG-CD1	7.31	1.49	1.38
1	C	276	PHE	CG-CD1	7.28	1.49	1.38
1	B	276	PHE	CG-CD1	7.16	1.49	1.38
1	A	276	PHE	CG-CD1	6.97	1.49	1.38
1	F	276	PHE	CG-CD1	6.90	1.49	1.38
1	D	276	PHE	CG-CD1	6.85	1.49	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	H	315	LYS	CE-NZ	6.66	1.65	1.49
1	F	13	GLU	CD-OE1	6.64	1.32	1.25
1	H	275	CYS	CB-SG	-6.51	1.71	1.82
1	F	108	SER	CB-OG	-6.40	1.33	1.42
1	E	184	GLU	CG-CD	6.12	1.61	1.51
1	E	382	GLU	CD-OE1	6.12	1.32	1.25
1	B	2	GLU	CD-OE1	5.93	1.32	1.25
1	A	251	GLU	CG-CD	-5.83	1.43	1.51
1	D	251	GLU	CG-CD	5.79	1.60	1.51
1	G	181	GLU	CG-CD	5.79	1.60	1.51
1	B	320	LYS	CD-CE	5.70	1.65	1.51
1	A	132	GLU	CD-OE1	5.70	1.31	1.25
1	A	330	GLU	CD-OE2	-5.68	1.19	1.25
1	B	340	ARG	CZ-NH2	-5.50	1.25	1.33
1	D	276	PHE	CB-CG	5.38	1.60	1.51
1	H	29	LYS	CE-NZ	5.36	1.62	1.49
1	H	362	PHE	CG-CD1	5.27	1.46	1.38
1	B	207	GLU	CD-OE1	5.25	1.31	1.25
1	E	330	GLU	CD-OE1	5.25	1.31	1.25
1	D	251	GLU	CD-OE1	5.24	1.31	1.25
1	G	276	PHE	CG-CD1	5.24	1.46	1.38
1	H	215	GLU	CD-OE2	5.09	1.31	1.25
1	A	251	GLU	CD-OE1	-5.08	1.20	1.25
1	A	362	PHE	CG-CD1	5.05	1.46	1.38

All (182) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	G	228	ARG	NE-CZ-NH2	-11.86	114.37	120.30
1	E	102	ASP	CB-CG-OD2	-11.52	107.94	118.30
1	G	340	ARG	NE-CZ-NH2	11.10	125.85	120.30
1	E	321	LEU	CB-CG-CD2	10.11	128.19	111.00
1	H	156	LEU	CA-CB-CG	10.11	138.55	115.30
1	C	156	LEU	CA-CB-CG	10.10	138.53	115.30
1	D	156	LEU	CA-CB-CG	10.06	138.45	115.30
1	C	323	LEU	CB-CG-CD2	-10.03	93.95	111.00
1	F	156	LEU	CA-CB-CG	9.96	138.21	115.30
1	G	156	LEU	CA-CB-CG	9.91	138.09	115.30
1	B	156	LEU	CA-CB-CG	9.86	137.98	115.30
1	E	156	LEU	CA-CB-CG	9.78	137.80	115.30
1	G	286	LYS	CD-CE-NZ	-9.53	89.79	111.70
1	H	11	ASP	CB-CG-OD2	9.13	126.52	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	340	ARG	NE-CZ-NH2	8.87	124.74	120.30
1	D	324	LEU	CA-CB-CG	8.79	135.51	115.30
1	F	385	LEU	CA-CB-CG	8.73	135.37	115.30
1	C	323	LEU	CA-CB-CG	8.60	135.09	115.30
1	A	228	ARG	NE-CZ-NH2	8.29	124.44	120.30
1	C	228	ARG	NE-CZ-NH2	8.24	124.42	120.30
1	C	242	LEU	CB-CG-CD2	-8.19	97.08	111.00
1	C	35	TYR	CB-CG-CD2	-8.19	116.09	121.00
1	B	298	LEU	CB-CG-CD1	8.17	124.89	111.00
1	G	195	ARG	NE-CZ-NH2	-8.17	116.22	120.30
1	D	320	LYS	CB-CA-C	8.07	126.55	110.40
1	A	331	LEU	CB-CG-CD1	7.99	124.59	111.00
1	G	301	GLN	CB-CA-C	7.95	126.31	110.40
1	A	12	LEU	CB-CG-CD2	7.89	124.41	111.00
1	A	385	LEU	CB-CG-CD2	-7.86	97.64	111.00
1	H	12	LEU	CB-CG-CD2	7.83	124.30	111.00
1	E	365	ARG	NE-CZ-NH1	-7.77	116.41	120.30
1	D	123	ARG	NE-CZ-NH1	-7.64	116.48	120.30
1	H	373	LYS	CD-CE-NZ	-7.62	94.16	111.70
1	C	286	LYS	CD-CE-NZ	-7.59	94.24	111.70
1	H	74	LEU	CB-CG-CD2	7.58	123.88	111.00
1	D	321	LEU	CA-CB-CG	7.54	132.63	115.30
1	C	35	TYR	CB-CG-CD1	7.52	125.51	121.00
1	H	72	LEU	CB-CG-CD1	7.43	123.63	111.00
1	B	323	LEU	CA-CB-CG	7.14	131.73	115.30
1	B	228	ARG	NE-CZ-NH2	-7.11	116.75	120.30
1	E	102	ASP	CB-CG-OD1	7.08	124.67	118.30
1	H	216	TYR	CB-CG-CD1	7.05	125.23	121.00
1	G	365	ARG	NE-CZ-NH2	-7.04	116.78	120.30
1	E	324	LEU	CB-CG-CD2	-6.92	99.23	111.00
1	B	340	ARG	CG-CD-NE	6.91	126.31	111.80
1	E	345	LYS	CD-CE-NZ	6.89	127.54	111.70
1	D	320	LYS	CA-CB-CG	6.87	128.51	113.40
1	F	255	LYS	CD-CE-NZ	6.78	127.28	111.70
1	E	327	ASN	CB-CA-C	-6.77	96.86	110.40
1	H	216	TYR	CB-CG-CD2	-6.77	116.94	121.00
1	D	323	LEU	CA-CB-CG	6.66	130.61	115.30
1	H	323	LEU	CA-CB-CG	6.64	130.56	115.30
1	G	157	LEU	CA-CB-CG	6.63	130.56	115.30
1	G	361	LYS	CD-CE-NZ	-6.62	96.48	111.70
1	H	365	ARG	NE-CZ-NH1	6.60	123.60	120.30
1	C	321	LEU	CA-CB-CG	6.59	130.45	115.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	E	195	ARG	NE-CZ-NH2	-6.58	117.01	120.30
1	D	189	ARG	NE-CZ-NH1	6.54	123.57	120.30
1	H	73	ASN	N-CA-CB	6.49	122.28	110.60
1	H	1	MSE	CG-SE-CE	6.47	113.14	98.90
1	B	1	MSE	CG-SE-CE	6.42	113.03	98.90
1	H	69	ASP	CB-CG-OD1	6.39	124.05	118.30
1	B	374	MSE	CG-SE-CE	6.36	112.90	98.90
1	E	296	MSE	CA-CB-CG	6.31	124.03	113.30
1	A	255	LYS	CD-CE-NZ	6.29	126.18	111.70
1	D	331	LEU	CB-CG-CD1	6.29	121.70	111.00
1	G	181	GLU	OE1-CD-OE2	-6.28	115.76	123.30
1	D	195	ARG	NE-CZ-NH2	-6.27	117.16	120.30
1	H	268	MSE	CG-SE-CE	6.26	112.68	98.90
1	F	341	LEU	CB-CG-CD2	6.26	121.64	111.00
1	F	195	ARG	NE-CZ-NH2	-6.23	117.19	120.30
1	B	110	MSE	CB-CA-C	-6.19	98.03	110.40
1	C	363	LEU	CB-CG-CD1	6.18	121.50	111.00
1	A	322	ASP	CB-CA-C	6.15	122.69	110.40
1	E	318	LEU	CB-CG-CD1	6.13	121.43	111.00
1	C	167	PHE	CB-CG-CD1	6.09	125.06	120.80
1	A	333	MSE	CG-SE-CE	-6.09	85.51	98.90
1	A	156	LEU	CA-CB-CG	6.08	129.28	115.30
1	C	293	ASP	CB-CG-OD1	6.05	123.75	118.30
1	F	214	ARG	NE-CZ-NH2	-6.03	117.28	120.30
1	D	322	ASP	CB-CA-C	6.03	122.45	110.40
1	D	228	ARG	NE-CZ-NH1	5.96	123.28	120.30
1	E	324	LEU	CB-CG-CD1	5.93	121.09	111.00
1	A	365	ARG	NE-CZ-NH2	-5.92	117.34	120.30
1	H	134	GLU	CA-CB-CG	5.90	126.38	113.40
1	B	268	MSE	CG-SE-CE	5.89	111.87	98.90
1	E	174	ILE	CG1-CB-CG2	5.89	124.37	111.40
1	H	211	GLU	OE1-CD-OE2	-5.89	116.23	123.30
1	C	195	ARG	NE-CZ-NH2	-5.88	117.36	120.30
1	F	316	GLU	CA-CB-CG	5.86	126.29	113.40
1	A	251	GLU	CG-CD-OE1	-5.86	106.59	118.30
1	A	138	ARG	CD-NE-CZ	5.82	131.74	123.60
1	D	369	LEU	CB-CG-CD1	5.81	120.88	111.00
1	F	157	LEU	CA-CB-CG	5.81	128.66	115.30
1	H	386	LEU	CB-CG-CD1	-5.78	101.18	111.00
1	F	228	ARG	NE-CZ-NH2	-5.76	117.42	120.30
1	A	75	ASP	CB-CG-OD1	5.75	123.47	118.30
1	B	195	ARG	NE-CZ-NH2	-5.74	117.43	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	F	340	ARG	CA-CB-CG	-5.73	100.79	113.40
1	B	322	ASP	CB-CA-C	5.72	121.83	110.40
1	H	242	LEU	CB-CG-CD2	-5.70	101.31	111.00
1	B	195	ARG	NE-CZ-NH1	5.68	123.14	120.30
1	D	195	ARG	NE-CZ-NH1	5.68	123.14	120.30
1	C	365	ARG	NE-CZ-NH1	5.66	123.13	120.30
1	D	316	GLU	CA-CB-CG	5.65	125.83	113.40
1	B	327	ASN	N-CA-CB	-5.63	100.46	110.60
1	H	365	ARG	NE-CZ-NH2	-5.60	117.50	120.30
1	G	154	ARG	NE-CZ-NH2	-5.58	117.51	120.30
1	D	100	LEU	CB-CG-CD2	5.57	120.47	111.00
1	B	138	ARG	CG-CD-NE	5.56	123.47	111.80
1	F	29	LYS	CD-CE-NZ	-5.56	98.91	111.70
1	F	293	ASP	CB-CG-OD1	5.56	123.30	118.30
1	C	111	LYS	CD-CE-NZ	-5.56	98.92	111.70
1	F	157	LEU	CB-CG-CD2	-5.54	101.59	111.00
1	E	363	LEU	CB-CG-CD1	5.53	120.40	111.00
1	C	315	LYS	CD-CE-NZ	-5.51	99.02	111.70
1	F	345	LYS	CD-CE-NZ	5.51	124.37	111.70
1	G	322	ASP	CB-CG-OD1	5.50	123.25	118.30
1	A	138	ARG	CG-CD-NE	5.50	123.35	111.80
1	C	110	MSE	CA-CB-CG	5.50	122.64	113.30
1	H	282	ARG	NE-CZ-NH1	5.48	123.04	120.30
1	G	363	LEU	CB-CG-CD1	5.45	120.26	111.00
1	H	188	ILE	CB-CG1-CD1	5.45	129.16	113.90
1	E	138	ARG	NE-CZ-NH2	-5.44	117.58	120.30
1	H	385	LEU	CA-CB-CG	5.44	127.81	115.30
1	F	322	ASP	CB-CA-C	5.41	121.23	110.40
1	D	385	LEU	CA-CB-CG	5.41	127.75	115.30
1	F	369	LEU	CB-CG-CD1	5.41	120.20	111.00
1	H	10	LYS	CB-CA-C	5.41	121.22	110.40
1	A	340	ARG	CA-CB-CG	-5.41	101.51	113.40
1	F	322	ASP	N-CA-CB	5.40	120.32	110.60
1	B	363	LEU	CB-CG-CD1	5.39	120.17	111.00
1	E	293	ASP	N-CA-CB	5.39	120.31	110.60
1	C	386	LEU	CB-CG-CD1	-5.39	101.84	111.00
1	C	215	GLU	CG-CD-OE1	5.33	128.96	118.30
1	G	295	ILE	CG1-CB-CG2	5.32	123.09	111.40
1	G	340	ARG	NH1-CZ-NH2	-5.31	113.56	119.40
1	B	110	MSE	N-CA-CB	-5.31	101.04	110.60
1	B	316	GLU	CA-CB-CG	5.29	125.05	113.40
1	D	300	GLU	OE1-CD-OE2	-5.29	116.96	123.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	G	148	GLU	CG-CD-OE2	5.28	128.86	118.30
1	E	369	LEU	CB-CG-CD2	5.28	119.97	111.00
1	G	282	ARG	NE-CZ-NH1	5.27	122.94	120.30
1	C	333	MSE	CG-SE-CE	-5.27	87.31	98.90
1	G	318	LEU	CB-CG-CD1	5.27	119.95	111.00
1	B	324	LEU	CB-CG-CD1	5.26	119.94	111.00
1	H	333	MSE	CG-SE-CE	-5.26	87.33	98.90
1	F	138	ARG	NE-CZ-NH2	-5.26	117.67	120.30
1	H	75	ASP	CB-CG-OD1	5.25	123.03	118.30
1	D	184	GLU	CB-CG-CD	-5.24	100.05	114.20
1	H	228	ARG	NE-CZ-NH2	-5.24	117.68	120.30
1	G	373	LYS	CD-CE-NZ	-5.24	99.66	111.70
1	H	313	LYS	CD-CE-NZ	-5.24	99.66	111.70
1	E	100	LEU	CB-CG-CD2	5.21	119.85	111.00
1	D	357	LYS	CD-CE-NZ	5.20	123.66	111.70
1	B	327	ASN	CB-CA-C	-5.20	100.01	110.40
1	E	228	ARG	NE-CZ-NH2	-5.19	117.70	120.30
1	F	1	MSE	CA-CB-CG	5.18	122.11	113.30
1	F	293	ASP	N-CA-CB	5.18	119.93	110.60
1	A	200	MSE	CG-SE-CE	5.17	110.28	98.90
1	E	330	GLU	CG-CD-OE1	5.17	128.64	118.30
1	H	340	ARG	NE-CZ-NH2	5.17	122.88	120.30
1	C	383	LEU	CB-CG-CD2	5.16	119.78	111.00
1	G	369	LEU	CB-CG-CD1	5.16	119.78	111.00
1	G	195	ARG	NE-CZ-NH1	5.15	122.87	120.30
1	C	293	ASP	CB-CG-OD2	-5.14	113.67	118.30
1	E	228	ARG	NE-CZ-NH1	5.14	122.87	120.30
1	A	195	ARG	NE-CZ-NH2	-5.12	117.74	120.30
1	C	195	ARG	NE-CZ-NH1	5.12	122.86	120.30
1	C	219	LYS	CD-CE-NZ	-5.12	99.94	111.70
1	A	13	GLU	CA-CB-CG	5.11	124.64	113.40
1	F	365	ARG	CD-NE-CZ	-5.11	116.45	123.60
1	E	322	ASP	CB-CA-C	-5.10	100.20	110.40
1	B	110	MSE	CA-CB-CG	5.09	121.95	113.30
1	B	167	PHE	CB-CG-CD1	5.09	124.36	120.80
1	B	340	ARG	NE-CZ-NH1	-5.07	117.77	120.30
1	C	295	ILE	CA-CB-CG1	5.07	120.63	111.00
1	D	363	LEU	CB-CG-CD1	5.06	119.61	111.00
1	F	282	ARG	NE-CZ-NH2	-5.03	117.79	120.30
1	G	43	LYS	CA-CB-CG	5.02	124.45	113.40
1	C	328	ASP	CB-CG-OD2	-5.02	113.78	118.30
1	D	175	LYS	CA-CB-CG	5.00	124.41	113.40

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	E	167	PHE	Sidechain
1	H	16	ASN	Sidechain

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3183	0	3179	51	0
1	B	3183	0	3179	44	1
1	C	3183	0	3179	41	0
1	D	3183	0	3179	48	0
1	E	3188	0	3188	62	0
1	F	3183	0	3179	54	0
1	G	3183	0	3179	47	0
1	H	3183	0	3179	90	1
2	A	44	0	0	3	0
2	B	27	0	0	2	0
2	C	36	0	0	1	0
2	D	29	0	0	2	0
2	E	20	0	0	1	0
2	F	21	0	0	2	0
2	G	28	0	0	0	0
2	H	6	0	0	0	0
All	All	25680	0	25441	416	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 8.

All (416) 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:H:170:MSE:O	1:H:174:ILE:HD11	1.40	1.21
1:A:167:PHE:HA	1:A:170:MSE:HE3	1.31	1.12
1:F:372:GLN:HE21	1:F:378:GLN:HG2	1.10	1.11

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:170:MSE:O	1:H:174:ILE:CD1	2.00	1.08
1:H:167:PHE:HA	1:H:170:MSE:HE3	1.34	1.06
1:D:167:PHE:HA	1:D:170:MSE:HE3	1.33	1.06
1:B:167:PHE:HA	1:B:170:MSE:HE3	1.33	1.06
1:C:167:PHE:HA	1:C:170:MSE:HE3	1.33	1.05
1:G:167:PHE:HA	1:G:170:MSE:HE3	1.32	1.05
1:H:172:GLN:HA	1:H:172:GLN:OE1	1.54	1.05
1:A:68:LYS:HG3	1:A:96:ILE:HD11	1.07	1.04
1:G:298:LEU:HB3	1:G:321:LEU:HD11	1.51	0.93
1:A:68:LYS:HG3	1:A:96:ILE:CD1	1.99	0.90
1:E:68:LYS:CG	1:E:96:ILE:HD11	2.00	0.90
1:A:68:LYS:CG	1:A:96:ILE:HD11	2.00	0.90
1:H:174:ILE:H	1:H:174:ILE:HD13	1.34	0.89
1:D:310:GLU:HG2	1:D:313:LYS:HD3	1.52	0.88
1:A:251:GLU:OE1	1:D:250:GLN:NE2	2.07	0.88
1:H:174:ILE:HG13	1:H:203:ILE:HD13	1.55	0.88
1:E:68:LYS:HG3	1:E:96:ILE:HD11	1.53	0.88
1:A:172:GLN:NE2	1:B:132:GLU:OE1	2.07	0.88
1:H:174:ILE:N	1:H:174:ILE:HD13	1.87	0.87
1:H:306:ILE:HD11	1:H:314:ALA:HB1	1.57	0.87
1:D:327:ASN:OD1	1:D:330:GLU:HG3	1.76	0.84
1:G:371:LEU:HD23	1:G:374:MSE:HE3	1.59	0.84
1:F:372:GLN:NE2	1:F:378:GLN:HG2	1.92	0.84
1:F:93:PHE:HB3	1:F:96:ILE:CD1	2.10	0.81
1:B:257:LEU:O	1:B:261:VAL:HG22	1.81	0.81
1:E:67:MSE:HE2	1:E:67:MSE:HA	1.61	0.81
1:F:93:PHE:HB3	1:F:96:ILE:HD13	1.61	0.81
1:H:174:ILE:HG13	1:H:203:ILE:CD1	2.11	0.81
1:D:282:ARG:NH2	1:D:340:ARG:NH2	2.28	0.80
1:F:372:GLN:HE21	1:F:378:GLN:CG	1.94	0.80
1:A:333:MSE:HE1	1:A:366:LEU:HD12	1.64	0.79
1:H:3:LEU:HG	1:H:69:ASP:OD2	1.82	0.79
1:H:158:LEU:HD13	1:H:173:LEU:HD23	1.65	0.79
1:A:307:ASN:OD1	1:A:340:ARG:NH2	2.16	0.78
1:F:333:MSE:HE1	1:F:366:LEU:HD12	1.65	0.78
1:H:306:ILE:HD11	1:H:314:ALA:CB	2.14	0.78
1:H:306:ILE:CD1	1:H:314:ALA:CB	2.63	0.77
1:H:200:MSE:HB3	1:H:216:TYR:CD2	2.19	0.77
1:C:383:LEU:HD13	1:D:352:ILE:HG12	1.68	0.76
1:H:96:ILE:HD12	1:H:96:ILE:N	2.00	0.76
1:E:55:VAL:HG21	1:E:67:MSE:HE3	1.68	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:298:LEU:CB	1:G:321:LEU:HD11	2.16	0.76
1:E:137:LYS:HG2	1:F:140:GLY:HA2	1.68	0.76
1:G:307:ASN:OD1	1:G:340:ARG:NH2	2.19	0.76
1:G:371:LEU:HD23	1:G:374:MSE:CE	2.16	0.76
1:C:333:MSE:HE1	1:C:366:LEU:HD23	1.69	0.74
1:B:298:LEU:HD23	1:B:317:VAL:HG13	1.70	0.74
1:G:333:MSE:HE1	1:G:366:LEU:HD12	1.68	0.73
1:H:2:GLU:CG	1:H:73:ASN:HD21	2.02	0.73
1:B:333:MSE:HE1	1:B:366:LEU:HD12	1.71	0.73
1:H:158:LEU:HD11	1:H:174:ILE:CD1	2.19	0.73
1:G:348:PHE:HD2	1:G:374:MSE:HE1	1.53	0.73
1:A:208:ASN:HD21	1:A:365:ARG:HH22	1.37	0.72
1:A:13:GLU:HB2	1:E:324:LEU:HG	1.69	0.72
1:H:83:SER:HA	1:H:188:ILE:HD11	1.70	0.72
1:C:172:GLN:NE2	1:D:132:GLU:OE1	2.23	0.71
1:A:208:ASN:HD21	1:A:365:ARG:NH2	1.89	0.71
1:B:327:ASN:CB	1:B:330:GLU:HG3	2.21	0.71
1:C:90:ALA:O	1:C:228:ARG:HG2	1.91	0.71
1:H:170:MSE:C	1:H:174:ILE:HD11	2.11	0.70
1:G:348:PHE:CD2	1:G:374:MSE:HE1	2.25	0.70
1:C:298:LEU:HB3	1:C:321:LEU:HD21	1.74	0.69
1:F:158:LEU:HD13	1:F:173:LEU:HD23	1.74	0.69
1:G:158:LEU:HD13	1:G:173:LEU:HD23	1.75	0.69
1:H:96:ILE:H	1:H:96:ILE:CD1	2.05	0.69
1:B:158:LEU:HD13	1:B:173:LEU:HD23	1.75	0.69
1:D:282:ARG:CZ	1:D:340:ARG:NH2	2.55	0.69
1:E:333:MSE:HE1	1:E:366:LEU:HD23	1.74	0.69
1:C:158:LEU:HD13	1:C:173:LEU:HD23	1.75	0.69
1:E:167:PHE:HD2	1:E:170:MSE:HE2	1.57	0.69
1:H:96:ILE:N	1:H:96:ILE:CD1	2.55	0.69
1:E:158:LEU:HD13	1:E:173:LEU:HD23	1.75	0.68
1:E:327:ASN:HB2	1:E:330:GLU:HG3	1.74	0.68
1:H:333:MSE:HE1	1:H:366:LEU:HD12	1.73	0.68
1:A:158:LEU:HD13	1:A:173:LEU:HD23	1.74	0.68
1:F:167:PHE:HD2	1:F:170:MSE:HE2	1.58	0.67
1:D:282:ARG:NH2	1:D:340:ARG:HH22	1.89	0.67
1:D:158:LEU:HD13	1:D:173:LEU:HD23	1.75	0.67
1:H:306:ILE:HD13	1:H:314:ALA:HB2	1.76	0.67
1:B:257:LEU:O	1:B:261:VAL:CG2	2.42	0.67
1:D:307:ASN:OD1	1:D:340:ARG:NH1	2.27	0.67
1:G:298:LEU:HB3	1:G:321:LEU:CD1	2.25	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:83:SER:HA	1:H:188:ILE:CD1	2.25	0.66
1:B:327:ASN:HB2	1:B:330:GLU:HG3	1.76	0.66
1:D:333:MSE:HE1	1:D:366:LEU:HD12	1.76	0.66
1:H:200:MSE:CB	1:H:216:TYR:CD2	2.79	0.66
1:D:228:ARG:NH1	2:D:401:HOH:O	2.28	0.66
1:A:326:HIS:CB	1:A:331:LEU:HD12	2.26	0.65
1:F:361:LYS:HD3	1:F:386:LEU:HD22	1.78	0.65
1:C:307:ASN:OD1	1:C:340:ARG:NH1	2.29	0.65
1:E:327:ASN:CB	1:E:330:GLU:HG3	2.27	0.65
1:E:170:MSE:HE3	1:E:203:ILE:HG12	1.79	0.65
1:D:329:ASN:ND2	1:D:358:SER:OG	2.30	0.64
1:A:340:ARG:HG2	1:A:340:ARG:NH1	2.11	0.64
1:H:12:LEU:HD11	1:H:19:MSE:HG2	1.80	0.64
1:H:46:ASN:H	1:H:46:ASN:ND2	1.96	0.64
1:A:326:HIS:HB2	1:A:331:LEU:CD1	2.27	0.64
1:H:174:ILE:CD1	1:H:174:ILE:H	1.95	0.63
1:A:30:ASN:OD1	1:A:32:ASN:HB2	1.98	0.63
1:E:243:PHE:HE1	1:E:366:LEU:HD13	1.63	0.63
1:F:289:ASN:OD1	1:F:291:GLU:HG2	1.98	0.63
1:A:340:ARG:HG2	1:A:340:ARG:HH11	1.64	0.63
1:H:306:ILE:CD1	1:H:314:ALA:HB1	2.27	0.62
1:F:167:PHE:HD2	1:F:170:MSE:CE	2.12	0.62
1:H:208:ASN:OD1	1:H:365:ARG:NH2	2.33	0.62
1:A:326:HIS:CB	1:A:331:LEU:CD1	2.77	0.62
1:E:167:PHE:HD2	1:E:170:MSE:CE	2.13	0.62
1:F:19:MSE:CE	1:F:31:PRO:HB3	2.29	0.62
1:F:338:LYS:O	1:F:342:GLU:HG2	1.99	0.62
1:A:39:ASN:ND2	1:E:322:ASP:O	2.33	0.62
1:D:282:ARG:CZ	1:D:340:ARG:HH22	2.10	0.61
1:E:12:LEU:HD11	1:E:19:MSE:HG2	1.82	0.61
1:C:30:ASN:OD1	1:C:32:ASN:HB2	2.00	0.61
1:G:30:ASN:OD1	1:G:32:ASN:HB2	2.01	0.61
1:H:153:SER:HA	1:H:156:LEU:HD13	1.83	0.61
1:D:326:HIS:CB	1:D:331:LEU:HD13	2.30	0.61
1:G:298:LEU:HD23	1:G:321:LEU:HD12	1.81	0.61
1:G:298:LEU:HD23	1:G:321:LEU:CD1	2.30	0.61
1:F:12:LEU:HD11	1:F:19:MSE:HG2	1.82	0.61
1:F:30:ASN:OD1	1:F:32:ASN:HB2	2.01	0.61
1:H:71:CYS:HA	1:H:74:LEU:HD12	1.83	0.61
1:E:167:PHE:CD2	1:E:170:MSE:HE2	2.36	0.61
1:D:30:ASN:OD1	1:D:32:ASN:HB2	2.00	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:153:SER:HA	1:F:156:LEU:HD13	1.83	0.60
1:H:167:PHE:HD1	1:H:170:MSE:CE	2.14	0.60
1:D:12:LEU:HD11	1:D:19:MSE:HG2	1.82	0.60
1:E:30:ASN:OD1	1:E:32:ASN:HB2	2.01	0.60
1:H:333:MSE:HE3	1:H:363:LEU:HD13	1.83	0.60
1:E:153:SER:HA	1:E:156:LEU:HD13	1.82	0.60
1:E:68:LYS:HG2	1:E:96:ILE:HD11	1.83	0.60
1:C:8:MSE:HG2	1:C:22:TRP:CH2	2.36	0.60
1:D:153:SER:HA	1:D:156:LEU:HD13	1.83	0.60
1:A:167:PHE:HD1	1:A:170:MSE:CE	2.15	0.60
1:H:8:MSE:HG2	1:H:22:TRP:CH2	2.37	0.60
1:C:109:ASN:ND2	1:C:112:SER:H	2.00	0.60
1:F:167:PHE:CD2	1:F:170:MSE:HE2	2.36	0.60
1:G:12:LEU:HD11	1:G:19:MSE:HG2	1.84	0.59
1:H:345:LYS:HE3	1:H:376:GLU:OE1	2.02	0.59
1:A:8:MSE:HG2	1:A:22:TRP:CH2	2.37	0.59
1:F:8:MSE:HG2	1:F:22:TRP:CH2	2.37	0.59
1:F:64:TYR:CE1	1:F:96:ILE:HD11	2.37	0.59
1:C:298:LEU:HB3	1:C:321:LEU:CD2	2.32	0.59
1:G:133:PHE:CZ	1:H:181:GLU:OE1	2.55	0.59
1:F:170:MSE:HE3	1:F:203:ILE:HG12	1.83	0.59
1:A:131:THR:OG1	1:A:134:GLU:HG2	2.02	0.59
1:F:333:MSE:HE2	1:F:355:PHE:HZ	1.68	0.59
1:D:333:MSE:HE2	1:D:355:PHE:HZ	1.67	0.59
1:C:167:PHE:HD1	1:C:170:MSE:CE	2.16	0.59
1:G:153:SER:HA	1:G:156:LEU:HD13	1.84	0.59
1:E:327:ASN:HB2	1:E:330:GLU:CG	2.33	0.58
1:B:167:PHE:HD1	1:B:170:MSE:CE	2.16	0.58
1:B:153:SER:HA	1:B:156:LEU:HD13	1.85	0.58
1:G:167:PHE:HD1	1:G:170:MSE:CE	2.16	0.58
1:B:180:SER:HA	1:B:189:ARG:NH2	2.18	0.58
1:C:320:LYS:O	1:C:323:LEU:HG	2.03	0.58
1:H:306:ILE:HD13	1:H:314:ALA:CB	2.32	0.58
1:A:333:MSE:HE1	1:A:366:LEU:CD1	2.32	0.58
1:G:133:PHE:HZ	1:H:181:GLU:OE1	1.87	0.58
1:A:132:GLU:OE1	1:B:172:GLN:NE2	2.37	0.58
1:E:140:GLY:HA2	1:F:137:LYS:HG2	1.86	0.58
1:A:345:LYS:HE2	1:A:376:GLU:OE1	2.03	0.57
1:B:333:MSE:HE2	1:B:355:PHE:HZ	1.69	0.57
1:C:153:SER:HA	1:C:156:LEU:HD13	1.86	0.57
1:G:333:MSE:HE2	1:G:355:PHE:HZ	1.69	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:334:HIS:HD2	2:A:408:HOH:O	1.86	0.57
1:H:200:MSE:HB3	1:H:216:TYR:CE2	2.38	0.57
1:B:8:MSE:HG2	1:B:22:TRP:CH2	2.39	0.57
1:C:377:ASN:HD22	1:C:377:ASN:C	2.07	0.57
1:B:327:ASN:HB3	1:B:330:GLU:HG3	1.86	0.57
1:E:136:VAL:HG22	1:F:136:VAL:HG22	1.86	0.57
1:C:109:ASN:HD22	1:C:112:SER:H	1.50	0.57
1:D:8:MSE:HG2	1:D:22:TRP:CH2	2.38	0.57
1:E:333:MSE:HE2	1:E:355:PHE:HZ	1.70	0.57
1:D:352:ILE:HD11	1:D:384:LEU:HD22	1.86	0.57
1:B:30:ASN:OD1	1:B:32:ASN:HB3	2.05	0.57
1:E:329:ASN:HD22	1:E:330:GLU:N	2.03	0.57
1:B:379:LYS:H	1:B:379:LYS:HE2	1.71	0.56
1:C:331:LEU:HD22	1:C:335:TYR:CE2	2.40	0.56
1:A:333:MSE:HE2	1:A:355:PHE:HZ	1.70	0.56
1:C:228:ARG:HG3	1:C:229:PHE:N	2.20	0.56
1:E:313:LYS:O	1:E:317:VAL:HG12	2.06	0.56
1:H:306:ILE:HD11	1:H:341:LEU:HD13	1.87	0.56
1:B:228:ARG:NH1	2:B:401:HOH:O	2.38	0.55
1:C:208:ASN:OD1	1:C:365:ARG:NH2	2.38	0.55
1:B:12:LEU:HD11	1:B:19:MSE:HG2	1.88	0.55
1:H:306:ILE:CD1	1:H:341:LEU:HD13	2.36	0.55
1:H:58:GLN:CG	1:H:59:TYR:CE1	2.90	0.55
1:B:110:MSE:HA	1:B:110:MSE:HE3	1.88	0.55
1:C:12:LEU:HD11	1:C:19:MSE:HG2	1.88	0.55
1:F:93:PHE:HB3	1:F:96:ILE:HD12	1.86	0.55
1:C:243:PHE:HE1	1:C:366:LEU:HD13	1.72	0.54
1:B:124:GLU:OE1	1:B:138:ARG:NH1	2.39	0.54
1:C:105:ILE:HD12	1:C:117:LYS:HG2	1.90	0.54
1:H:158:LEU:HD11	1:H:174:ILE:HD13	1.89	0.54
1:E:105:ILE:HD12	1:E:117:LYS:HG2	1.89	0.54
1:G:272:GLN:HE21	1:G:296:MSE:HE1	1.73	0.54
1:G:331:LEU:HD22	1:G:335:TYR:CE2	2.42	0.54
1:C:167:PHE:CA	1:C:170:MSE:HE3	2.23	0.54
1:A:167:PHE:HD1	1:A:170:MSE:HE1	1.73	0.53
1:H:162:LEU:HA	1:H:170:MSE:HE1	1.90	0.53
1:E:361:LYS:NZ	1:E:386:LEU:HD22	2.23	0.53
1:D:352:ILE:HD13	1:D:384:LEU:HD13	1.90	0.53
1:E:327:ASN:HB2	1:E:330:GLU:OE1	2.09	0.53
1:F:105:ILE:HD12	1:F:117:LYS:HG2	1.90	0.53
1:E:137:LYS:O	1:F:140:GLY:HA3	2.09	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:58:GLN:HG3	1:H:59:TYR:CE1	2.43	0.53
1:C:162:LEU:HA	1:C:170:MSE:HE1	1.91	0.53
1:C:333:MSE:HE2	1:C:355:PHE:HZ	1.73	0.53
1:H:21:LYS:HB3	1:H:21:LYS:NZ	2.24	0.53
1:B:180:SER:HA	1:B:189:ARG:HH21	1.74	0.52
1:G:167:PHE:HD1	1:G:170:MSE:HE1	1.75	0.52
1:H:172:GLN:OE1	1:H:172:GLN:CA	2.43	0.52
1:H:9:LYS:HZ3	1:H:38:LEU:HB3	1.74	0.52
1:H:200:MSE:CB	1:H:216:TYR:CE2	2.93	0.52
1:D:105:ILE:HD12	1:D:117:LYS:HG2	1.92	0.52
1:A:162:LEU:HA	1:A:170:MSE:HE1	1.91	0.52
1:E:327:ASN:HB2	1:E:330:GLU:CD	2.30	0.52
1:F:132:GLU:O	1:F:136:VAL:HG12	2.10	0.52
1:H:167:PHE:CA	1:H:170:MSE:HE3	2.25	0.52
1:B:162:LEU:HA	1:B:170:MSE:HE1	1.92	0.52
1:H:21:LYS:HZ3	1:H:21:LYS:HB3	1.75	0.52
1:H:331:LEU:HD22	1:H:335:TYR:CE2	2.45	0.52
1:H:333:MSE:HE2	1:H:355:PHE:HZ	1.75	0.51
1:E:8:MSE:HG2	1:E:22:TRP:CH2	2.44	0.51
1:H:9:LYS:NZ	1:H:38:LEU:HB3	2.25	0.51
1:G:71:CYS:HA	1:G:74:LEU:HD22	1.93	0.51
1:G:8:MSE:HG2	1:G:22:TRP:CH2	2.45	0.51
1:A:208:ASN:ND2	1:A:365:ARG:HH22	2.06	0.51
1:H:30:ASN:OD1	1:H:32:ASN:HB2	2.11	0.51
1:B:71:CYS:HA	1:B:74:LEU:HD22	1.93	0.51
1:F:141:LYS:O	1:F:141:LYS:HG3	2.10	0.51
1:B:167:PHE:HD1	1:B:170:MSE:HE1	1.75	0.51
1:H:2:GLU:HG2	1:H:73:ASN:HD21	1.73	0.51
1:D:162:LEU:HA	1:D:170:MSE:HE1	1.92	0.51
1:G:132:GLU:O	1:G:136:VAL:HG12	2.11	0.51
1:C:377:ASN:HD22	1:C:378:GLN:N	2.08	0.51
1:H:170:MSE:O	1:H:174:ILE:CG1	2.57	0.51
1:C:71:CYS:HA	1:C:74:LEU:HD22	1.93	0.51
1:H:2:GLU:HG3	1:H:73:ASN:HD21	1.75	0.51
1:H:167:PHE:HD1	1:H:170:MSE:HE1	1.75	0.50
1:G:167:PHE:CA	1:G:170:MSE:HE3	2.23	0.50
1:F:71:CYS:HA	1:F:74:LEU:HD22	1.92	0.50
1:C:167:PHE:HD1	1:C:170:MSE:HE1	1.76	0.50
1:D:326:HIS:HB2	1:D:331:LEU:HD13	1.94	0.50
1:G:162:LEU:HA	1:G:170:MSE:HE1	1.93	0.50
1:H:368:LEU:HD23	1:H:385:LEU:HD13	1.94	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:67:MSE:CE	1:E:67:MSE:HA	2.35	0.50
1:D:348:PHE:O	1:D:352:ILE:HG23	2.12	0.50
1:H:111:LYS:HD2	1:H:146:THR:CG2	2.42	0.50
1:E:132:GLU:O	1:E:136:VAL:HG12	2.12	0.49
1:E:331:LEU:HD23	1:E:335:TYR:CE2	2.47	0.49
1:C:132:GLU:O	1:C:136:VAL:HG12	2.12	0.49
1:H:333:MSE:HE1	1:H:366:LEU:CD1	2.43	0.49
1:B:105:ILE:HD12	1:B:117:LYS:HG2	1.93	0.49
1:E:71:CYS:HA	1:E:74:LEU:HD22	1.93	0.49
1:H:105:ILE:HD12	1:H:117:LYS:HG2	1.94	0.49
1:B:132:GLU:O	1:B:136:VAL:HG12	2.12	0.49
1:H:132:GLU:O	1:H:136:VAL:HG12	2.13	0.49
1:A:71:CYS:HA	1:A:74:LEU:HD22	1.94	0.49
1:D:71:CYS:HA	1:D:74:LEU:HD22	1.93	0.48
1:D:132:GLU:O	1:D:136:VAL:HG12	2.12	0.48
1:A:132:GLU:O	1:A:136:VAL:HG12	2.13	0.48
1:B:167:PHE:CA	1:B:170:MSE:HE3	2.24	0.48
1:G:36:ASP:HB3	1:G:43:LYS:HG3	1.96	0.48
1:H:96:ILE:HD13	1:H:96:ILE:H	1.79	0.48
1:H:313:LYS:O	1:H:317:VAL:HG12	2.13	0.48
1:D:295:ILE:HD13	1:D:330:GLU:OE2	2.14	0.47
1:F:76:VAL:HG13	1:F:104:MSE:HG3	1.95	0.47
1:H:184:GLU:OE2	1:H:185:ASN:HB2	2.14	0.47
1:B:333:MSE:HE1	1:B:366:LEU:CD1	2.41	0.47
1:D:310:GLU:HG2	1:D:313:LYS:CD	2.36	0.47
1:H:174:ILE:CD1	1:H:203:ILE:HD11	2.44	0.47
1:H:76:VAL:HG13	1:H:104:MSE:HG3	1.95	0.47
1:B:89:ASP:OD2	1:B:97:GLU:OE2	2.32	0.47
1:A:167:PHE:CA	1:A:170:MSE:HE3	2.22	0.47
1:B:242:LEU:HD23	1:B:243:PHE:CE1	2.49	0.47
1:C:167:PHE:HA	1:C:170:MSE:CE	2.24	0.47
1:F:170:MSE:HE3	1:F:203:ILE:CG1	2.43	0.47
1:E:348:PHE:CZ	1:E:370:GLU:HG3	2.49	0.47
1:H:318:LEU:CD2	1:H:341:LEU:HD22	2.45	0.47
1:D:348:PHE:CZ	1:D:370:GLU:HG3	2.51	0.46
1:D:333:MSE:HE1	1:D:366:LEU:CD1	2.43	0.46
1:F:96:ILE:HD12	2:F:410:HOH:O	2.16	0.46
1:G:133:PHE:HB2	1:H:176:GLN:OE1	2.15	0.46
1:G:336:TYR:CE1	1:G:366:LEU:HB3	2.51	0.46
1:D:329:ASN:HA	1:D:329:ASN:HD22	1.52	0.46
1:H:89:ASP:OD2	1:H:97:GLU:OE2	2.34	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:76:VAL:HG21	1:B:103:SER:HB2	1.97	0.46
1:A:9:LYS:HG2	1:E:323:LEU:O	2.15	0.46
1:F:228:ARG:NH1	2:F:401:HOH:O	2.48	0.46
1:A:76:VAL:HG13	1:A:104:MSE:HG3	1.98	0.46
1:A:326:HIS:HB3	1:A:331:LEU:CD1	2.46	0.46
1:G:272:GLN:NE2	1:G:296:MSE:HE1	2.30	0.46
1:H:167:PHE:HD1	1:H:170:MSE:HE3	1.80	0.46
1:A:327:ASN:ND2	1:A:330:GLU:H	2.14	0.46
1:E:76:VAL:HG13	1:E:104:MSE:HG3	1.98	0.46
1:E:167:PHE:CD2	1:E:170:MSE:CE	2.96	0.46
1:H:336:TYR:CE1	1:H:366:LEU:HB3	2.50	0.46
1:C:39:ASN:HB3	2:C:408:HOH:O	2.15	0.46
1:D:76:VAL:HG13	1:D:104:MSE:HG3	1.97	0.46
1:E:43:LYS:HE2	2:E:402:HOH:O	2.15	0.46
1:B:336:TYR:CE1	1:B:366:LEU:HB3	2.51	0.45
1:B:4:ILE:HG22	2:B:408:HOH:O	2.16	0.45
1:E:55:VAL:HG21	1:E:67:MSE:CE	2.41	0.45
1:D:336:TYR:CE1	1:D:366:LEU:HB3	2.51	0.45
1:A:348:PHE:CZ	1:A:370:GLU:HG3	2.51	0.45
1:A:70:TYR:HE1	2:A:419:HOH:O	1.98	0.45
1:D:352:ILE:CD1	1:D:384:LEU:HD13	2.47	0.45
1:E:137:LYS:HG2	1:F:140:GLY:CA	2.43	0.45
1:E:336:TYR:CE1	1:E:366:LEU:HB3	2.52	0.45
1:H:167:PHE:HA	1:H:170:MSE:CE	2.25	0.45
1:B:76:VAL:HG13	1:B:104:MSE:HG3	1.98	0.45
1:F:336:TYR:CE1	1:F:366:LEU:HB3	2.52	0.45
1:F:262:GLN:NE2	1:F:262:GLN:H	2.15	0.45
1:H:79:LYS:HE3	1:H:184:GLU:HG2	1.99	0.45
1:E:262:GLN:H	1:E:262:GLN:NE2	2.16	0.44
1:E:334:HIS:HE1	1:E:338:LYS:HE3	1.82	0.44
1:F:361:LYS:CD	1:F:386:LEU:HD22	2.46	0.44
1:H:318:LEU:HD22	1:H:341:LEU:HD22	1.99	0.44
1:A:336:TYR:CE1	1:A:366:LEU:HB3	2.52	0.44
1:A:340:ARG:CG	1:A:340:ARG:HH11	2.28	0.44
1:E:170:MSE:HE3	1:E:203:ILE:CG1	2.46	0.44
1:F:89:ASP:OD2	1:F:97:GLU:OE2	2.36	0.44
1:F:93:PHE:CB	1:F:96:ILE:HD13	2.40	0.44
1:C:76:VAL:HG21	1:C:103:SER:HB2	2.00	0.44
1:F:167:PHE:CD2	1:F:170:MSE:CE	2.95	0.44
1:G:333:MSE:HE1	1:G:366:LEU:CD1	2.40	0.44
1:H:208:ASN:CG	1:H:365:ARG:HH22	2.21	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:336:TYR:CE1	1:C:366:LEU:HB3	2.51	0.44
1:H:197:HIS:CE1	1:H:219:LYS:HD2	2.51	0.44
1:D:76:VAL:HG21	1:D:103:SER:HB2	2.00	0.44
1:A:326:HIS:CB	1:A:331:LEU:HD13	2.48	0.44
1:G:262:GLN:NE2	1:G:262:GLN:H	2.15	0.44
1:E:76:VAL:HG21	1:E:103:SER:HB2	2.00	0.43
1:A:167:PHE:HD1	1:A:170:MSE:HE3	1.83	0.43
1:B:167:PHE:HA	1:B:170:MSE:CE	2.24	0.43
1:F:348:PHE:CZ	1:F:370:GLU:HG3	2.53	0.43
1:H:68:LYS:O	1:H:72:LEU:HD23	2.18	0.43
1:A:262:GLN:H	1:A:262:GLN:NE2	2.16	0.43
1:B:262:GLN:NE2	1:B:262:GLN:H	2.16	0.43
1:G:104:MSE:HG2	1:G:112:SER:HB3	2.01	0.43
1:G:76:VAL:HG21	1:G:103:SER:HB2	2.00	0.43
1:C:348:PHE:CZ	1:C:370:GLU:HG3	2.53	0.43
1:E:136:VAL:HG13	1:F:136:VAL:HG21	2.01	0.43
1:A:115:TYR:HA	1:A:149:MSE:SE	2.69	0.43
1:B:231:VAL:HG13	1:B:270:PHE:CE2	2.53	0.43
1:G:296:MSE:HE2	1:G:296:MSE:HB3	1.91	0.43
1:D:167:PHE:CA	1:D:170:MSE:HE3	2.24	0.43
1:F:191:THR:O	1:F:195:ARG:HG3	2.19	0.43
1:H:174:ILE:CD1	1:H:174:ILE:N	2.58	0.43
1:F:333:MSE:HE1	1:F:366:LEU:CD1	2.41	0.43
1:D:262:GLN:H	1:D:262:GLN:NE2	2.16	0.42
1:G:348:PHE:CD2	1:G:374:MSE:CE	3.01	0.42
1:H:331:LEU:HD22	1:H:335:TYR:HE2	1.84	0.42
1:E:349:TYR:CE1	1:F:380:LEU:HD13	2.54	0.42
1:D:16:ASN:OD1	1:G:247:GLU:OE2	2.36	0.42
1:F:167:PHE:CE2	1:F:206:ASN:HB2	2.54	0.42
1:D:231:VAL:HG13	1:D:270:PHE:CE2	2.54	0.42
1:G:191:THR:O	1:G:195:ARG:HG3	2.19	0.42
1:A:315:LYS:HE3	1:A:315:LYS:HB2	1.89	0.42
1:C:377:ASN:ND2	1:C:377:ASN:C	2.72	0.42
1:D:208:ASN:HD21	1:D:365:ARG:HH12	1.68	0.42
1:E:133:PHE:CZ	1:E:137:LYS:HD2	2.55	0.42
1:E:231:VAL:HG13	1:E:270:PHE:CE2	2.55	0.42
1:E:288:ILE:HD11	1:E:304:CYS:HB2	2.02	0.42
1:F:231:VAL:HG13	1:F:270:PHE:CE2	2.55	0.42
1:E:243:PHE:CE1	1:E:366:LEU:HD13	2.48	0.42
1:F:288:ILE:HD11	1:F:304:CYS:HB2	2.01	0.42
1:C:282:ARG:HG3	1:C:307:ASN:CG	2.40	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:379:LYS:HG2	1:D:349:TYR:CE2	2.55	0.42
1:F:286:LYS:HD3	1:F:287:TRP:CE2	2.55	0.42
1:G:76:VAL:HG13	1:G:104:MSE:HG3	2.02	0.42
1:H:115:TYR:HA	1:H:149:MSE:SE	2.69	0.42
1:H:231:VAL:HG13	1:H:270:PHE:CE2	2.55	0.42
1:A:334:HIS:CD2	2:A:408:HOH:O	2.67	0.42
1:C:76:VAL:HG13	1:C:104:MSE:HG3	2.01	0.42
1:C:262:GLN:H	1:C:262:GLN:NE2	2.17	0.42
1:C:231:VAL:HG13	1:C:270:PHE:CE2	2.55	0.42
1:H:200:MSE:HB2	1:H:216:TYR:CD2	2.55	0.42
1:A:231:VAL:HG13	1:A:270:PHE:CE2	2.55	0.41
1:D:104:MSE:HG2	1:D:112:SER:HB3	2.02	0.41
1:F:282:ARG:HG3	1:F:307:ASN:CG	2.40	0.41
1:B:115:TYR:HA	1:B:149:MSE:SE	2.70	0.41
1:B:331:LEU:HD22	1:B:335:TYR:CE2	2.55	0.41
1:E:385:LEU:O	1:E:386:LEU:HB2	2.20	0.41
1:E:191:THR:O	1:E:195:ARG:HG3	2.19	0.41
1:G:115:TYR:HA	1:G:149:MSE:SE	2.70	0.41
1:G:167:PHE:HD1	1:G:170:MSE:HE3	1.84	0.41
1:E:101:ILE:O	1:E:105:ILE:HG12	2.20	0.41
1:E:282:ARG:HG3	1:E:307:ASN:CG	2.41	0.41
1:F:101:ILE:O	1:F:105:ILE:HG12	2.21	0.41
1:G:348:PHE:CZ	1:G:370:GLU:HG3	2.56	0.41
1:H:174:ILE:CG1	1:H:203:ILE:CD1	2.92	0.41
1:B:348:PHE:CZ	1:B:370:GLU:HG3	2.56	0.41
1:G:231:VAL:HG13	1:G:270:PHE:CE2	2.56	0.41
1:B:101:ILE:O	1:B:105:ILE:HG12	2.21	0.41
1:E:115:TYR:HA	1:E:149:MSE:SE	2.71	0.41
1:E:104:MSE:HG2	1:E:112:SER:HB3	2.03	0.41
1:F:331:LEU:HD22	1:F:335:TYR:CE2	2.56	0.41
1:H:145:LYS:HB3	1:H:145:LYS:HE3	1.87	0.41
1:D:115:TYR:HA	1:D:149:MSE:SE	2.71	0.41
1:A:326:HIS:HB3	1:A:331:LEU:HD12	2.02	0.40
1:G:288:ILE:HD11	1:G:304:CYS:HB2	2.02	0.40
1:H:101:ILE:O	1:H:105:ILE:HG12	2.20	0.40
1:G:380:LEU:HD13	1:H:349:TYR:CE1	2.57	0.40
1:A:248:LEU:HD22	2:D:405:HOH:O	2.22	0.40
1:E:329:ASN:ND2	1:E:330:GLU:N	2.68	0.40
1:E:71:CYS:O	1:E:74:LEU:HB2	2.21	0.40
1:A:22:TRP:CZ2	1:A:58:GLN:HG2	2.57	0.40
1:B:86:GLU:HA	1:B:86:GLU:OE1	2.22	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:101:ILE:O	1:D:105:ILE:HG12	2.20	0.40
1:D:379:LYS:HD2	1:D:379:LYS:HA	1.91	0.40
1:F:71:CYS:O	1:F:74:LEU:HB2	2.22	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:B:46:ASN:ND2	1:H:378:GLN:OE1[1_455]	1.97	0.23

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	384/386 (100%)	378 (98%)	6 (2%)	0	100	100
1	B	384/386 (100%)	378 (98%)	6 (2%)	0	100	100
1	C	384/386 (100%)	376 (98%)	8 (2%)	0	100	100
1	D	384/386 (100%)	378 (98%)	6 (2%)	0	100	100
1	E	385/386 (100%)	377 (98%)	8 (2%)	0	100	100
1	F	384/386 (100%)	378 (98%)	6 (2%)	0	100	100
1	G	384/386 (100%)	377 (98%)	7 (2%)	0	100	100
1	H	384/386 (100%)	377 (98%)	7 (2%)	0	100	100
All	All	3073/3088 (100%)	3019 (98%)	54 (2%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	360/345 (104%)	324 (90%)	36 (10%)	7 18
1	B	360/345 (104%)	316 (88%)	44 (12%)	5 11
1	C	360/345 (104%)	321 (89%)	39 (11%)	6 15
1	D	360/345 (104%)	312 (87%)	48 (13%)	4 9
1	E	361/345 (105%)	319 (88%)	42 (12%)	5 12
1	F	360/345 (104%)	316 (88%)	44 (12%)	5 11
1	G	360/345 (104%)	324 (90%)	36 (10%)	7 18
1	H	360/345 (104%)	314 (87%)	46 (13%)	4 10
All	All	2881/2760 (104%)	2546 (88%)	335 (12%)	5 12

All (335) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	12	LEU
1	A	49	SER
1	A	65	GLU
1	A	74	LEU
1	A	76	VAL
1	A	95	GLU
1	A	104	MSE
1	A	134	GLU
1	A	136	VAL
1	A	137	LYS
1	A	138	ARG
1	A	145	LYS
1	A	156	LEU
1	A	158	LEU
1	A	168	SER
1	A	198	VAL
1	A	211	GLU
1	A	228	ARG
1	A	248	LEU

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Mol	Chain	Res	Type
1	A	262	GLN
1	A	276	PHE
1	A	286	LYS
1	A	309	ASN
1	A	312	SER
1	A	315	LYS
1	A	324	LEU
1	A	327	ASN
1	A	340	ARG
1	A	341	LEU
1	A	343	GLN
1	A	363	LEU
1	A	368	LEU
1	A	369	LEU
1	A	370	GLU
1	A	380	LEU
1	A	385	LEU
1	B	1	MSE
1	B	20	ASN
1	B	21	LYS
1	B	32	ASN
1	B	49	SER
1	B	65	GLU
1	B	74	LEU
1	B	76	VAL
1	B	95	GLU
1	B	100	LEU
1	B	103	SER
1	B	104	MSE
1	B	110	MSE
1	B	136	VAL
1	B	138	ARG
1	B	141	LYS
1	B	156	LEU
1	B	158	LEU
1	B	168	SER
1	B	189	ARG
1	B	198	VAL
1	B	217	SER
1	B	218	LYS
1	B	228	ARG
1	B	242	LEU

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Mol	Chain	Res	Type
1	B	250	GLN
1	B	262	GLN
1	B	276	PHE
1	B	296	MSE
1	B	298	LEU
1	B	310	GLU
1	B	320	LYS
1	B	324	LEU
1	B	327	ASN
1	B	329	ASN
1	B	331	LEU
1	B	338	LYS
1	B	341	LEU
1	B	363	LEU
1	B	368	LEU
1	B	370	GLU
1	B	373	LYS
1	B	379	LYS
1	B	380	LEU
1	C	49	SER
1	C	65	GLU
1	C	74	LEU
1	C	76	VAL
1	C	95	GLU
1	C	100	LEU
1	C	103	SER
1	C	109	ASN
1	C	110	MSE
1	C	136	VAL
1	C	137	LYS
1	C	138	ARG
1	C	141	LYS
1	C	145	LYS
1	C	156	LEU
1	C	158	LEU
1	C	168	SER
1	C	184	GLU
1	C	198	VAL
1	C	228	ARG
1	C	262	GLN
1	C	268	MSE
1	C	276	PHE

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Mol	Chain	Res	Type
1	C	282	ARG
1	C	286	LYS
1	C	295	ILE
1	C	298	LEU
1	C	309	ASN
1	C	324	LEU
1	C	341	LEU
1	C	363	LEU
1	C	365	ARG
1	C	366	LEU
1	C	368	LEU
1	C	369	LEU
1	C	370	GLU
1	C	377	ASN
1	C	379	LYS
1	C	380	LEU
1	D	2	GLU
1	D	49	SER
1	D	68	LYS
1	D	74	LEU
1	D	76	VAL
1	D	95	GLU
1	D	102	ASP
1	D	103	SER
1	D	110	MSE
1	D	134	GLU
1	D	136	VAL
1	D	137	LYS
1	D	138	ARG
1	D	141	LYS
1	D	145	LYS
1	D	156	LEU
1	D	158	LEU
1	D	168	SER
1	D	175	LYS
1	D	198	VAL
1	D	218	LYS
1	D	228	ARG
1	D	242	LEU
1	D	262	GLN
1	D	276	PHE
1	D	282	ARG

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Mol	Chain	Res	Type
1	D	296	MSE
1	D	298	LEU
1	D	309	ASN
1	D	310	GLU
1	D	316	GLU
1	D	320	LYS
1	D	321	LEU
1	D	324	LEU
1	D	329	ASN
1	D	331	LEU
1	D	338	LYS
1	D	341	LEU
1	D	352	ILE
1	D	356	LYS
1	D	363	LEU
1	D	368	LEU
1	D	369	LEU
1	D	370	GLU
1	D	379	LYS
1	D	380	LEU
1	D	385	LEU
1	D	386	LEU
1	E	49	SER
1	E	65	GLU
1	E	68	LYS
1	E	74	LEU
1	E	76	VAL
1	E	77	LYS
1	E	95	GLU
1	E	103	SER
1	E	134	GLU
1	E	136	VAL
1	E	137	LYS
1	E	138	ARG
1	E	141	LYS
1	E	156	LEU
1	E	158	LEU
1	E	168	SER
1	E	174	ILE
1	E	184	GLU
1	E	198	VAL
1	E	211	GLU

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Mol	Chain	Res	Type
1	E	228	ARG
1	E	242	LEU
1	E	262	GLN
1	E	276	PHE
1	E	282	ARG
1	E	286	LYS
1	E	293	ASP
1	E	309	ASN
1	E	313	LYS
1	E	317	VAL
1	E	318	LEU
1	E	320	LYS
1	E	324	LEU
1	E	327	ASN
1	E	329	ASN
1	E	331	LEU
1	E	340	ARG
1	E	363	LEU
1	E	366	LEU
1	E	368	LEU
1	E	370	GLU
1	E	380	LEU
1	F	49	SER
1	F	65	GLU
1	F	74	LEU
1	F	76	VAL
1	F	100	LEU
1	F	102	ASP
1	F	104	MSE
1	F	108	SER
1	F	111	LYS
1	F	134	GLU
1	F	136	VAL
1	F	137	LYS
1	F	138	ARG
1	F	141	LYS
1	F	156	LEU
1	F	158	LEU
1	F	168	SER
1	F	172	GLN
1	F	183	SER
1	F	198	VAL

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Mol	Chain	Res	Type
1	F	209	SER
1	F	228	ARG
1	F	242	LEU
1	F	262	GLN
1	F	276	PHE
1	F	282	ARG
1	F	286	LYS
1	F	293	ASP
1	F	309	ASN
1	F	310	GLU
1	F	316	GLU
1	F	320	LYS
1	F	321	LEU
1	F	324	LEU
1	F	331	LEU
1	F	338	LYS
1	F	341	LEU
1	F	342	GLU
1	F	343	GLN
1	F	368	LEU
1	F	369	LEU
1	F	370	GLU
1	F	380	LEU
1	F	385	LEU
1	G	13	GLU
1	G	39	ASN
1	G	49	SER
1	G	74	LEU
1	G	76	VAL
1	G	95	GLU
1	G	100	LEU
1	G	102	ASP
1	G	103	SER
1	G	136	VAL
1	G	137	LYS
1	G	138	ARG
1	G	156	LEU
1	G	158	LEU
1	G	168	SER
1	G	184	GLU
1	G	211	GLU
1	G	218	LYS

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Mol	Chain	Res	Type
1	G	228	ARG
1	G	242	LEU
1	G	262	GLN
1	G	276	PHE
1	G	282	ARG
1	G	295	ILE
1	G	309	ASN
1	G	318	LEU
1	G	324	LEU
1	G	327	ASN
1	G	331	LEU
1	G	341	LEU
1	G	356	LYS
1	G	363	LEU
1	G	368	LEU
1	G	370	GLU
1	G	379	LYS
1	G	380	LEU
1	H	10	LYS
1	H	39	ASN
1	H	44	THR
1	H	46	ASN
1	H	49	SER
1	H	73	ASN
1	H	74	LEU
1	H	76	VAL
1	H	95	GLU
1	H	96	ILE
1	H	102	ASP
1	H	104	MSE
1	H	111	LYS
1	H	136	VAL
1	H	137	LYS
1	H	138	ARG
1	H	150	ASN
1	H	154	ARG
1	H	156	LEU
1	H	158	LEU
1	H	168	SER
1	H	172	GLN
1	H	174	ILE
1	H	180	SER

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Mol	Chain	Res	Type
1	H	184	GLU
1	H	198	VAL
1	H	209	SER
1	H	228	ARG
1	H	276	PHE
1	H	286	LYS
1	H	309	ASN
1	H	310	GLU
1	H	317	VAL
1	H	318	LEU
1	H	327	ASN
1	H	331	LEU
1	H	345	LYS
1	H	357	LYS
1	H	365	ARG
1	H	368	LEU
1	H	369	LEU
1	H	370	GLU
1	H	378	GLN
1	H	379	LYS
1	H	380	LEU
1	H	385	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (65) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	20	ASN
1	A	39	ASN
1	A	166	ASN
1	A	190	ASN
1	A	208	ASN
1	A	262	GLN
1	A	265	ASN
1	A	311	ASN
1	A	327	ASN
1	A	359	ASN
1	B	32	ASN
1	B	172	GLN
1	B	208	ASN
1	B	262	GLN
1	B	265	ASN
1	B	311	ASN

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Mol	Chain	Res	Type
1	B	359	ASN
1	C	109	ASN
1	C	190	ASN
1	C	250	GLN
1	C	262	GLN
1	C	265	ASN
1	C	301	GLN
1	C	359	ASN
1	C	377	ASN
1	D	143	ASN
1	D	190	ASN
1	D	206	ASN
1	D	208	ASN
1	D	262	GLN
1	D	265	ASN
1	D	329	ASN
1	D	359	ASN
1	E	16	ASN
1	E	190	ASN
1	E	206	ASN
1	E	262	GLN
1	E	265	ASN
1	E	329	ASN
1	E	334	HIS
1	E	359	ASN
1	F	73	ASN
1	F	172	GLN
1	F	190	ASN
1	F	262	GLN
1	F	265	ASN
1	F	301	GLN
1	F	359	ASN
1	F	372	GLN
1	G	190	ASN
1	G	262	GLN
1	G	265	ASN
1	G	271	GLN
1	G	272	GLN
1	G	327	ASN
1	G	334	HIS
1	G	359	ASN
1	H	46	ASN

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Mol	Chain	Res	Type
1	H	73	ASN
1	H	190	ASN
1	H	265	ASN
1	H	311	ASN
1	H	327	ASN
1	H	334	HIS
1	H	359	ASN

5.3.3 RNA

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates

There are no carbohydrates in this entry.

5.6 Ligand geometry

There are no ligands in this entry.

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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	A	371/386 (96%)	0.08	3 (0%) 86 87	33, 51, 81, 100	0
1	B	371/386 (96%)	0.35	11 (2%) 50 51	26, 62, 106, 142	0
1	C	371/386 (96%)	0.22	5 (1%) 77 78	34, 57, 91, 117	0
1	D	371/386 (96%)	0.26	11 (2%) 50 51	34, 58, 99, 144	0
1	E	371/386 (96%)	0.40	11 (2%) 50 51	39, 65, 90, 108	0
1	F	371/386 (96%)	0.32	16 (4%) 35 33	37, 69, 109, 131	0
1	G	371/386 (96%)	0.20	5 (1%) 77 78	31, 57, 95, 114	0
1	H	371/386 (96%)	1.07	74 (19%) 1 0	41, 79, 135, 183	0
All	All	2968/3088 (96%)	0.36	136 (4%) 32 31	26, 61, 106, 183	0

All (136) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	H	13	GLU	8.8
1	H	16	ASN	7.4
1	H	12	LEU	6.8
1	H	81	ALA	6.3
1	H	85	LEU	6.3
1	F	37	PHE	6.0
1	E	96	ILE	5.0
1	H	113	LYS	4.8
1	H	37	PHE	4.7
1	H	105	ILE	4.7
1	H	115	TYR	4.7
1	B	40	HIS	4.5
1	H	150	ASN	4.3
1	H	72	LEU	4.1
1	D	20	ASN	4.1
1	H	17	SER	4.0

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Mol	Chain	Res	Type	RSRZ
1	H	106	SER	4.0
1	H	122	HIS	3.9
1	B	42	GLY	3.9
1	H	84	ALA	3.8
1	H	139	LEU	3.8
1	H	28	LEU	3.8
1	H	11	ASP	3.7
1	H	192	TYR	3.7
1	B	317	VAL	3.7
1	H	76	VAL	3.6
1	D	21	LYS	3.4
1	F	13	GLU	3.4
1	H	20	ASN	3.4
1	H	191	THR	3.3
1	H	189	ARG	3.3
1	H	42	GLY	3.2
1	F	48	PHE	3.2
1	H	119	TYR	3.2
1	H	35	TYR	3.2
1	H	94	PHE	3.2
1	H	177	ILE	3.1
1	H	48	PHE	3.0
1	H	45	PHE	3.0
1	G	183	SER	3.0
1	H	188	ILE	3.0
1	E	45	PHE	3.0
1	H	34	LEU	3.0
1	H	144	ILE	3.0
1	H	9	LYS	3.0
1	F	119	TYR	2.9
1	G	25	VAL	2.9
1	E	42	GLY	2.9
1	C	105	ILE	2.9
1	D	324	LEU	2.8
1	E	101	ILE	2.8
1	H	142	LEU	2.8
1	E	323	LEU	2.8
1	H	203	ILE	2.8
1	H	369	LEU	2.8
1	H	145	LYS	2.8
1	F	162	LEU	2.8
1	D	182	ILE	2.7

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Mol	Chain	Res	Type	RSRZ
1	D	293	ASP	2.7
1	H	4	ILE	2.7
1	F	4	ILE	2.7
1	H	59	TYR	2.7
1	H	73	ASN	2.6
1	H	24	THR	2.6
1	H	210	LEU	2.6
1	H	153	SER	2.6
1	H	22	TRP	2.6
1	H	124	GLU	2.6
1	G	184	GLU	2.5
1	E	85	LEU	2.5
1	E	174	ILE	2.5
1	H	167	PHE	2.5
1	H	41	ASP	2.5
1	F	164	THR	2.5
1	H	146	THR	2.5
1	B	48	PHE	2.5
1	H	93	PHE	2.5
1	G	276	PHE	2.5
1	H	120	LYS	2.5
1	H	64	TYR	2.5
1	H	201	SER	2.4
1	B	41	ASP	2.4
1	F	35	TYR	2.4
1	B	85	LEU	2.4
1	C	101	ILE	2.4
1	H	165	GLY	2.4
1	F	276	PHE	2.4
1	B	167	PHE	2.4
1	E	169	PRO	2.4
1	D	25	VAL	2.3
1	H	138	ARG	2.3
1	F	45	PHE	2.3
1	A	35	TYR	2.3
1	H	112	SER	2.3
1	H	179	LEU	2.3
1	F	188	ILE	2.3
1	H	103	SER	2.3
1	H	152	PHE	2.3
1	H	18	LEU	2.3
1	C	133	PHE	2.3

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Mol	Chain	Res	Type	RSRZ
1	H	99	VAL	2.3
1	A	276	PHE	2.2
1	G	21	LYS	2.2
1	B	295	ILE	2.2
1	E	248	LEU	2.2
1	F	26	ALA	2.2
1	D	29	LYS	2.2
1	C	276	PHE	2.2
1	D	16	ASN	2.2
1	H	143	ASN	2.2
1	H	232	PHE	2.2
1	A	335	TYR	2.1
1	F	97	GLU	2.1
1	B	106	SER	2.1
1	H	185	ASN	2.1
1	H	36	ASP	2.1
1	H	251	GLU	2.1
1	F	33	PRO	2.1
1	H	27	GLY	2.1
1	H	102	ASP	2.1
1	H	47	GLU	2.1
1	D	18	LEU	2.1
1	H	137	LYS	2.1
1	E	24	THR	2.1
1	B	37	PHE	2.1
1	D	325	VAL	2.1
1	H	51	ILE	2.1
1	H	46	ASN	2.1
1	D	318	LEU	2.0
1	F	18	LEU	2.0
1	H	199	LEU	2.0
1	B	105	ILE	2.0
1	C	31	PRO	2.0
1	E	359	ASN	2.0
1	H	228	ARG	2.0
1	F	84	ALA	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

There are no carbohydrates in this entry.

6.4 Ligands

There are no ligands in this entry.

6.5 Other polymers

There are no such residues in this entry.