



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 12, 2026 – 06:17 PM UTC

PDB ID : 3VS9 / pdb_00003vs9
Title : Crystal structure of type III PKS ArsC mutant
Authors : Satou, R.; Miyanaga, A.; Ozawa, H.; Funa, N.; Miyazono, K.; Tanokura, M.;
Ohnishi, Y.; Horinouchi, S.
Deposited on : 2012-04-23
Resolution : 1.99 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
Mogul : 2022.3.0, CSD as543be (2022)
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

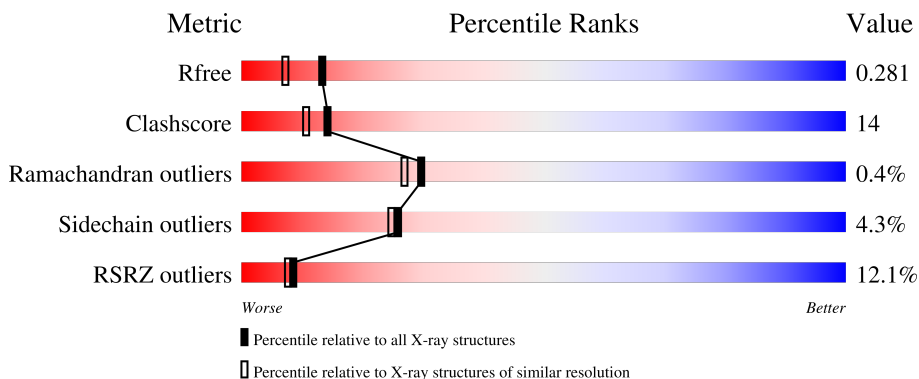
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.99 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.



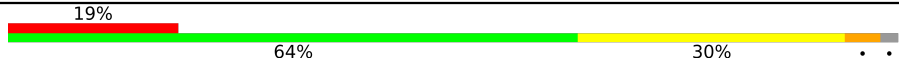


Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	10052 (2.00-2.00)
Clashscore	190562	11152 (2.00-2.00)
Ramachandran outliers	187476	11031 (2.00-2.00)
Sidechain outliers	187428	11029 (2.00-2.00)
RSRZ outliers	180081	10067 (2.00-2.00)

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	410	
1	B	410	
1	C	410	
1	D	410	
1	E	410	

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Mol	Chain	Length	Quality of chain
1	F	410	
1	G	410	
1	H	410	

2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 27142 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 Type III polyketide synthase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	401	3117	1985	540	577	15	0	0	0
1	B	397	3086	1966	536	569	15	0	0	0
1	C	396	3072	1956	532	569	15	0	0	0
1	D	401	3110	1978	540	577	15	0	0	0
1	E	400	3106	1976	539	576	15	0	0	0
1	F	401	3117	1985	540	577	15	0	0	0
1	G	397	3076	1961	536	564	15	0	0	0
1	H	383	2977	1899	519	544	15	0	0	0

- Molecule 2 is SODIUM ION (CCD ID: NA) (formula: Na).

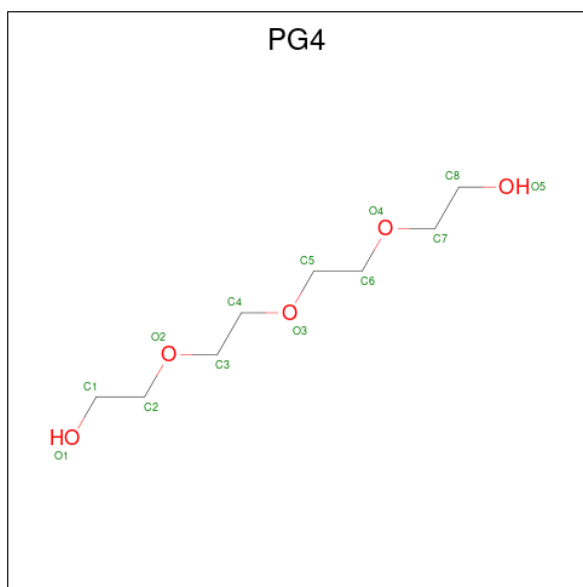
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	1	Total	Na	0	0
			1	1		
2	B	1	Total	Na	0	0
			1	1		
2	C	1	Total	Na	0	0
			1	1		
2	D	1	Total	Na	0	0
			1	1		
2	E	1	Total	Na	0	0
			1	1		
2	F	1	Total	Na	0	0
			1	1		

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	G	1	Total Na 1 1	0	0
2	H	1	Total Na 1 1	0	0

- Molecule 3 is TETRAETHYLENE GLYCOL (CCD ID: PG4) (formula: C₈H₁₈O₅).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total C O 13 8 5	0	0
3	B	1	Total C O 13 8 5	0	0
3	C	1	Total C O 13 8 5	0	0
3	D	1	Total C O 13 8 5	0	0
3	E	1	Total C O 13 8 5	0	0
3	F	1	Total C O 13 8 5	0	0
3	G	1	Total C O 13 8 5	0	0
3	H	1	Total C O 13 8 5	0	0

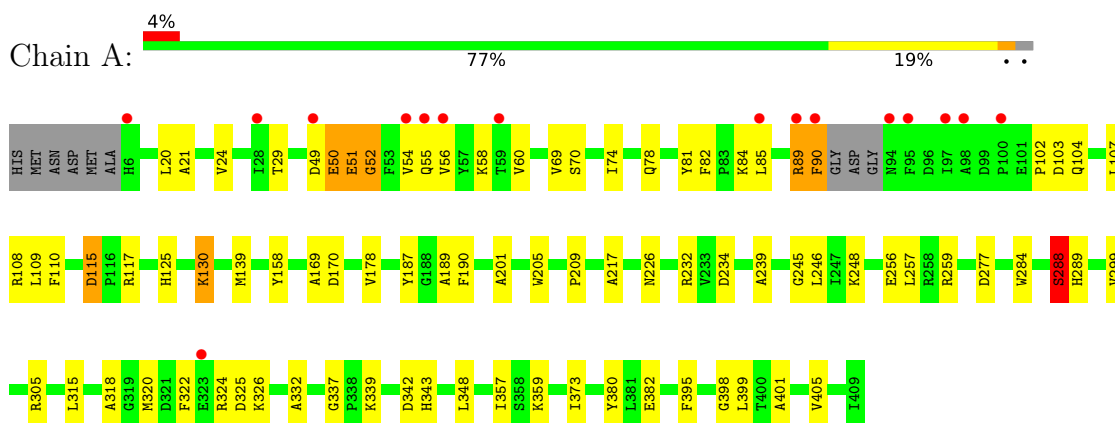
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	372	Total 372	O 372	0	0
4	B	243	Total 243	O 243	0	0
4	C	338	Total 338	O 338	0	0
4	D	343	Total 343	O 343	0	0
4	E	368	Total 368	O 368	0	0
4	F	270	Total 270	O 270	0	0
4	G	235	Total 235	O 235	0	0
4	H	200	Total 200	O 200	0	0

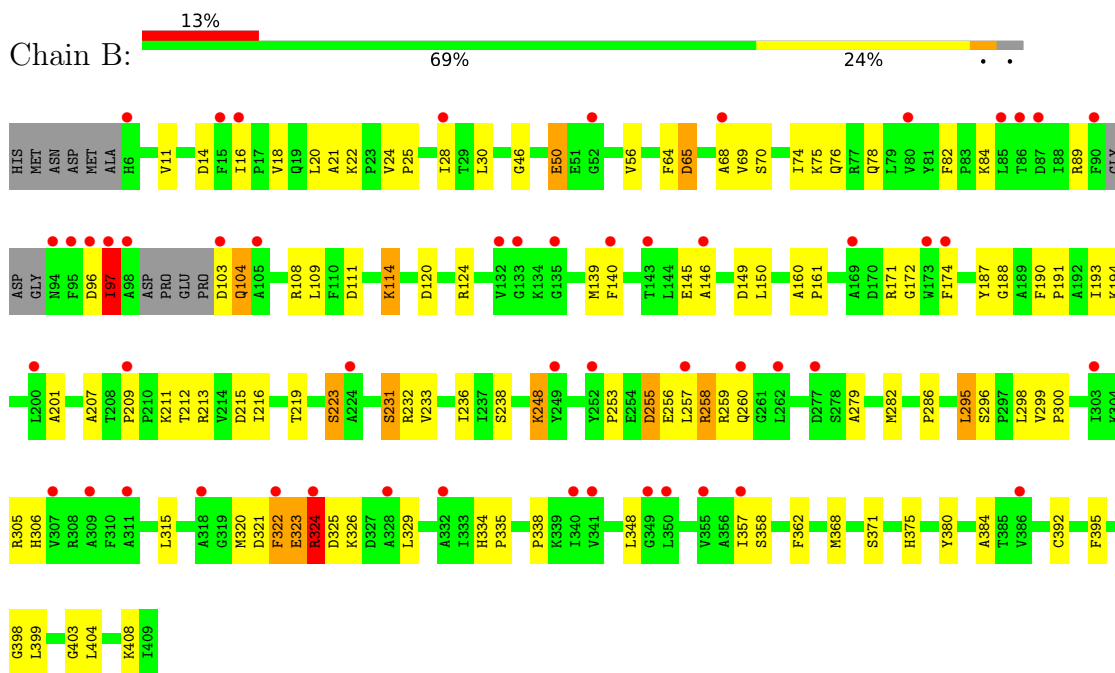
3 Residue-property plots [i](#)

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.

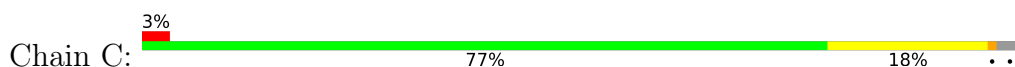
- Molecule 1: Type III polyketide synthase

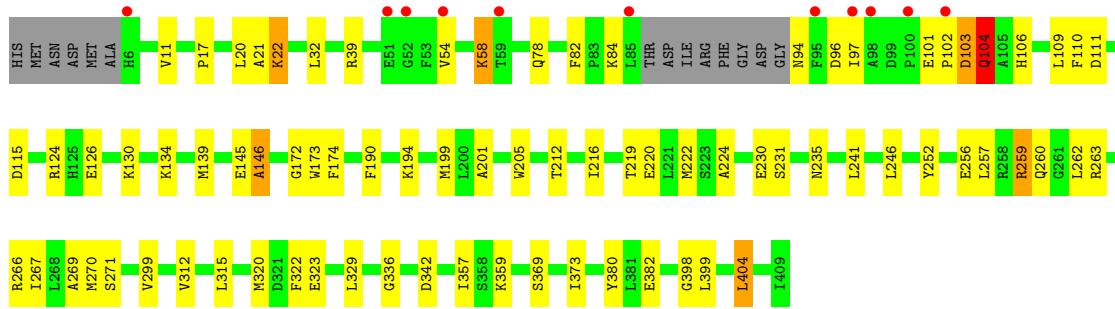


- Molecule 1: Type III polyketide synthase

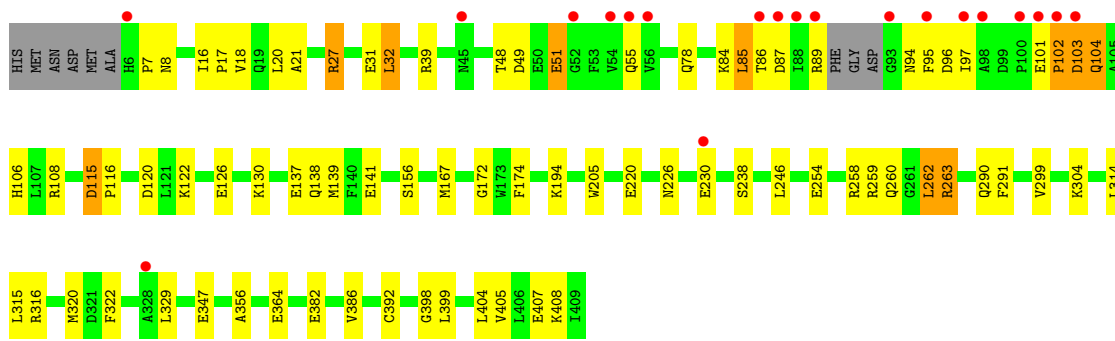
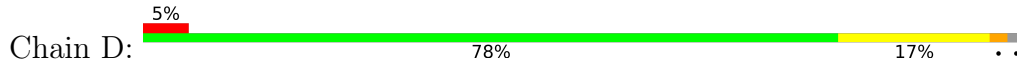


- Molecule 1: Type III polyketide synthase

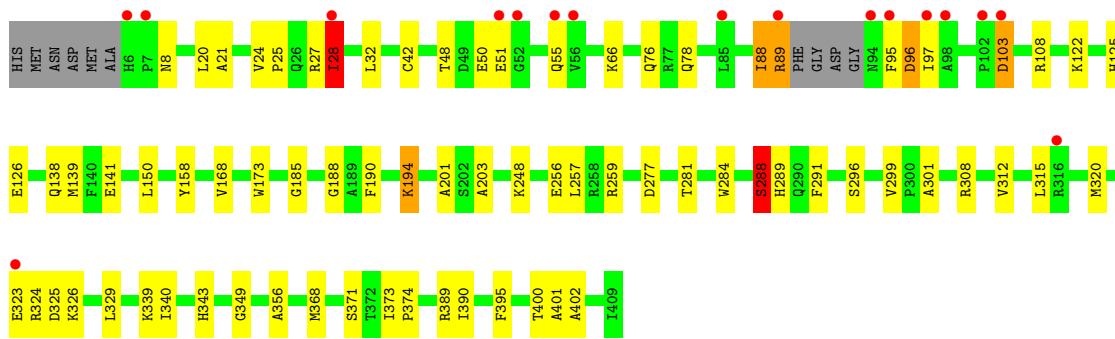
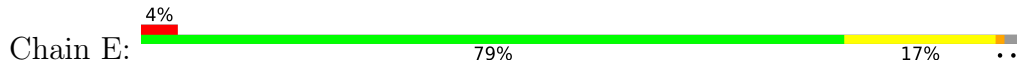




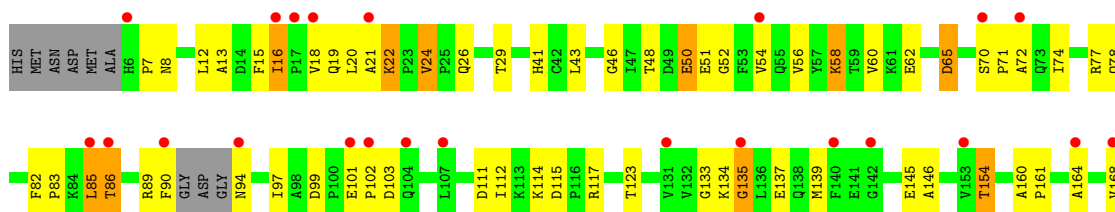
• Molecule 1: Type III polyketide synthase

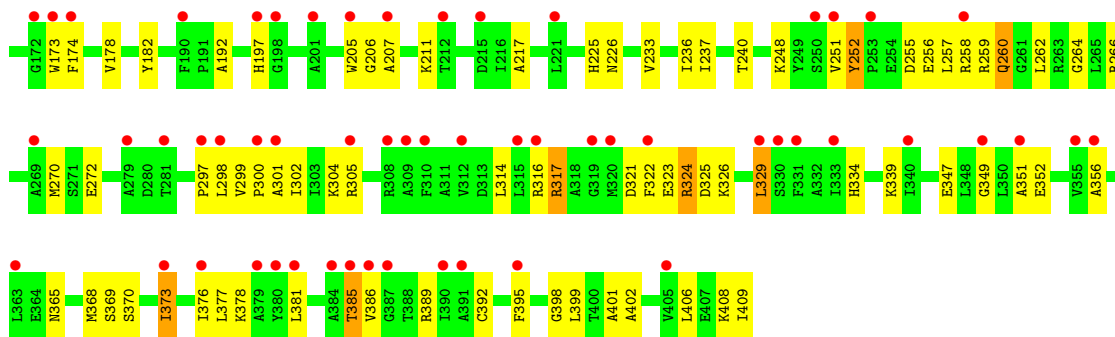


• Molecule 1: Type III polyketide synthase

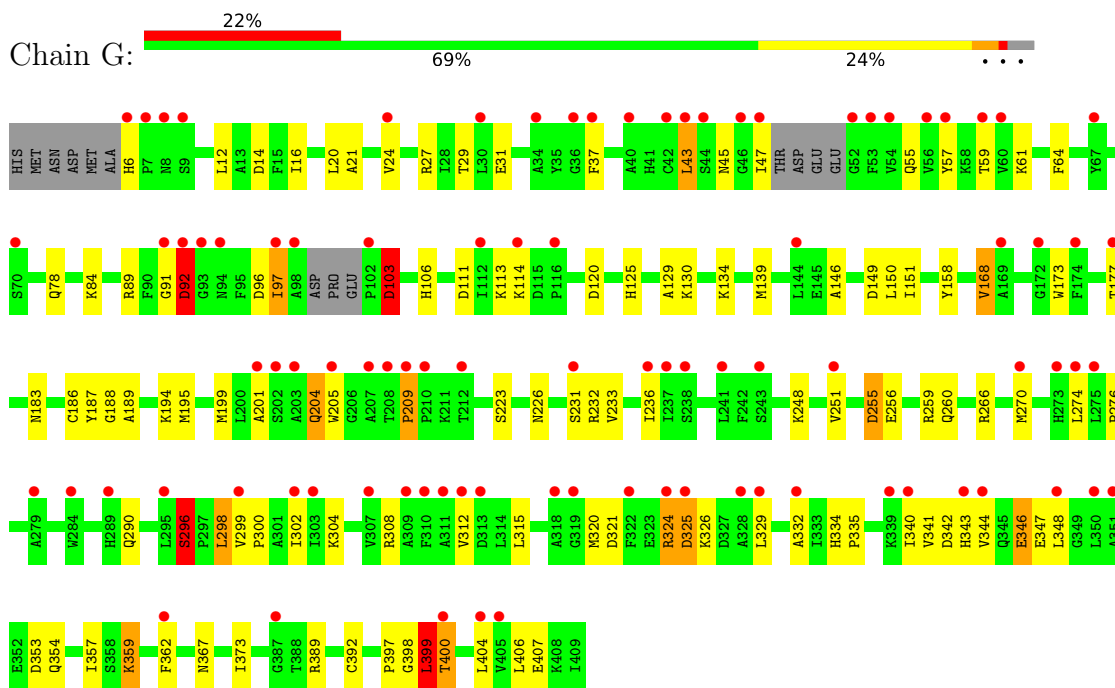


• Molecule 1: Type III polyketide synthase

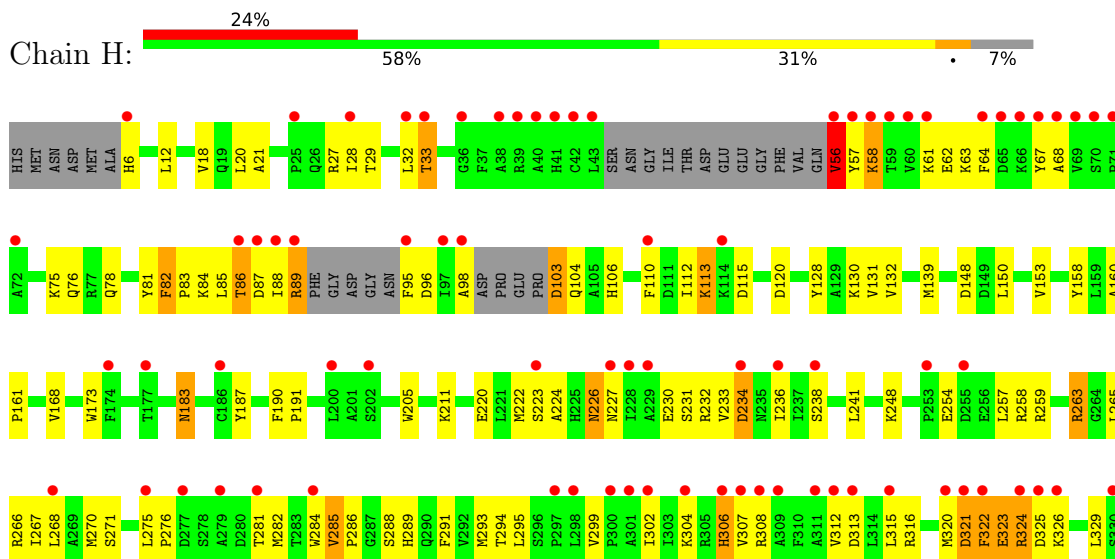




• Molecule 1: Type III polyketide synthase



• Molecule 1: Type III polyketide synthase





4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	102.92Å 142.72Å 129.87Å 90.00° 110.43° 90.00°	Depositor
Resolution (Å)	37.78 – 1.99 37.78 – 1.99	Depositor EDS
% Data completeness (in resolution range)	96.9 (37.78-1.99) 96.9 (37.78-1.99)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.21 (at 1.98Å)	Xtrriage
Refinement program	REFMAC 5.5.0066	Depositor
R, R_{free}	0.205 , 0.273 0.218 , 0.281	Depositor DCC
R_{free} test set	11676 reflections (5.02%)	wwPDB-VP
Wilson B-factor (Å ²)	26.6	Xtrriage
Anisotropy	0.110	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 47.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtrriage
Estimated twinning fraction	0.044 for h,-k,-h-l	Xtrriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	27142	wwPDB-VP
Average B, all atoms (Å ²)	37.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 77.56 % 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 8.2928e-07. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

¹Intensities estimated from amplitudes.

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.

5 Model quality i

5.1 Standard geometry i

Bond lengths and bond angles in the following residue types are not validated in this section: NA, PG4

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	A	1.29	8/3189 (0.3%)	1.20	15/4325 (0.3%)
1	B	1.30	8/3155 (0.3%)	1.22	15/4275 (0.4%)
1	C	1.31	9/3143 (0.3%)	1.18	9/4263 (0.2%)
1	D	1.25	4/3181 (0.1%)	1.16	7/4314 (0.2%)
1	E	1.28	7/3177 (0.2%)	1.18	14/4309 (0.3%)
1	F	1.28	6/3189 (0.2%)	1.32	22/4325 (0.5%)
1	G	1.24	9/3146 (0.3%)	1.20	13/4262 (0.3%)
1	H	1.22	5/3043 (0.2%)	1.21	14/4122 (0.3%)
All	All	1.27	56/25223 (0.2%)	1.21	109/34195 (0.3%)

All (56) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	E	299	VAL	CA-CB	11.92	1.60	1.54
1	G	373	ILE	CA-CB	9.64	1.59	1.54
1	A	373	ILE	CA-CB	9.52	1.59	1.54
1	B	213	ARG	N-CA	8.13	1.55	1.46
1	C	219	THR	CA-CB	7.58	1.64	1.52
1	C	373	ILE	CA-CB	7.44	1.58	1.54
1	A	299	VAL	CA-CB	7.31	1.57	1.54
1	G	168	VAL	CA-CB	-7.14	1.45	1.54
1	H	306	HIS	CD2-NE2	7.10	1.45	1.37
1	C	266	ARG	C-O	-7.05	1.15	1.23
1	D	16	ILE	CA-CB	-6.69	1.48	1.54
1	D	299	VAL	CA-CB	6.43	1.57	1.54
1	F	178	VAL	N-CA	6.38	1.54	1.46
1	B	219	THR	CA-CB	6.31	1.61	1.52
1	C	267	ILE	CA-CB	6.27	1.61	1.54
1	B	194	LYS	C-O	6.17	1.31	1.24
1	H	132	VAL	CA-CB	6.15	1.62	1.54
1	G	209	PRO	CA-C	6.00	1.57	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	F	16	ILE	CA-C	5.90	1.59	1.52
1	A	332	ALA	CA-CB	5.87	1.61	1.53
1	G	24	VAL	CA-CB	5.85	1.61	1.54
1	E	401	ALA	CA-CB	5.81	1.62	1.53
1	A	169	ALA	CA-CB	5.73	1.62	1.53
1	D	167	MET	C-O	-5.69	1.17	1.24
1	G	189	ALA	CA-CB	5.69	1.62	1.53
1	H	18	VAL	CA-CB	5.62	1.61	1.54
1	G	129	ALA	CA-CB	5.62	1.62	1.53
1	A	70	SER	N-CA	5.56	1.52	1.46
1	H	56	VAL	CB-CG2	5.54	1.70	1.52
1	A	178	VAL	CA-CB	5.52	1.60	1.54
1	B	209	PRO	CA-C	5.50	1.57	1.52
1	E	373	ILE	CA-CB	5.49	1.57	1.53
1	F	192	ALA	C-O	5.47	1.30	1.24
1	E	203	ALA	N-CA	5.46	1.52	1.46
1	G	359	LYS	C-O	5.43	1.30	1.24
1	G	29	THR	CA-CB	5.37	1.61	1.53
1	B	97	ILE	CA-CB	5.36	1.60	1.54
1	F	154	THR	N-CA	5.33	1.52	1.46
1	D	17	PRO	CA-C	5.31	1.58	1.52
1	B	193	ILE	C-O	5.30	1.30	1.24
1	E	301	ALA	CA-CB	5.29	1.61	1.53
1	C	216	ILE	CA-CB	5.22	1.60	1.54
1	C	269	ALA	CA-CB	5.20	1.62	1.53
1	B	223	SER	N-CA	5.19	1.52	1.46
1	E	194	LYS	C-O	-5.14	1.18	1.24
1	F	192	ALA	N-CA	5.13	1.52	1.46
1	E	356	ALA	CA-CB	5.12	1.61	1.53
1	A	401	ALA	CA-CB	5.10	1.61	1.53
1	C	312	VAL	CA-CB	5.09	1.60	1.54
1	F	123	THR	CA-CB	5.08	1.61	1.53
1	C	17	PRO	CA-C	5.08	1.59	1.52
1	H	153	VAL	CA-CB	5.07	1.60	1.54
1	G	367	ASN	C-O	5.06	1.30	1.23
1	A	190	PHE	CA-C	5.06	1.58	1.52
1	C	299	VAL	CA-C	5.03	1.57	1.52
1	B	236	ILE	C-O	-5.03	1.18	1.24

All (109) bond angle outliers are listed below:

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	252	TYR	CA-C-N	-10.54	108.92	119.78
1	F	252	TYR	C-N-CA	-10.54	108.92	119.78
1	F	233	VAL	N-CA-C	9.70	120.55	110.36
1	H	115	ASP	CA-C-N	8.51	128.72	119.87
1	H	115	ASP	C-N-CA	8.51	128.72	119.87
1	H	82	PHE	N-CA-C	-8.23	98.95	110.31
1	H	275	LEU	CA-C-N	-8.02	111.13	120.11
1	H	275	LEU	C-N-CA	-8.02	111.13	120.11
1	B	187	TYR	N-CA-C	-7.87	104.11	112.93
1	G	188	GLY	N-CA-C	7.30	122.98	113.27
1	E	188	GLY	N-CA-C	7.24	122.44	114.40
1	G	6	HIS	CA-C-N	7.04	127.00	120.03
1	G	6	HIS	C-N-CA	7.04	127.00	120.03
1	H	376	ILE	N-CA-C	-6.95	104.00	110.53
1	E	190	PHE	CA-C-N	-6.87	111.90	119.19
1	E	190	PHE	C-N-CA	-6.87	111.90	119.19
1	G	146	ALA	CA-C-N	-6.87	113.22	120.03
1	G	146	ALA	C-N-CA	-6.87	113.22	120.03
1	F	16	ILE	CA-C-N	-6.86	113.73	120.52
1	F	16	ILE	C-N-CA	-6.86	113.73	120.52
1	H	58	LYS	N-CA-C	6.85	118.40	111.07
1	A	288	SER	CA-CB-OG	-6.84	97.42	111.10
1	A	82	PHE	CA-C-N	-6.79	112.79	119.78
1	A	82	PHE	C-N-CA	-6.79	112.79	119.78
1	B	65	ASP	N-CA-C	-6.68	103.09	111.11
1	B	70	SER	CA-C-N	6.66	126.60	119.28
1	B	70	SER	C-N-CA	6.66	126.60	119.28
1	H	299	VAL	CA-C-N	-6.55	112.08	119.28
1	H	299	VAL	C-N-CA	-6.55	112.08	119.28
1	H	187	TYR	N-CA-C	-6.49	104.94	112.92
1	B	82	PHE	N-CA-C	-6.44	101.96	110.07
1	G	255	ASP	N-CA-C	6.43	119.28	111.82
1	F	135	GLY	N-CA-C	-6.41	105.04	112.73
1	D	115	ASP	CA-C-N	6.40	126.09	119.56
1	D	115	ASP	C-N-CA	6.40	126.09	119.56
1	F	324	ARG	N-CA-C	6.22	119.04	111.82
1	C	252	TYR	CA-C-N	-6.14	113.43	119.76
1	C	252	TYR	C-N-CA	-6.14	113.43	119.76
1	F	16	ILE	N-CA-C	6.02	114.11	108.15
1	H	183	ASN	CB-CA-C	-6.00	103.21	111.73
1	B	324	ARG	N-CA-C	5.96	117.86	111.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	317	ARG	N-CA-C	5.83	118.38	111.33
1	D	356	ALA	N-CA-C	5.82	117.30	111.07
1	F	402	ALA	CA-C-N	-5.80	115.95	121.46
1	F	402	ALA	C-N-CA	-5.80	115.95	121.46
1	C	82	PHE	N-CA-C	-5.77	102.80	110.07
1	F	302	ILE	N-CA-C	-5.74	105.14	110.53
1	A	189	ALA	N-CA-C	-5.72	105.19	111.82
1	E	402	ALA	CA-C-N	-5.68	116.70	121.58
1	E	402	ALA	C-N-CA	-5.68	116.70	121.58
1	G	187	TYR	N-CA-C	-5.66	105.95	112.92
1	F	395	PHE	N-CA-C	5.66	118.29	109.52
1	F	99	ASP	CA-C-N	-5.66	114.43	120.03
1	F	99	ASP	C-N-CA	-5.66	114.43	120.03
1	A	337	GLY	CA-C-N	5.61	125.98	119.47
1	A	337	GLY	C-N-CA	5.61	125.98	119.47
1	A	115	ASP	CA-C-N	5.57	125.24	119.56
1	A	115	ASP	C-N-CA	5.57	125.24	119.56
1	H	131	VAL	N-CA-C	-5.56	105.10	110.72
1	B	146	ALA	CA-C-N	-5.56	114.86	120.31
1	B	146	ALA	C-N-CA	-5.56	114.86	120.31
1	G	399	LEU	CA-C-N	-5.55	114.61	122.94
1	G	399	LEU	C-N-CA	-5.55	114.61	122.94
1	B	236	ILE	N-CA-C	-5.53	105.14	110.72
1	B	358	SER	N-CA-C	-5.51	105.36	111.36
1	C	199	MET	N-CA-C	-5.49	105.32	112.23
1	F	41	HIS	N-CA-C	-5.47	105.22	111.07
1	E	28	ILE	N-CA-C	5.46	116.23	110.72
1	F	82	PHE	CA-C-N	-5.46	114.16	119.78
1	F	82	PHE	C-N-CA	-5.46	114.16	119.78
1	C	146	ALA	CA-C-N	-5.45	114.97	120.31
1	C	146	ALA	C-N-CA	-5.45	114.97	120.31
1	A	102	PRO	CA-C-N	-5.40	113.68	122.65
1	A	102	PRO	C-N-CA	-5.40	113.68	122.65
1	A	29	THR	N-CA-C	-5.38	105.50	111.36
1	F	206	GLY	N-CA-C	-5.35	107.65	115.63
1	E	340	ILE	N-CA-C	5.35	115.56	110.42
1	G	296	SER	CA-C-N	-5.34	114.19	120.12
1	G	296	SER	C-N-CA	-5.34	114.19	120.12
1	G	103	ASP	N-CA-C	-5.33	105.04	112.45
1	H	128	TYR	N-CA-C	-5.32	105.48	111.28
1	H	323	GLU	N-CA-C	5.30	117.27	108.20
1	D	137	GLU	CB-CA-C	-5.30	102.56	110.88

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	271	SER	CB-CA-C	-5.29	100.48	110.16
1	E	48	THR	CA-C-N	5.28	128.35	120.95
1	E	48	THR	C-N-CA	5.28	128.35	120.95
1	A	58	LYS	N-CA-C	-5.26	105.62	111.36
1	F	52	GLY	N-CA-C	-5.25	106.44	112.73
1	B	368	MET	N-CA-C	-5.23	107.43	112.97
1	F	16	ILE	N-CA-CB	-5.20	106.00	111.36
1	B	11	VAL	N-CA-C	5.20	115.76	108.17
1	D	291	PHE	N-CA-C	-5.14	101.59	109.76
1	B	24	VAL	CA-C-O	5.14	122.53	119.19
1	C	190	PHE	CA-C-N	-5.13	113.63	119.28
1	C	190	PHE	C-N-CA	-5.13	113.63	119.28
1	G	357	ILE	N-CA-C	5.12	115.33	110.42
1	A	51	GLU	N-CA-C	-5.09	105.91	111.82
1	E	185	GLY	N-CA-C	5.09	120.39	111.78
1	B	216	ILE	N-CA-C	-5.08	100.80	108.12
1	A	52	GLY	N-CA-C	-5.07	106.61	112.50
1	A	187	TYR	N-CA-C	-5.07	106.93	113.02
1	E	42	CYS	N-CA-C	-5.07	105.83	111.36
1	E	291	PHE	N-CA-C	-5.07	101.71	109.76
1	F	65	ASP	N-CA-C	-5.07	105.88	111.71
1	E	368	MET	N-CA-C	-5.05	107.62	112.97
1	B	233	VAL	N-CA-C	5.04	116.36	110.62
1	E	288	SER	CA-CB-OG	-5.02	101.06	111.10
1	D	238	SER	N-CA-C	5.02	117.13	111.11
1	D	364	GLU	N-CA-C	5.00	119.09	112.89

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	3117	0	3108	66	0
1	B	3086	0	3083	104	0
1	C	3072	0	3064	67	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	D	3110	0	3102	77	1
1	E	3106	0	3099	61	0
1	F	3117	0	3108	121	0
1	G	3076	0	3078	104	0
1	H	2977	0	2990	129	2
2	A	1	0	0	0	0
2	B	1	0	0	0	0
2	C	1	0	0	0	0
2	D	1	0	0	0	0
2	E	1	0	0	0	0
2	F	1	0	0	0	0
2	G	1	0	0	0	0
2	H	1	0	0	0	0
3	A	13	0	18	1	0
3	B	13	0	18	2	0
3	C	13	0	18	1	0
3	D	13	0	18	2	0
3	E	13	0	18	0	0
3	F	13	0	18	1	0
3	G	13	0	18	1	0
3	H	13	0	18	2	0
4	A	372	0	0	15	0
4	B	243	0	0	11	0
4	C	338	0	0	4	0
4	D	343	0	0	7	0
4	E	368	0	0	10	1
4	F	270	0	0	27	0
4	G	235	0	0	13	0
4	H	200	0	0	9	0
All	All	27142	0	24776	705	2

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 14.

All (705) 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:263:ARG:HH11	1:H:263:ARG:CG	1.43	1.31
1:H:226:ASN:HD22	1:H:226:ASN:C	1.40	1.26
1:G:298:LEU:HD12	4:G:801:HOH:O	1.08	1.24
1:E:89:ARG:HG2	1:E:89:ARG:HH11	1.09	1.12

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:139:MET:HE3	1:B:248:LYS:CB	1.78	1.11
1:F:300:PRO:HG2	4:F:777:HOH:O	1.50	1.09
1:A:89:ARG:HH11	1:A:89:ARG:CG	1.65	1.09
1:B:139:MET:HE3	1:B:248:LYS:HB2	1.36	1.08
1:C:101:GLU:HB2	1:C:103:ASP:HB3	1.35	1.07
1:H:263:ARG:NH1	1:H:263:ARG:HG2	1.30	1.07
1:B:22:LYS:H	1:B:84:LYS:NZ	1.55	1.05
1:H:226:ASN:ND2	1:H:226:ASN:O	1.89	1.04
1:C:101:GLU:CB	1:C:103:ASP:HB3	1.88	1.03
1:F:18:VAL:HG21	1:F:139:MET:HG2	1.42	1.02
1:G:324:ARG:HH11	1:G:324:ARG:HG2	0.86	0.99
1:H:226:ASN:C	1:H:226:ASN:ND2	2.16	0.99
1:F:323:GLU:HG2	4:F:842:HOH:O	1.62	0.98
1:E:89:ARG:HH11	1:E:89:ARG:CG	1.76	0.98
1:A:89:ARG:NH1	1:A:89:ARG:HG2	1.48	0.97
1:G:324:ARG:HH11	1:G:324:ARG:CG	1.75	0.97
1:B:139:MET:CE	1:B:248:LYS:HB2	1.93	0.97
1:E:108:ARG:NH2	4:E:962:HOH:O	1.98	0.96
1:G:324:ARG:HG2	1:G:324:ARG:NH1	1.69	0.95
1:H:33:THR:HG21	4:H:759:HOH:O	1.65	0.94
1:H:89:ARG:HD2	1:H:96:ASP:O	1.68	0.94
1:B:75:LYS:C	1:B:76:GLN:HG3	1.92	0.94
1:B:22:LYS:H	1:B:84:LYS:HZ1	0.97	0.94
1:C:101:GLU:HB3	1:C:103:ASP:CB	1.97	0.94
1:D:104:GLN:OE1	1:D:104:GLN:HA	1.67	0.94
1:H:320:MET:HE1	1:H:329:LEU:HD21	1.51	0.93
1:B:223:SER:HA	3:B:502:PG4:H61	1.51	0.93
1:B:320:MET:HE1	1:B:329:LEU:HD11	1.50	0.93
1:D:39:ARG:NH2	1:D:94:ASN:ND2	2.17	0.93
1:D:27:ARG:HG2	4:D:638:HOH:O	1.71	0.91
1:H:288:SER:OG	1:H:289:HIS:HD2	1.52	0.91
1:B:139:MET:HE3	1:B:248:LYS:HB3	1.54	0.90
1:B:75:LYS:O	1:B:76:GLN:HG3	1.72	0.90
1:E:95:PHE:O	1:E:96:ASP:HB2	1.70	0.89
1:H:112:ILE:HG13	1:H:112:ILE:O	1.73	0.89
1:H:20:LEU:H	1:H:78:GLN:HE22	1.17	0.88
1:D:304:LYS:HZ3	1:D:347:GLU:HB2	1.38	0.88
1:F:205:TRP:HE1	1:G:204:GLN:HG2	1.39	0.87
1:H:58:LYS:HD2	1:H:58:LYS:O	1.73	0.87
1:F:85:LEU:N	1:F:85:LEU:HD23	1.88	0.87
1:A:89:ARG:HH11	1:A:89:ARG:HG2	0.75	0.86

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:89:ARG:HG2	1:E:89:ARG:NH1	1.87	0.86
1:F:211:LYS:NZ	4:F:617:HOH:O	2.09	0.86
1:H:220:GLU:HB3	1:H:222:MET:HE3	1.55	0.86
1:A:320:MET:HE1	1:A:405:VAL:HG11	1.56	0.85
1:D:320:MET:HE1	1:D:329:LEU:HD21	1.59	0.85
1:A:90:PHE:N	1:A:90:PHE:CD2	2.44	0.85
1:C:101:GLU:CB	1:C:103:ASP:CB	2.53	0.84
1:G:20:LEU:H	1:G:78:GLN:NE2	1.75	0.84
1:H:263:ARG:HH11	1:H:263:ARG:HG2	0.69	0.84
1:B:371:SER:O	1:B:375:HIS:HD2	1.60	0.84
1:F:20:LEU:H	1:F:78:GLN:NE2	1.76	0.84
1:D:39:ARG:NH2	1:D:94:ASN:HD22	1.75	0.83
1:B:76:GLN:NE2	4:B:730:HOH:O	2.08	0.83
1:H:139:MET:HE3	1:H:248:LYS:HB3	1.60	0.83
1:C:101:GLU:HB3	1:C:103:ASP:HB2	1.58	0.83
1:E:277:ASP:OD2	4:E:745:HOH:O	1.96	0.83
1:G:20:LEU:H	1:G:78:GLN:HE22	1.26	0.83
1:H:110:PHE:HB3	1:H:226:ASN:OD1	1.79	0.83
1:F:18:VAL:CG2	1:F:139:MET:HG2	2.09	0.82
1:F:24:VAL:HG21	1:F:29:THR:HG22	1.61	0.82
1:E:126:GLU:OE2	4:E:724:HOH:O	1.97	0.82
1:B:22:LYS:N	1:B:84:LYS:HZ1	1.78	0.81
1:B:14:ASP:O	1:B:16:ILE:HD12	1.80	0.81
1:D:20:LEU:H	1:D:78:GLN:HE22	1.25	0.81
1:A:320:MET:CE	1:A:405:VAL:HG11	2.10	0.80
1:G:329:LEU:HD22	1:G:389:ARG:HB2	1.63	0.80
1:B:25:PRO:HG2	1:B:28:ILE:HD12	1.63	0.79
1:F:24:VAL:CG2	1:F:29:THR:CG2	2.59	0.79
1:H:112:ILE:O	1:H:113:LYS:HG3	1.82	0.79
1:H:263:ARG:CG	1:H:263:ARG:NH1	2.15	0.79
1:A:256:GLU:OE1	1:A:259:ARG:NH2	2.12	0.79
1:A:20:LEU:H	1:A:78:GLN:NE2	1.81	0.79
1:F:18:VAL:HG21	1:F:139:MET:CG	2.13	0.79
1:F:20:LEU:H	1:F:78:GLN:HE22	1.30	0.78
1:H:293:MET:HE2	1:H:295:LEU:HD13	1.65	0.78
1:D:101:GLU:O	1:D:104:GLN:N	2.17	0.78
1:E:125:HIS:CE1	1:E:158:TYR:H	2.00	0.78
1:C:220:GLU:HB3	1:C:222:MET:CE	2.13	0.78
1:G:341:VAL:HG23	4:G:647:HOH:O	1.83	0.78
1:F:300:PRO:CG	4:F:777:HOH:O	2.19	0.77
1:B:259:ARG:NH1	1:B:260:GLN:CG	2.48	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:20:LEU:H	1:H:78:GLN:NE2	1.83	0.76
1:F:24:VAL:HG21	1:F:29:THR:CG2	2.15	0.76
1:E:32:LEU:CD1	1:E:88:ILE:HD13	2.15	0.76
1:F:205:TRP:NE1	1:G:204:GLN:HG2	1.99	0.76
1:A:125:HIS:CE1	1:A:158:TYR:H	2.04	0.76
1:F:164:ALA:O	1:F:168:VAL:HG23	1.86	0.76
1:E:20:LEU:H	1:E:78:GLN:HE22	1.30	0.76
1:G:139:MET:HE3	1:G:248:LYS:HB3	1.68	0.76
1:C:20:LEU:H	1:C:78:GLN:HE22	1.33	0.75
1:A:277:ASP:OD2	4:A:703:HOH:O	2.04	0.75
1:D:226:ASN:HB3	3:D:502:PG4:H51	1.69	0.75
1:H:351:ALA:H	1:H:354:GLN:HE21	1.32	0.75
1:G:299:VAL:HB	1:G:300:PRO:HD3	1.69	0.75
1:C:101:GLU:C	1:C:103:ASP:N	2.40	0.75
1:E:20:LEU:H	1:E:78:GLN:NE2	1.85	0.75
1:E:323:GLU:HB3	4:E:864:HOH:O	1.86	0.74
1:G:256:GLU:OE2	1:G:259:ARG:NH2	2.19	0.74
1:E:25:PRO:O	1:E:28:ILE:CG2	2.35	0.74
1:H:106:HIS:CE1	1:H:130:LYS:HZ2	2.05	0.74
1:A:20:LEU:H	1:A:78:GLN:HE22	1.36	0.74
1:G:89:ARG:HG3	1:G:96:ASP:HB3	1.69	0.74
1:B:395:PHE:HD2	4:B:649:HOH:O	1.69	0.73
1:C:22:LYS:HB2	1:C:22:LYS:NZ	2.03	0.73
1:C:220:GLU:HB3	1:C:222:MET:HE2	1.69	0.73
1:B:320:MET:HE2	1:B:325:ASP:HB3	1.70	0.73
1:D:55:GLN:OE1	1:D:55:GLN:HA	1.88	0.73
1:H:383:GLU:OE2	4:H:652:HOH:O	2.07	0.73
1:A:239:ALA:HA	3:A:502:PG4:H72	1.70	0.73
1:G:97:ILE:N	1:G:97:ILE:CD1	2.52	0.73
1:H:308:ARG:O	1:H:312:VAL:HG23	1.88	0.73
1:E:32:LEU:HD11	1:E:88:ILE:HD13	1.71	0.73
1:D:101:GLU:O	1:D:103:ASP:N	2.23	0.72
1:A:90:PHE:N	1:A:90:PHE:HD2	1.84	0.72
1:D:21:ALA:H	1:D:78:GLN:HE21	1.38	0.72
1:E:323:GLU:CB	4:E:864:HOH:O	2.36	0.72
1:F:15:PHE:CB	1:F:378:LYS:HB2	2.20	0.71
1:G:407:GLU:OE1	4:G:830:HOH:O	2.08	0.71
1:A:339:LYS:O	1:A:343:HIS:HD2	1.74	0.71
1:B:21:ALA:HB1	1:B:84:LYS:HE3	1.72	0.70
1:B:76:GLN:HG2	4:B:744:HOH:O	1.91	0.70
1:B:223:SER:HA	3:B:502:PG4:C6	2.21	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:205:TRP:HE1	1:G:204:GLN:CG	2.03	0.70
1:H:29:THR:O	1:H:33:THR:HG23	1.91	0.70
1:E:320:MET:HE1	1:E:329:LEU:HD21	1.73	0.70
1:A:288:SER:HB3	1:A:289:HIS:CD2	2.26	0.70
1:D:20:LEU:H	1:D:78:GLN:NE2	1.89	0.70
1:B:14:ASP:OD1	1:B:16:ILE:HD11	1.90	0.70
1:H:106:HIS:CE1	1:H:130:LYS:NZ	2.59	0.70
1:D:382:GLU:OE1	4:D:727:HOH:O	2.09	0.69
1:A:89:ARG:CG	1:A:89:ARG:NH1	2.35	0.69
1:D:263:ARG:HG2	1:D:263:ARG:HH11	1.56	0.69
1:E:89:ARG:CG	1:E:89:ARG:NH1	2.49	0.69
1:B:22:LYS:H	1:B:84:LYS:CE	2.05	0.69
1:F:256:GLU:OE2	1:F:259:ARG:NH2	2.25	0.69
1:C:39:ARG:NH2	1:C:94:ASN:OD1	2.26	0.69
1:H:282:MET:HE2	1:H:295:LEU:HD11	1.74	0.69
1:H:21:ALA:H	1:H:78:GLN:HE21	1.40	0.69
1:D:263:ARG:HG2	1:D:263:ARG:NH1	2.07	0.68
1:H:321:ASP:O	1:H:325:ASP:HB2	1.92	0.68
1:D:39:ARG:HH21	1:D:94:ASN:HD22	1.38	0.68
1:E:25:PRO:O	1:E:28:ILE:HG22	1.93	0.68
1:B:259:ARG:NH1	1:B:260:GLN:HG2	2.08	0.68
1:B:321:ASP:OD1	1:B:324:ARG:HB3	1.94	0.68
1:A:305:ARG:CD	4:A:747:HOH:O	2.42	0.68
1:F:65:ASP:HB2	4:F:785:HOH:O	1.94	0.68
1:C:323:GLU:HB2	4:C:866:HOH:O	1.94	0.68
1:G:125:HIS:CE1	1:G:158:TYR:H	2.11	0.67
1:H:58:LYS:HD2	1:H:58:LYS:C	2.19	0.67
1:C:323:GLU:OE1	4:C:866:HOH:O	2.12	0.67
1:G:14:ASP:OD2	4:G:760:HOH:O	2.12	0.67
1:A:90:PHE:HD2	1:A:90:PHE:H	1.34	0.67
1:G:97:ILE:N	1:G:97:ILE:HD13	2.10	0.67
1:A:284:TRP:CD1	4:A:722:HOH:O	2.47	0.67
1:B:322:PHE:CE2	1:B:326:LYS:HD3	2.29	0.67
1:H:276:PRO:HD2	1:H:306:HIS:CE1	2.30	0.67
1:G:57:TYR:O	1:G:61:LYS:HG3	1.95	0.66
1:G:397:PRO:O	1:G:400:THR:HG23	1.94	0.66
1:C:126:GLU:OE1	4:C:811:HOH:O	2.13	0.66
1:B:258:ARG:CG	1:B:258:ARG:HH11	2.08	0.66
1:F:300:PRO:CD	4:F:777:HOH:O	2.41	0.66
1:A:139:MET:HE3	1:A:248:LYS:HB3	1.76	0.66
1:G:92:ASP:OD1	1:G:92:ASP:N	2.24	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:89:ARG:HD3	1:D:96:ASP:O	1.95	0.66
1:E:339:LYS:HB3	1:E:343:HIS:NE2	2.10	0.66
1:F:329:LEU:HD11	1:F:389:ARG:HB2	1.78	0.66
1:H:220:GLU:HB3	1:H:222:MET:CE	2.24	0.66
1:H:288:SER:OG	1:H:289:HIS:CD2	2.43	0.66
1:F:71:PRO:HD2	4:F:608:HOH:O	1.96	0.65
1:F:21:ALA:H	1:F:78:GLN:HE21	1.43	0.65
1:H:89:ARG:NH2	1:H:98:ALA:HB2	2.11	0.65
1:H:270:MET:HG2	4:H:668:HOH:O	1.96	0.65
1:H:89:ARG:HD3	1:H:96:ASP:HB3	1.79	0.65
1:A:289:HIS:HE1	4:A:907:HOH:O	1.79	0.65
1:C:230:GLU:O	1:C:235:ASN:ND2	2.29	0.65
1:D:101:GLU:C	1:D:103:ASP:N	2.55	0.65
1:D:101:GLU:HB3	1:D:103:ASP:OD2	1.97	0.65
1:H:324:ARG:HB3	1:H:324:ARG:NH1	2.11	0.65
1:H:267:ILE:HG21	1:H:270:MET:HE2	1.77	0.65
1:B:103:ASP:N	1:B:103:ASP:OD1	2.26	0.65
1:B:259:ARG:HH12	1:B:260:GLN:CG	2.10	0.64
1:C:58:LYS:HZ2	1:C:58:LYS:CB	2.08	0.64
1:H:353:ASP:HA	4:H:764:HOH:O	1.97	0.64
1:D:97:ILE:HG22	1:D:108:ARG:HH22	1.63	0.64
1:F:86:THR:O	1:F:89:ARG:NH1	2.29	0.64
1:G:347:GLU:OE2	4:G:751:HOH:O	2.15	0.64
1:B:14:ASP:CG	1:B:16:ILE:HD11	2.22	0.64
1:B:321:ASP:O	1:B:325:ASP:HB2	1.96	0.64
1:H:32:LEU:HD12	1:H:95:PHE:CD2	2.33	0.64
1:B:103:ASP:CG	1:B:104:GLN:H	2.04	0.64
1:F:207:ALA:HB1	1:G:270:MET:HE2	1.80	0.64
1:A:21:ALA:H	1:A:78:GLN:HE21	1.46	0.64
1:F:349:GLY:HA2	4:F:866:HOH:O	1.97	0.64
1:A:339:LYS:O	1:A:343:HIS:CD2	2.51	0.63
1:G:324:ARG:CG	1:G:324:ARG:NH1	2.46	0.63
1:D:263:ARG:HG3	1:F:46:GLY:HA3	1.78	0.63
1:B:258:ARG:HH11	1:B:258:ARG:HG3	1.63	0.63
1:H:75:LYS:HE2	1:H:364:GLU:OE2	1.99	0.63
1:H:351:ALA:H	1:H:354:GLN:NE2	1.96	0.63
1:A:339:LYS:CG	4:A:642:HOH:O	2.45	0.63
1:B:334:HIS:ND1	4:B:606:HOH:O	2.30	0.63
1:C:20:LEU:H	1:C:78:GLN:NE2	1.96	0.63
1:B:50:GLU:OE1	1:B:50:GLU:HA	1.98	0.62
1:F:300:PRO:HD2	4:F:777:HOH:O	1.98	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:304:LYS:HZ2	1:F:347:GLU:HB2	1.65	0.62
1:B:305:ARG:NH2	1:F:103:ASP:HB2	2.13	0.62
1:F:154:THR:HG22	1:F:182:TYR:CE1	2.35	0.62
1:F:19:GLN:HE22	1:F:22:LYS:NZ	1.98	0.62
1:F:323:GLU:HB3	4:F:784:HOH:O	1.98	0.62
1:A:320:MET:HE1	1:A:405:VAL:CG1	2.29	0.62
1:F:85:LEU:HD23	1:F:85:LEU:H	1.62	0.62
1:D:89:ARG:NE	1:D:96:ASP:HB3	2.15	0.62
1:D:104:GLN:OE1	1:D:104:GLN:CA	2.44	0.62
1:H:20:LEU:N	1:H:78:GLN:HE22	1.94	0.62
1:C:101:GLU:O	1:C:104:GLN:N	2.24	0.61
1:C:320:MET:HE1	1:C:329:LEU:HD21	1.81	0.61
1:G:12:LEU:HD23	1:G:251:VAL:HG22	1.82	0.61
1:B:22:LYS:N	1:B:84:LYS:CE	2.64	0.61
1:E:25:PRO:O	1:E:28:ILE:HG23	1.99	0.61
1:B:89:ARG:HB2	1:B:96:ASP:HB2	1.82	0.61
1:D:304:LYS:NZ	1:D:347:GLU:OE1	2.34	0.61
1:H:263:ARG:HH11	1:H:263:ARG:CB	2.11	0.61
1:G:103:ASP:O	1:G:106:HIS:HD2	1.83	0.61
1:G:168:VAL:HG13	1:G:173:TRP:HB2	1.82	0.61
1:H:282:MET:HG3	1:H:295:LEU:CD1	2.30	0.61
1:F:329:LEU:CD1	1:F:389:ARG:HB2	2.31	0.61
1:G:404:LEU:HD13	4:G:674:HOH:O	2.00	0.61
1:H:29:THR:O	1:H:33:THR:CG2	2.49	0.61
1:H:263:ARG:HH11	1:H:263:ARG:CA	2.13	0.61
1:G:89:ARG:HG2	4:G:809:HOH:O	2.00	0.61
1:B:139:MET:HE2	1:B:140:PHE:CE2	2.36	0.60
1:B:256:GLU:OE2	1:B:260:GLN:OE1	2.18	0.60
1:E:21:ALA:H	1:E:78:GLN:HE21	1.48	0.60
1:F:356:ALA:O	4:F:662:HOH:O	2.16	0.60
1:F:197:HIS:CB	1:F:270:MET:HE1	2.31	0.60
1:B:20:LEU:H	1:B:78:GLN:HE22	1.48	0.60
1:E:339:LYS:O	1:E:343:HIS:CD2	2.55	0.60
1:E:324:ARG:NH1	1:E:325:ASP:OD1	2.34	0.60
1:A:305:ARG:HD3	4:A:747:HOH:O	2.00	0.60
1:B:139:MET:HE1	1:B:248:LYS:HB2	1.81	0.60
1:C:22:LYS:HB2	1:C:22:LYS:HZ3	1.67	0.60
1:G:324:ARG:HB2	1:G:325:ASP:OD1	2.02	0.60
1:F:205:TRP:CZ2	1:G:201:ALA:HA	2.37	0.59
1:C:22:LYS:NZ	1:C:22:LYS:CB	2.65	0.59
1:F:255:ASP:O	4:F:800:HOH:O	2.17	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:288:SER:HB2	4:E:632:HOH:O	2.03	0.59
1:F:259:ARG:HG2	1:F:259:ARG:HH11	1.67	0.59
1:A:305:ARG:HD2	4:A:747:HOH:O	2.01	0.59
1:A:288:SER:HB3	1:A:289:HIS:HD2	1.65	0.58
1:B:259:ARG:HH12	1:B:260:GLN:HG2	1.67	0.58
1:A:339:LYS:HB2	4:A:642:HOH:O	2.02	0.58
1:F:70:SER:HB2	1:F:71:PRO:CD	2.34	0.58
1:G:150:LEU:C	1:G:150:LEU:HD23	2.28	0.58
1:G:321:ASP:CB	1:G:324:ARG:HD3	2.34	0.58
1:D:101:GLU:OE1	1:D:103:ASP:OD2	2.21	0.58
1:H:232:ARG:O	1:H:233:VAL:C	2.46	0.58
1:H:398:GLY:N	1:H:399:LEU:HA	2.19	0.58
1:G:64:PHE:CE2	1:G:236:ILE:HG23	2.39	0.58
1:A:342:ASP:OD1	1:A:359:LYS:HE2	2.03	0.58
1:E:32:LEU:HD12	1:E:88:ILE:HD13	1.84	0.57
1:B:22:LYS:O	1:B:84:LYS:HE2	2.04	0.57
1:C:21:ALA:H	1:C:78:GLN:HE21	1.52	0.57
1:D:101:GLU:O	1:D:102:PRO:C	2.47	0.57
1:E:103:ASP:OD2	1:E:103:ASP:N	2.33	0.57
1:D:97:ILE:CG2	1:D:108:ARG:NH2	2.68	0.57
1:H:110:PHE:C	1:H:110:PHE:CD2	2.82	0.57
1:H:89:ARG:HH22	1:H:98:ALA:HB2	1.69	0.57
1:B:139:MET:CE	1:B:248:LYS:CB	2.60	0.56
1:D:382:GLU:HG2	4:F:776:HOH:O	2.05	0.56
1:G:325:ASP:OD1	1:G:325:ASP:N	2.36	0.56
1:A:56:VAL:O	1:A:60:VAL:HG23	2.05	0.56
1:B:259:ARG:NH1	1:B:260:GLN:HG3	2.20	0.56
1:H:227:ASN:ND2	1:H:230:GLU:HG3	2.20	0.56
1:E:24:VAL:HG12	1:E:28:ILE:HG23	1.87	0.56
1:G:300:PRO:HB3	1:G:343:HIS:CD2	2.40	0.56
1:G:353:ASP:OD1	1:G:353:ASP:C	2.49	0.56
1:F:205:TRP:CE2	1:G:204:GLN:HG2	2.40	0.56
1:E:89:ARG:HH11	1:E:89:ARG:N	2.04	0.56
1:F:90:PHE:CD1	1:F:90:PHE:C	2.83	0.56
1:A:201:ALA:HA	1:C:205:TRP:CZ2	2.41	0.56
1:A:382:GLU:OE2	4:A:801:HOH:O	2.18	0.56
1:E:284:TRP:CD1	4:E:767:HOH:O	2.59	0.56
1:E:339:LYS:HB3	1:E:343:HIS:CD2	2.40	0.56
1:F:392:CYS:SG	1:F:406:LEU:HD12	2.46	0.56
4:F:603:HOH:O	1:G:400:THR:HG21	2.05	0.56
1:F:133:GLY:O	1:F:137:GLU:HG3	2.06	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:22:LYS:N	1:B:84:LYS:HE2	2.21	0.55
1:B:46:GLY:HA3	1:C:263:ARG:HG3	1.88	0.55
1:F:298:LEU:C	1:F:300:PRO:HD2	2.30	0.55
1:G:43:LEU:HD11	1:G:113:LYS:C	2.31	0.55
1:G:340:ILE:O	1:G:344:VAL:HG23	2.06	0.55
1:D:260:GLN:HB2	1:D:262:LEU:HD13	1.88	0.55
1:G:274:LEU:HD23	1:G:400:THR:HG22	1.88	0.55
1:C:130:LYS:HZ2	1:C:134:LYS:HE3	1.71	0.55
1:D:49:ASP:OD2	1:D:51:GLU:HB3	2.06	0.55
1:D:101:GLU:C	1:D:103:ASP:H	2.14	0.55
1:D:138:GLN:O	1:D:141:GLU:HG2	2.07	0.55
1:G:300:PRO:HB3	1:G:343:HIS:HD2	1.72	0.55
1:C:212:THR:HB	1:C:256:GLU:HG2	1.87	0.55
1:H:32:LEU:HD12	1:H:95:PHE:CE2	2.42	0.55
1:B:150:LEU:HD12	1:B:215:ASP:O	2.07	0.55
1:B:299:VAL:HB	1:B:300:PRO:HD3	1.89	0.55
1:A:69:VAL:HG11	1:A:74:ILE:HD12	1.89	0.55
1:B:56:VAL:HG23	4:B:702:HOH:O	2.06	0.55
1:D:102:PRO:C	1:D:104:GLN:H	2.15	0.55
1:F:24:VAL:HG23	1:F:29:THR:HG23	1.89	0.55
1:H:241:LEU:HD21	1:H:336:GLY:O	2.07	0.55
1:B:384:ALA:O	1:B:408:LYS:NZ	2.37	0.55
1:A:339:LYS:CB	4:A:642:HOH:O	2.54	0.54
1:E:371:SER:C	1:E:374:PRO:HD2	2.32	0.54
1:F:101:GLU:HB3	4:F:832:HOH:O	2.07	0.54
1:G:321:ASP:HB3	1:G:324:ARG:HD3	1.88	0.54
1:G:353:ASP:OD1	1:G:354:GLN:N	2.40	0.54
1:C:102:PRO:C	1:C:104:GLN:N	2.63	0.54
1:F:325:ASP:O	1:F:329:LEU:HD22	2.07	0.54
1:B:320:MET:HE1	1:B:329:LEU:CD1	2.30	0.54
1:C:101:GLU:O	1:C:102:PRO:C	2.47	0.54
1:D:260:GLN:CB	1:D:262:LEU:HD13	2.38	0.54
1:G:332:ALA:O	1:G:392:CYS:HA	2.08	0.54
1:C:104:GLN:HA	1:C:106:HIS:HD2	1.72	0.54
1:F:260:GLN:HB3	1:F:262:LEU:HG	1.88	0.54
1:E:32:LEU:HD12	1:E:88:ILE:CD1	2.37	0.54
1:A:50:GLU:O	1:A:54:VAL:HG23	2.07	0.54
1:B:201:ALA:HA	1:H:205:TRP:CZ2	2.42	0.54
1:D:263:ARG:HH11	1:D:263:ARG:CG	2.21	0.54
1:G:226:ASN:ND2	4:G:716:HOH:O	2.41	0.54
1:F:15:PHE:HB2	1:F:378:LYS:HB2	1.88	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:304:LYS:NZ	1:F:347:GLU:HB2	2.23	0.54
1:B:120:ASP:C	1:B:120:ASP:OD1	2.50	0.53
1:H:57:TYR:CE1	1:H:61:LYS:HD2	2.43	0.53
1:E:150:LEU:C	1:E:150:LEU:HD23	2.34	0.53
1:G:195:MET:O	1:G:199:MET:HG3	2.09	0.53
1:F:301:ALA:O	4:F:860:HOH:O	2.19	0.53
1:G:398:GLY:N	1:G:399:LEU:HA	2.23	0.53
1:H:63:LYS:HD2	1:H:236:ILE:HD11	1.90	0.53
1:H:268:LEU:HD12	1:H:405:VAL:HG12	1.90	0.53
1:F:226:ASN:HB3	3:F:502:PG4:H52	1.89	0.53
1:F:146:ALA:HB2	1:F:173:TRP:CD1	2.44	0.53
1:H:85:LEU:O	1:H:87:ASP:N	2.42	0.53
1:C:256:GLU:OE1	1:C:259:ARG:NH2	2.38	0.53
1:F:205:TRP:CZ2	1:G:204:GLN:HG2	2.44	0.53
1:B:21:ALA:H	1:B:78:GLN:HE21	1.55	0.53
1:D:85:LEU:HD22	4:D:661:HOH:O	2.09	0.53
1:E:125:HIS:HE1	1:E:158:TYR:H	1.54	0.53
1:F:314:LEU:O	1:F:317:ARG:HB2	2.08	0.53
1:D:101:GLU:O	1:D:104:GLN:HB2	2.09	0.53
1:G:21:ALA:H	1:G:78:GLN:HE21	1.57	0.53
1:G:342:ASP:OD2	4:G:768:HOH:O	2.19	0.53
1:H:282:MET:HG3	1:H:295:LEU:HD12	1.91	0.53
1:F:182:TYR:HE2	1:G:183:ASN:HD22	1.58	0.52
1:H:63:LYS:HD2	1:H:236:ILE:CD1	2.39	0.52
1:B:253:PRO:HB2	1:B:255:ASP:OD1	2.10	0.52
1:D:32:LEU:HD22	1:D:95:PHE:CE1	2.45	0.52
1:H:190:PHE:HB2	1:H:191:PRO:CD	2.39	0.52
1:G:304:LYS:HD2	1:G:343:HIS:HB3	1.91	0.52
1:F:334:HIS:HB3	4:F:712:HOH:O	2.10	0.52
1:G:57:TYR:CE1	1:G:61:LYS:HD3	2.45	0.52
1:G:397:PRO:O	1:G:400:THR:CG2	2.57	0.52
1:H:227:ASN:HD21	1:H:230:GLU:HG3	1.74	0.52
1:B:322:PHE:O	1:B:323:GLU:C	2.52	0.52
1:C:222:MET:O	3:C:502:PG4:H81	2.10	0.52
1:G:20:LEU:N	1:G:78:GLN:NE2	2.53	0.52
1:G:150:LEU:HD23	1:G:151:ILE:N	2.26	0.52
1:B:259:ARG:HH11	1:B:260:GLN:HG3	1.74	0.51
1:F:373:ILE:HD13	1:F:376:ILE:HD12	1.92	0.51
1:F:381:LEU:O	1:F:408:LYS:NZ	2.37	0.51
1:E:288:SER:HB3	1:E:289:HIS:ND1	2.24	0.51
1:H:329:LEU:CD2	1:H:389:ARG:HB2	2.41	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:74:ILE:HG21	1:F:77:ARG:HG3	1.92	0.51
1:B:190:PHE:HB2	1:B:191:PRO:HD3	1.93	0.51
1:D:97:ILE:HG22	1:D:108:ARG:NH2	2.26	0.51
1:A:395:PHE:HD2	4:A:690:HOH:O	1.93	0.51
1:C:222:MET:HE3	1:C:369:SER:HB3	1.91	0.51
1:D:122:LYS:HE3	1:D:126:GLU:OE2	2.10	0.51
1:C:220:GLU:HB3	1:C:222:MET:HE3	1.90	0.51
1:B:69:VAL:HG11	1:B:74:ILE:CD1	2.40	0.51
1:D:139:MET:HE2	1:D:246:LEU:HB3	1.92	0.51
1:H:63:LYS:HG2	1:H:67:TYR:HD1	1.76	0.51
1:H:315:LEU:HD22	1:H:322:PHE:HA	1.92	0.51
1:H:342:ASP:OD1	1:H:359:LYS:HE2	2.10	0.51
1:E:27:ARG:NH2	4:E:681:HOH:O	2.44	0.51
1:E:324:ARG:CZ	1:E:325:ASP:OD1	2.59	0.51
1:C:241:LEU:HD21	1:C:336:GLY:O	2.11	0.51
1:D:18:VAL:HG23	4:D:913:HOH:O	2.11	0.51
1:D:51:GLU:OE1	1:D:51:GLU:HA	2.11	0.51
1:H:263:ARG:NH1	1:H:263:ARG:HA	2.24	0.51
1:A:315:LEU:CD2	1:A:322:PHE:HA	2.41	0.50
1:F:260:GLN:HG2	1:F:262:LEU:HD11	1.92	0.50
1:A:125:HIS:HE1	1:A:158:TYR:H	1.56	0.50
1:C:103:ASP:C	1:C:104:GLN:HG2	2.36	0.50
1:F:135:GLY:O	1:F:139:MET:HG3	2.11	0.50
1:H:324:ARG:HB3	1:H:324:ARG:CZ	2.40	0.50
1:A:104:GLN:NE2	1:A:107:LEU:CD1	2.75	0.50
1:G:270:MET:HG2	4:G:674:HOH:O	2.12	0.50
1:F:12:LEU:HD23	1:F:251:VAL:HG22	1.93	0.50
1:F:24:VAL:HG23	1:F:29:THR:CG2	2.37	0.50
1:F:225:HIS:O	1:F:226:ASN:C	2.54	0.50
1:H:63:LYS:CD	1:H:236:ILE:CD1	2.89	0.50
1:C:130:LYS:HZ2	1:C:134:LYS:CE	2.24	0.50
1:H:64:PHE:O	1:H:68:ALA:HB3	2.11	0.50
1:B:20:LEU:H	1:B:78:GLN:NE2	2.09	0.50
1:B:255:ASP:OD1	1:B:255:ASP:N	2.44	0.50
1:F:90:PHE:C	1:F:90:PHE:HD1	2.19	0.50
1:H:323:GLU:OE1	1:H:323:GLU:HA	2.12	0.50
1:B:392:CYS:HB2	1:B:404:LEU:HB3	1.94	0.49
1:G:91:GLY:O	1:G:92:ASP:C	2.54	0.49
1:C:11:VAL:HG11	1:C:257:LEU:HD22	1.94	0.49
1:F:266:ARG:HD3	4:F:753:HOH:O	2.12	0.49
1:B:338:PRO:HD2	4:B:601:HOH:O	2.11	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:346:GLU:O	1:G:346:GLU:HG3	2.03	0.49
1:H:20:LEU:N	1:H:78:GLN:NE2	2.55	0.49
1:H:64:PHE:O	1:H:68:ALA:CB	2.60	0.49
1:G:308:ARG:HA	1:G:348:LEU:HD21	1.95	0.49
1:H:263:ARG:NH1	1:H:263:ARG:CA	2.75	0.49
1:D:315:LEU:HD12	1:D:322:PHE:HA	1.95	0.49
1:A:49:ASP:OD2	1:A:52:GLY:N	2.46	0.49
1:B:149:ASP:OD2	1:B:211:LYS:NZ	2.34	0.49
1:G:223:SER:HA	3:G:502:PG4:H32	1.95	0.49
1:A:315:LEU:HD23	1:A:322:PHE:HA	1.95	0.49
1:C:101:GLU:C	1:C:103:ASP:H	2.16	0.49
1:C:102:PRO:C	1:C:104:GLN:H	2.19	0.49
1:B:282:MET:HG3	1:B:295:LEU:HD13	1.95	0.48
1:G:20:LEU:N	1:G:78:GLN:HE22	2.05	0.48
1:B:160:ALA:HA	1:B:161:PRO:C	2.37	0.48
1:F:13:ALA:HB3	1:F:252:TYR:CE2	2.48	0.48
1:F:139:MET:HE1	1:F:217:ALA:HB1	1.95	0.48
1:H:120:ASP:OD1	1:H:120:ASP:C	2.57	0.48
1:D:205:TRP:CZ2	1:E:201:ALA:HA	2.48	0.48
1:D:258:ARG:O	1:D:259:ARG:C	2.56	0.48
1:F:197:HIS:HB3	1:F:270:MET:HE1	1.94	0.48
1:F:326:LYS:HG2	4:F:630:HOH:O	2.12	0.48
1:H:82:PHE:CG	1:H:83:PRO:HD2	2.48	0.48
1:H:304:LYS:O	1:H:307:VAL:HG12	2.14	0.48
1:A:104:GLN:NE2	1:A:107:LEU:HD12	2.28	0.48
1:D:20:LEU:N	1:D:78:GLN:HE22	2.04	0.48
1:H:75:LYS:HE2	1:H:364:GLU:CD	2.38	0.48
1:A:205:TRP:CZ2	1:C:201:ALA:HA	2.49	0.48
1:F:160:ALA:HA	1:F:161:PRO:C	2.38	0.48
1:G:103:ASP:O	1:G:106:HIS:CD2	2.66	0.48
1:A:108:ARG:NH2	4:A:846:HOH:O	1.98	0.47
1:B:207:ALA:HB1	1:H:270:MET:HE3	1.95	0.47
1:D:39:ARG:HH22	1:D:94:ASN:ND2	2.08	0.47
1:F:317:ARG:HG2	1:G:209:PRO:HD3	1.96	0.47
1:F:323:GLU:CB	4:F:784:HOH:O	2.61	0.47
1:H:27:ARG:HG3	1:H:28:ILE:N	2.28	0.47
1:E:138:GLN:O	1:E:141:GLU:HG2	2.14	0.47
1:G:326:LYS:O	1:G:354:GLN:NE2	2.48	0.47
1:H:223:SER:HA	3:H:502:PG4:H32	1.96	0.47
1:G:233:VAL:HG23	4:G:657:HOH:O	2.14	0.47
1:H:83:PRO:HG2	1:H:88:ILE:HD11	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:357:ILE:HD12	1:A:380:TYR:CE1	2.50	0.47
1:E:168:VAL:HG13	1:E:173:TRP:HB2	1.96	0.47
1:E:395:PHE:HA	1:E:400:THR:O	2.14	0.47
1:B:84:LYS:HD2	4:B:788:HOH:O	2.14	0.47
4:B:624:HOH:O	1:F:134:LYS:HD2	2.14	0.47
1:A:115:ASP:OD2	1:A:117:ARG:NH2	2.32	0.47
1:A:130:LYS:HG2	4:A:811:HOH:O	2.14	0.47
1:B:315:LEU:HD12	1:B:315:LEU:N	2.28	0.47
1:D:304:LYS:NZ	1:D:347:GLU:HB2	2.19	0.47
1:B:14:ASP:O	1:B:16:ILE:CD1	2.58	0.47
1:B:69:VAL:HG11	1:B:74:ILE:HD12	1.97	0.47
1:G:27:ARG:HD2	1:G:31:GLU:OE2	2.15	0.47
1:G:120:ASP:C	1:G:120:ASP:OD1	2.56	0.47
1:B:371:SER:O	1:B:375:HIS:CD2	2.52	0.47
1:G:315:LEU:HG	1:G:320:MET:HE3	1.97	0.47
1:H:284:TRP:CD1	4:H:686:HOH:O	2.68	0.47
1:E:256:GLU:OE1	1:E:259:ARG:NH2	2.26	0.47
1:G:298:LEU:O	1:G:302:ILE:HG13	2.14	0.47
1:A:170:ASP:O	4:A:909:HOH:O	2.20	0.47
1:E:339:LYS:O	1:E:343:HIS:HD2	1.96	0.47
1:E:389:ARG:C	1:E:390:ILE:HG13	2.40	0.47
1:H:315:LEU:HD22	1:H:322:PHE:HD1	1.80	0.47
1:A:51:GLU:OE2	1:A:55:GLN:HG2	2.15	0.46
1:G:398:GLY:HA3	1:G:400:THR:HG22	1.97	0.46
1:G:335:PRO:HB2	1:G:362:PHE:CD1	2.51	0.46
1:C:222:MET:HE3	1:C:369:SER:CB	2.46	0.46
1:E:89:ARG:HH11	1:E:89:ARG:CB	2.25	0.46
1:F:50:GLU:HA	1:F:50:GLU:OE1	2.16	0.46
1:F:174:PHE:CZ	1:G:276:PRO:HA	2.51	0.46
1:G:392:CYS:HB2	1:G:404:LEU:HB3	1.97	0.46
1:H:395:PHE:HA	1:H:400:THR:O	2.15	0.46
1:D:20:LEU:N	1:D:78:GLN:NE2	2.62	0.46
1:F:373:ILE:HD13	1:F:373:ILE:HA	1.71	0.46
1:B:64:PHE:O	1:B:65:ASP:C	2.59	0.46
1:A:232:ARG:NH1	1:A:234:ASP:OD1	2.42	0.46
1:D:226:ASN:CB	3:D:502:PG4:H51	2.42	0.46
1:C:256:GLU:O	1:C:260:GLN:HG3	2.15	0.46
1:F:236:ILE:O	1:F:237:ILE:C	2.55	0.46
1:F:272:GLU:HA	1:F:401:ALA:O	2.16	0.46
1:H:285:VAL:HA	1:H:286:PRO:HD3	1.80	0.46
1:E:339:LYS:CB	1:E:343:HIS:NE2	2.79	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:111:ASP:OD1	1:B:111:ASP:C	2.59	0.46
1:B:306:HIS:HB3	4:B:645:HOH:O	2.15	0.46
1:C:146:ALA:HB2	1:C:173:TRP:CD1	2.51	0.46
1:B:335:PRO:HB2	1:B:362:PHE:CD1	2.50	0.45
1:F:299:VAL:N	1:F:300:PRO:CD	2.79	0.45
1:A:339:LYS:HB3	1:A:343:HIS:CD2	2.52	0.45
1:B:104:GLN:O	1:B:104:GLN:HG3	2.16	0.45
1:B:398:GLY:N	1:B:399:LEU:HA	2.31	0.45
1:F:83:PRO:HG3	1:F:97:ILE:HD12	1.98	0.45
1:H:190:PHE:HB2	1:H:191:PRO:HD2	1.98	0.45
1:H:315:LEU:HD21	1:H:329:LEU:CD1	2.46	0.45
1:B:97:ILE:HD13	1:B:108:ARG:HH12	1.81	0.45
1:B:326:LYS:HE3	1:B:326:LYS:HB3	1.79	0.45
1:H:266:ARG:O	1:H:406:LEU:HA	2.17	0.45
1:A:104:GLN:HE21	1:A:107:LEU:HD12	1.82	0.45
1:B:231:SER:O	1:B:232:ARG:C	2.59	0.45
1:H:371:SER:C	1:H:374:PRO:HD2	2.42	0.45
1:D:407:GLU:OE2	4:D:871:HOH:O	2.21	0.45
1:F:297:PRO:O	1:F:300:PRO:HD2	2.16	0.45
1:H:226:ASN:ND2	4:H:691:HOH:O	2.06	0.45
1:C:130:LYS:NZ	1:C:134:LYS:CE	2.80	0.45
1:H:329:LEU:HD23	1:H:389:ARG:HB2	1.99	0.45
1:C:382:GLU:OE1	4:C:809:HOH:O	2.21	0.45
1:A:318:ALA:HB3	1:A:320:MET:HE3	1.99	0.45
1:B:305:ARG:HH22	1:F:103:ASP:HB2	1.78	0.45
1:F:339:LYS:HD3	4:F:744:HOH:O	2.17	0.45
1:H:103:ASP:CG	1:H:104:GLN:N	2.75	0.45
1:C:109:LEU:HD13	1:C:124:ARG:HG2	1.98	0.45
1:E:326:LYS:NZ	1:E:349:GLY:O	2.50	0.45
1:H:291:PHE:N	1:H:291:PHE:CD1	2.83	0.45
1:H:183:ASN:CG	1:H:183:ASN:O	2.59	0.44
1:H:345:GLN:HG3	1:H:350:LEU:HB2	2.00	0.44
1:A:130:LYS:HB3	1:A:130:LYS:HE3	1.44	0.44
1:E:32:LEU:HA	1:E:32:LEU:HD23	1.55	0.44
1:H:168:VAL:HG13	1:H:173:TRP:HB2	2.00	0.44
1:A:110:PHE:HB3	1:A:226:ASN:HD21	1.83	0.44
1:D:263:ARG:HA	1:D:263:ARG:HD3	1.90	0.44
1:D:398:GLY:N	1:D:399:LEU:HA	2.31	0.44
1:B:298:LEU:CD2	1:F:102:PRO:HG2	2.48	0.44
4:B:659:HOH:O	1:C:382:GLU:HG2	2.17	0.44
1:A:245:GLY:C	1:A:246:LEU:HD12	2.42	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:316:ARG:HD2	4:D:942:HOH:O	2.17	0.44
1:F:111:ASP:OD2	1:F:115:ASP:N	2.46	0.44
1:F:329:LEU:HD12	1:F:389:ARG:O	2.18	0.44
1:H:84:LYS:O	1:H:85:LEU:C	2.60	0.44
1:A:139:MET:HE1	1:A:217:ALA:HB1	1.98	0.44
1:C:111:ASP:HB3	1:C:115:ASP:O	2.18	0.44
1:E:89:ARG:NH1	1:E:89:ARG:N	2.66	0.44
1:E:308:ARG:O	1:E:312:VAL:HG23	2.18	0.44
1:F:205:TRP:HZ2	1:G:204:GLN:HB3	1.82	0.44
1:B:322:PHE:CZ	1:B:326:LYS:HD3	2.52	0.44
1:D:103:ASP:O	1:D:104:GLN:OE1	2.36	0.44
1:F:24:VAL:CG2	1:F:24:VAL:O	2.63	0.44
1:F:145:GLU:OE2	1:F:145:GLU:HA	2.18	0.44
1:F:316:ARG:HD2	4:F:737:HOH:O	2.17	0.44
1:F:385:THR:O	1:F:386:VAL:C	2.61	0.44
1:F:408:LYS:HG2	1:F:409:ILE:N	2.32	0.44
1:B:161:PRO:HD2	4:B:607:HOH:O	2.18	0.43
1:F:255:ASP:CG	4:F:786:HOH:O	2.61	0.43
1:G:186:CYS:HB3	1:G:334:HIS:NE2	2.33	0.43
1:G:256:GLU:CD	1:G:259:ARG:HH21	2.24	0.43
1:D:194:LYS:HD2	1:D:194:LYS:C	2.43	0.43
1:D:382:GLU:HG2	1:F:48:THR:OG1	2.18	0.43
1:F:8:ASN:HA	1:G:205:TRP:CZ2	2.53	0.43
1:F:369:SER:OG	1:F:370:SER:N	2.52	0.43
1:C:101:GLU:O	1:C:103:ASP:N	2.52	0.43
1:E:139:MET:SD	1:E:248:LYS:HB3	2.58	0.43
1:E:315:LEU:HD21	1:E:329:LEU:HD11	2.01	0.43
1:F:322:PHE:O	1:F:326:LYS:HD2	2.18	0.43
1:B:279:ALA:HA	1:B:398:GLY:O	2.19	0.43
1:B:357:ILE:HD12	1:B:380:TYR:CE2	2.53	0.43
1:E:281:THR:HB	1:E:296:SER:HB3	2.00	0.43
1:G:149:ASP:OD1	1:G:177:THR:HB	2.18	0.43
1:H:148:ASP:HB3	1:H:211:LYS:HG2	2.00	0.43
1:H:322:PHE:O	1:H:326:LYS:HB3	2.18	0.43
1:F:70:SER:HB2	1:F:71:PRO:HD2	2.00	0.43
1:H:6:HIS:HB2	1:H:254:GLU:OE1	2.18	0.43
1:H:190:PHE:CB	1:H:191:PRO:CD	2.97	0.43
1:A:322:PHE:CZ	1:A:326:LYS:HD2	2.53	0.43
1:B:97:ILE:HD13	1:B:108:ARG:NH1	2.33	0.43
1:F:97:ILE:HB	4:F:798:HOH:O	2.18	0.43
1:G:347:GLU:CD	4:G:751:HOH:O	2.60	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:321:ASP:O	1:H:323:GLU:N	2.51	0.43
1:B:75:LYS:C	1:B:76:GLN:CG	2.76	0.43
1:B:111:ASP:OD2	1:B:114:LYS:HB2	2.19	0.43
1:B:172:GLY:HA2	1:B:174:PHE:CE2	2.54	0.43
1:D:85:LEU:C	1:D:87:ASP:H	2.27	0.43
1:F:398:GLY:N	1:F:399:LEU:HA	2.34	0.43
1:A:398:GLY:N	1:A:399:LEU:HA	2.33	0.43
1:D:156:SER:OG	1:D:220:GLU:HA	2.18	0.43
1:D:260:GLN:O	1:D:262:LEU:HD13	2.19	0.43
1:G:111:ASP:OD2	1:G:114:LYS:HG3	2.18	0.43
1:H:313:ASP:OD1	1:H:316:ARG:NH2	2.52	0.43
1:A:24:VAL:O	1:A:24:VAL:HG23	2.18	0.43
1:B:212:THR:O	1:B:253:PRO:HD2	2.19	0.43
1:C:315:LEU:HD12	1:C:322:PHE:HA	2.01	0.43
1:D:115:ASP:HA	1:D:116:PRO:HD2	1.83	0.43
1:F:26:GLN:HB2	1:F:74:ILE:O	2.18	0.43
1:H:81:TYR:CE1	1:H:224:ALA:HB2	2.54	0.43
1:H:324:ARG:HG2	1:H:324:ARG:O	2.19	0.43
1:E:8:ASN:N	1:E:8:ASN:HD22	2.17	0.42
1:G:106:HIS:NE2	1:G:130:LYS:HE3	2.34	0.42
1:D:85:LEU:C	1:D:87:ASP:N	2.76	0.42
1:D:254:GLU:O	1:D:258:ARG:HG2	2.19	0.42
1:E:339:LYS:HA	1:E:339:LYS:HD3	1.73	0.42
1:F:94:ASN:HB2	4:F:847:HOH:O	2.19	0.42
1:F:240:THR:HG22	4:F:681:HOH:O	2.18	0.42
1:G:341:VAL:HG11	1:G:359:LYS:HG3	2.01	0.42
1:H:234:ASP:OD2	1:H:294:THR:HA	2.19	0.42
1:D:386:VAL:HA	1:D:408:LYS:HG2	2.01	0.42
1:D:106:HIS:CE1	1:D:130:LYS:CE	3.02	0.42
1:G:37:PHE:O	4:G:767:HOH:O	2.21	0.42
1:B:392:CYS:O	1:B:403:GLY:HA2	2.19	0.42
1:H:58:LYS:NZ	1:H:62:GLU:OE2	2.49	0.42
1:H:112:ILE:O	1:H:112:ILE:CG1	2.43	0.42
1:H:353:ASP:CA	4:H:764:HOH:O	2.64	0.42
1:G:84:LYS:HB2	1:G:84:LYS:HE2	1.76	0.42
1:H:84:LYS:HB3	1:H:84:LYS:HE2	1.82	0.42
1:H:258:ARG:O	1:H:259:ARG:C	2.60	0.42
1:A:339:LYS:HG2	4:A:642:HOH:O	2.12	0.42
1:D:27:ARG:O	1:D:31:GLU:HG3	2.19	0.42
1:E:194:LYS:HE2	1:E:194:LYS:HB3	1.91	0.42
1:C:103:ASP:OD1	1:C:103:ASP:O	2.37	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:290:GLN:NE2	4:D:663:HOH:O	2.53	0.42
1:F:324:ARG:O	1:F:324:ARG:HG2	2.18	0.42
1:H:56:VAL:HB	1:H:57:TYR:H	1.56	0.42
1:H:76:GLN:HB3	4:H:773:HOH:O	2.20	0.42
1:B:171:ARG:HD2	1:B:171:ARG:HA	1.80	0.42
1:D:120:ASP:OD2	1:D:120:ASP:C	2.61	0.42
1:E:95:PHE:O	1:E:96:ASP:CB	2.51	0.42
1:F:56:VAL:O	1:F:60:VAL:HG23	2.19	0.42
1:G:150:LEU:C	1:G:150:LEU:CD2	2.93	0.42
1:B:188:GLY:O	1:B:191:PRO:HD2	2.19	0.42
1:D:172:GLY:HA2	1:D:174:PHE:CE2	2.55	0.42
1:F:72:ALA:N	4:F:608:HOH:O	2.49	0.42
1:G:183:ASN:CG	1:G:183:ASN:O	2.62	0.42
1:G:266:ARG:O	1:G:406:LEU:HA	2.20	0.42
1:H:12:LEU:HB2	1:H:265:LEU:HB2	2.02	0.42
1:H:67:TYR:CD2	1:H:233:VAL:HG13	2.55	0.42
1:H:315:LEU:CD2	1:H:322:PHE:HA	2.50	0.42
1:C:110:PHE:CD1	1:C:110:PHE:C	2.98	0.41
1:F:15:PHE:CG	1:F:378:LYS:HB2	2.55	0.41
1:F:264:GLY:O	1:F:408:LYS:HA	2.20	0.41
1:B:64:PHE:O	1:B:68:ALA:CB	2.68	0.41
1:B:109:LEU:HD13	1:B:124:ARG:HG2	2.02	0.41
1:C:58:LYS:HZ3	1:C:58:LYS:HG2	1.61	0.41
1:H:139:MET:CE	1:H:248:LYS:HB3	2.40	0.41
1:H:335:PRO:HG3	1:H:362:PHE:HB2	2.03	0.41
1:A:84:LYS:O	1:A:85:LEU:C	2.61	0.41
1:A:324:ARG:NE	1:A:325:ASP:OD1	2.40	0.41
1:C:104:GLN:C	1:C:106:HIS:N	2.77	0.41
1:D:7:PRO:O	1:D:8:ASN:C	2.62	0.41
1:E:97:ILE:HD12	1:E:97:ILE:N	2.34	0.41
1:G:64:PHE:CZ	1:G:236:ILE:HG23	2.56	0.41
1:H:226:ASN:HA	3:H:502:PG4:H31	2.01	0.41
1:B:321:ASP:N	1:B:325:ASP:OD2	2.43	0.41
1:E:122:LYS:HE3	4:E:724:HOH:O	2.20	0.41
1:F:43:LEU:HD11	1:F:112:ILE:C	2.45	0.41
1:G:16:ILE:HD12	1:G:248:LYS:NZ	2.36	0.41
1:B:296:SER:O	1:B:299:VAL:HG23	2.20	0.41
1:F:259:ARG:HG2	1:F:259:ARG:NH1	2.33	0.41
1:F:365:ASN:HB2	1:F:368:MET:HE2	2.02	0.41
1:H:148:ASP:CB	1:H:211:LYS:HG2	2.51	0.41
1:H:150:LEU:C	1:H:150:LEU:HD23	2.44	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:233:VAL:HA	1:H:236:ILE:HD12	2.02	0.41
1:A:84:LYS:HE3	1:A:84:LYS:HB2	1.76	0.41
1:F:13:ALA:HB3	1:F:252:TYR:HE2	1.84	0.41
1:F:351:ALA:O	1:F:352:GLU:C	2.63	0.41
1:H:341:VAL:HG23	4:H:678:HOH:O	2.20	0.41
1:B:258:ARG:CG	1:B:258:ARG:NH1	2.76	0.41
1:D:89:ARG:NE	1:D:96:ASP:CB	2.83	0.41
1:D:314:LEU:HD11	1:D:405:VAL:HG23	2.01	0.41
1:F:58:LYS:HD3	1:F:62:GLU:OE2	2.20	0.41
1:G:97:ILE:N	1:G:97:ILE:HD12	2.33	0.41
1:B:103:ASP:CG	1:B:104:GLN:N	2.73	0.41
1:C:102:PRO:O	1:C:104:GLN:N	2.53	0.41
1:G:103:ASP:OD1	1:G:103:ASP:N	2.50	0.41
1:H:281:THR:HG21	1:H:302:ILE:CD1	2.51	0.41
1:A:81:TYR:CE1	1:A:109:LEU:HD11	2.56	0.41
1:C:104:GLN:C	1:C:106:HIS:H	2.29	0.41
1:C:172:GLY:HA2	1:C:174:PHE:CE2	2.56	0.41
1:C:194:LYS:HE2	1:C:194:LYS:HB3	1.97	0.41
1:C:398:GLY:N	1:C:399:LEU:HA	2.34	0.41
1:F:373:ILE:O	1:F:377:LEU:HG	2.21	0.41
1:G:226:ASN:ND2	1:G:226:ASN:O	2.53	0.41
1:G:256:GLU:O	1:G:260:GLN:HG3	2.20	0.41
1:G:308:ARG:O	1:G:312:VAL:HG23	2.20	0.41
1:D:392:CYS:HB2	1:D:404:LEU:HB3	2.03	0.41
1:E:51:GLU:O	1:E:55:GLN:HG2	2.21	0.41
1:C:22:LYS:HB2	1:C:22:LYS:HZ2	1.85	0.40
1:C:270:MET:HE2	1:C:270:MET:HB2	1.91	0.40
1:C:342:ASP:OD1	1:C:359:LYS:HE2	2.21	0.40
1:C:357:ILE:HD12	1:C:380:TYR:CE2	2.57	0.40
1:F:7:PRO:O	1:F:8:ASN:C	2.63	0.40
1:B:286:PRO:HD2	1:H:158:TYR:O	2.21	0.40
1:C:139:MET:HE2	1:C:246:LEU:HB3	2.02	0.40
1:C:270:MET:HG2	1:C:404:LEU:HD23	2.02	0.40
1:E:323:GLU:HA	4:E:864:HOH:O	2.20	0.40
1:D:106:HIS:CE1	1:D:130:LYS:HE3	2.57	0.40
1:G:194:LYS:HA	1:G:270:MET:SD	2.61	0.40
1:G:231:SER:O	1:G:232:ARG:C	2.64	0.40
1:H:6:HIS:HB2	1:H:254:GLU:CD	2.46	0.40
1:H:160:ALA:HA	1:H:161:PRO:C	2.44	0.40
1:C:124:ARG:HD3	1:C:224:ALA:O	2.22	0.40
1:C:260:GLN:HB2	1:C:262:LEU:HG	2.02	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:296:SER:OG	1:G:298:LEU:HB2	2.21	0.40
1:G:324:ARG:C	1:G:325:ASP:OD1	2.65	0.40
1:D:97:ILE:HG21	1:D:108:ARG:CZ	2.51	0.40
1:G:321:ASP:OD2	1:G:324:ARG:CD	2.69	0.40

All (2) 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:H:324:ARG:NE	4:E:866:HOH:O[1_656]	2.09	0.11
1:D:230:GLU:OE2	1:H:321:ASP:OD2[1_454]	2.17	0.03

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	397/410 (97%)	385 (97%)	12 (3%)	0	100	100
1	B	391/410 (95%)	371 (95%)	18 (5%)	2 (0%)	24	21
1	C	392/410 (96%)	380 (97%)	10 (3%)	2 (0%)	24	21
1	D	397/410 (97%)	385 (97%)	10 (2%)	2 (0%)	24	21
1	E	396/410 (97%)	381 (96%)	14 (4%)	1 (0%)	36	35
1	F	397/410 (97%)	379 (96%)	18 (4%)	0	100	100
1	G	391/410 (95%)	376 (96%)	13 (3%)	2 (0%)	24	21
1	H	375/410 (92%)	356 (95%)	15 (4%)	4 (1%)	11	7
All	All	3136/3280 (96%)	3013 (96%)	110 (4%)	13 (0%)	30	27

All (13) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	322	PHE
1	B	323	GLU
1	E	96	ASP
1	C	103	ASP
1	C	104	GLN
1	H	86	THR
1	G	45	ASN
1	G	92	ASP
1	H	113	LYS
1	H	322	PHE
1	D	86	THR
1	D	102	PRO
1	H	234	ASP

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	333/339 (98%)	324 (97%)	9 (3%)	39	42
1	B	329/339 (97%)	313 (95%)	16 (5%)	22	20
1	C	328/339 (97%)	316 (96%)	12 (4%)	30	30
1	D	332/339 (98%)	322 (97%)	10 (3%)	36	38
1	E	332/339 (98%)	323 (97%)	9 (3%)	39	42
1	F	333/339 (98%)	313 (94%)	20 (6%)	17	14
1	G	327/339 (96%)	309 (94%)	18 (6%)	19	17
1	H	317/339 (94%)	299 (94%)	18 (6%)	18	15
All	All	2631/2712 (97%)	2519 (96%)	112 (4%)	26	25

All (112) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	50	GLU
1	A	89	ARG
1	A	90	PHE

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Mol	Chain	Res	Type
1	A	103	ASP
1	A	130	LYS
1	A	209	PRO
1	A	257	LEU
1	A	288	SER
1	A	348	LEU
1	B	18	VAL
1	B	30	LEU
1	B	50	GLU
1	B	97	ILE
1	B	104	GLN
1	B	114	LYS
1	B	145	GLU
1	B	231	SER
1	B	238	SER
1	B	248	LYS
1	B	255	ASP
1	B	257	LEU
1	B	258	ARG
1	B	295	LEU
1	B	324	ARG
1	B	348	LEU
1	C	22	LYS
1	C	32	LEU
1	C	54	VAL
1	C	58	LYS
1	C	84	LYS
1	C	96	ASP
1	C	97	ILE
1	C	104	GLN
1	C	145	GLU
1	C	231	SER
1	C	259	ARG
1	C	404	LEU
1	D	27	ARG
1	D	32	LEU
1	D	48	THR
1	D	51	GLU
1	D	84	LYS
1	D	85	LEU
1	D	103	ASP
1	D	104	GLN

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Mol	Chain	Res	Type
1	D	262	LEU
1	D	263	ARG
1	E	28	ILE
1	E	50	GLU
1	E	66	LYS
1	E	76	GLN
1	E	88	ILE
1	E	89	ARG
1	E	103	ASP
1	E	257	LEU
1	E	288	SER
1	F	16	ILE
1	F	22	LYS
1	F	24	VAL
1	F	50	GLU
1	F	51	GLU
1	F	54	VAL
1	F	58	LYS
1	F	85	LEU
1	F	86	THR
1	F	114	LYS
1	F	117	ARG
1	F	248	LYS
1	F	257	LEU
1	F	258	ARG
1	F	260	GLN
1	F	305	ARG
1	F	321	ASP
1	F	329	LEU
1	F	373	ILE
1	F	385	THR
1	G	43	LEU
1	G	47	ILE
1	G	55	GLN
1	G	59	THR
1	G	92	ASP
1	G	97	ILE
1	G	103	ASP
1	G	134	LYS
1	G	204	GLN
1	G	255	ASP
1	G	290	GLN

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Mol	Chain	Res	Type
1	G	296	SER
1	G	298	LEU
1	G	324	ARG
1	G	325	ASP
1	G	346	GLU
1	G	399	LEU
1	G	400	THR
1	H	33	THR
1	H	56	VAL
1	H	86	THR
1	H	89	ARG
1	H	103	ASP
1	H	226	ASN
1	H	231	SER
1	H	238	SER
1	H	257	LEU
1	H	263	ARG
1	H	271	SER
1	H	285	VAL
1	H	321	ASP
1	H	324	ARG
1	H	346	GLU
1	H	348	LEU
1	H	373	ILE
1	H	386	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (52) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	41	HIS
1	A	78	GLN
1	A	104	GLN
1	A	125	HIS
1	A	226	ASN
1	A	289	HIS
1	A	343	HIS
1	B	55	GLN
1	B	78	GLN
1	B	138	GLN
1	B	226	ASN
1	B	260	GLN
1	B	289	HIS

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Mol	Chain	Res	Type
1	B	375	HIS
1	C	78	GLN
1	C	104	GLN
1	C	138	GLN
1	C	226	ASN
1	D	78	GLN
1	D	94	ASN
1	D	227	ASN
1	D	290	GLN
1	D	343	HIS
1	E	8	ASN
1	E	19	GLN
1	E	41	HIS
1	E	78	GLN
1	E	104	GLN
1	E	125	HIS
1	E	138	GLN
1	E	226	ASN
1	E	260	GLN
1	E	343	HIS
1	F	19	GLN
1	F	78	GLN
1	F	290	GLN
1	F	343	HIS
1	G	6	HIS
1	G	55	GLN
1	G	78	GLN
1	G	106	HIS
1	G	125	HIS
1	G	183	ASN
1	G	226	ASN
1	G	290	GLN
1	G	343	HIS
1	H	78	GLN
1	H	106	HIS
1	H	226	ASN
1	H	289	HIS
1	H	290	GLN
1	H	354	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 16 ligands modelled in this entry, 8 are monoatomic - leaving 8 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
3	PG4	B	502	-	12,12,12	0.64	0	11,11,11	0.50	0
3	PG4	H	502	-	12,12,12	0.51	0	11,11,11	0.34	0
3	PG4	D	502	-	12,12,12	0.61	0	11,11,11	0.51	0
3	PG4	C	502	-	12,12,12	0.58	0	11,11,11	0.62	0
3	PG4	F	502	-	12,12,12	0.61	0	11,11,11	0.31	0
3	PG4	G	502	-	12,12,12	0.56	0	11,11,11	0.38	0
3	PG4	A	502	-	12,12,12	0.55	0	11,11,11	0.66	0
3	PG4	E	502	-	12,12,12	0.43	0	11,11,11	0.84	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '2' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	PG4	B	502	-	-	5/10/10/10	-
3	PG4	H	502	-	-	7/10/10/10	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	PG4	D	502	-	-	4/10/10/10	-
3	PG4	C	502	-	-	5/10/10/10	-
3	PG4	F	502	-	-	2/10/10/10	-
3	PG4	G	502	-	-	6/10/10/10	-
3	PG4	A	502	-	-	8/10/10/10	-
3	PG4	E	502	-	-	5/10/10/10	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (42) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	F	502	PG4	O2-C3-C4-O3
3	E	502	PG4	O2-C3-C4-O3
3	C	502	PG4	O1-C1-C2-O2
3	B	502	PG4	O2-C3-C4-O3
3	B	502	PG4	O4-C7-C8-O5
3	H	502	PG4	O4-C7-C8-O5
3	C	502	PG4	O2-C3-C4-O3
3	A	502	PG4	O4-C7-C8-O5
3	D	502	PG4	O1-C1-C2-O2
3	G	502	PG4	O4-C7-C8-O5
3	H	502	PG4	O2-C3-C4-O3
3	G	502	PG4	O1-C1-C2-O2
3	A	502	PG4	O2-C3-C4-O3
3	H	502	PG4	O1-C1-C2-O2
3	E	502	PG4	C3-C4-O3-C5
3	E	502	PG4	O3-C5-C6-O4
3	C	502	PG4	C1-C2-O2-C3
3	F	502	PG4	C1-C2-O2-C3
3	C	502	PG4	C4-C3-O2-C2
3	B	502	PG4	C5-C6-O4-C7
3	G	502	PG4	C8-C7-O4-C6
3	E	502	PG4	C8-C7-O4-C6
3	H	502	PG4	C1-C2-O2-C3
3	G	502	PG4	C4-C3-O2-C2
3	C	502	PG4	O4-C7-C8-O5
3	A	502	PG4	C4-C3-O2-C2

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Mol	Chain	Res	Type	Atoms
3	A	502	PG4	O3-C5-C6-O4
3	B	502	PG4	C8-C7-O4-C6
3	A	502	PG4	C5-C6-O4-C7
3	A	502	PG4	C6-C5-O3-C4
3	D	502	PG4	O2-C3-C4-O3
3	H	502	PG4	C3-C4-O3-C5
3	A	502	PG4	C8-C7-O4-C6
3	G	502	PG4	O2-C3-C4-O3
3	A	502	PG4	C1-C2-O2-C3
3	H	502	PG4	O3-C5-C6-O4
3	E	502	PG4	O1-C1-C2-O2
3	H	502	PG4	C8-C7-O4-C6
3	D	502	PG4	C3-C4-O3-C5
3	D	502	PG4	O3-C5-C6-O4
3	G	502	PG4	O3-C5-C6-O4
3	B	502	PG4	C4-C3-O2-C2

There are no ring outliers.

7 monomers are involved in 10 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	502	PG4	2	0
3	H	502	PG4	2	0
3	D	502	PG4	2	0
3	C	502	PG4	1	0
3	F	502	PG4	1	0
3	G	502	PG4	1	0
3	A	502	PG4	1	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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	401/410 (97%)	0.23	16 (3%) 42 41	19, 29, 50, 68	0
1	B	397/410 (96%)	1.07	52 (13%) 7 6	27, 38, 59, 84	0
1	C	396/410 (96%)	0.18	11 (2%) 55 54	18, 29, 55, 77	0
1	D	401/410 (97%)	0.29	20 (4%) 34 33	20, 30, 64, 80	0
1	E	400/410 (97%)	0.24	17 (4%) 40 39	20, 29, 52, 70	0
1	F	401/410 (97%)	1.34	79 (19%) 3 3	28, 41, 60, 71	0
1	G	397/410 (96%)	1.24	92 (23%) 2 2	25, 41, 69, 88	0
1	H	383/410 (93%)	1.37	97 (25%) 1 1	26, 41, 70, 89	0
All	All	3176/3280 (96%)	0.74	384 (12%) 8 8	18, 35, 63, 89	0

All (384) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	H	56	VAL	10.4
1	G	52	GLY	6.9
1	B	98	ALA	6.7
1	H	43	LEU	6.3
1	A	90	PHE	5.7
1	H	311	ALA	5.6
1	F	329	LEU	5.5
1	F	340	ILE	5.4
1	H	306	HIS	4.8
1	B	97	ILE	4.6
1	C	52	GLY	4.5
1	H	59	THR	4.4
1	H	71	PRO	4.4
1	F	355	VAL	4.2
1	C	97	ILE	4.2
1	G	328	ALA	4.1

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Mol	Chain	Res	Type	RSRZ
1	H	351	ALA	4.0
1	G	53	PHE	4.0
1	F	90	PHE	4.0
1	H	238	SER	4.0
1	H	300	PRO	3.9
1	H	60	VAL	3.9
1	F	107	LEU	3.9
1	G	54	VAL	3.9
1	H	42	CYS	3.8
1	B	350	LEU	3.8
1	G	42	CYS	3.8
1	G	344	VAL	3.8
1	H	69	VAL	3.8
1	G	46	GLY	3.7
1	F	85	LEU	3.7
1	H	337	GLY	3.7
1	H	57	TYR	3.6
1	D	6	HIS	3.6
1	H	40	ALA	3.6
1	G	93	GLY	3.6
1	G	47	ILE	3.6
1	C	100	PRO	3.6
1	F	312	VAL	3.6
1	F	391	ALA	3.5
1	D	87	ASP	3.5
1	H	68	ALA	3.5
1	H	236	ILE	3.5
1	H	307	VAL	3.5
1	F	298	LEU	3.5
1	F	384	ALA	3.5
1	H	330	SER	3.4
1	F	351	ALA	3.4
1	H	41	HIS	3.4
1	D	88	ILE	3.4
1	B	307	VAL	3.4
1	B	96	ASP	3.3
1	H	28	ILE	3.3
1	H	98	ALA	3.3
1	H	324	ARG	3.3
1	H	399	LEU	3.3
1	H	95	PHE	3.3
1	F	86	THR	3.3

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Mol	Chain	Res	Type	RSRZ
1	G	6	HIS	3.3
1	G	236	ILE	3.3
1	D	56	VAL	3.3
1	E	98	ALA	3.3
1	G	319	GLY	3.3
1	G	231	SER	3.3
1	B	340	ILE	3.2
1	F	373	ILE	3.2
1	G	67	TYR	3.2
1	F	349	GLY	3.2
1	D	97	ILE	3.2
1	G	307	VAL	3.2
1	F	72	ALA	3.2
1	F	101	GLU	3.2
1	F	102	PRO	3.2
1	G	348	LEU	3.2
1	H	350	LEU	3.2
1	F	174	PHE	3.2
1	D	103	ASP	3.2
1	F	201	ALA	3.1
1	G	279	ALA	3.1
1	D	93	GLY	3.1
1	H	61	LYS	3.1
1	B	90	PHE	3.1
1	B	328	ALA	3.1
1	G	7	PRO	3.1
1	E	94	ASN	3.1
1	F	381	LEU	3.0
1	G	275	LEU	3.0
1	H	284	TRP	3.0
1	B	103	ASP	3.0
1	G	295	LEU	3.0
1	D	54	VAL	3.0
1	E	323	GLU	3.0
1	G	322	PHE	3.0
1	H	38	ALA	3.0
1	B	357	ILE	3.0
1	A	54	VAL	3.0
1	F	309	ALA	3.0
1	H	32	LEU	2.9
1	D	86	THR	2.9
1	F	135	GLY	2.9

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Mol	Chain	Res	Type	RSRZ
1	F	319	GLY	2.9
1	G	400	THR	2.9
1	B	95	PHE	2.9
1	H	322	PHE	2.9
1	F	173	TRP	2.9
1	H	301	ALA	2.9
1	F	330	SER	2.9
1	D	89	ARG	2.9
1	F	168	VAL	2.9
1	H	67	TYR	2.9
1	G	205	TRP	2.9
1	E	28	ILE	2.9
1	G	208	THR	2.9
1	H	253	PRO	2.9
1	B	169	ALA	2.9
1	B	311	ALA	2.9
1	H	309	ALA	2.9
1	G	60	VAL	2.8
1	F	297	PRO	2.8
1	G	102	PRO	2.8
1	G	210	PRO	2.8
1	H	297	PRO	2.8
1	C	6	HIS	2.8
1	F	104	GLN	2.8
1	G	98	ALA	2.8
1	B	85	LEU	2.8
1	F	333	ILE	2.8
1	F	258	ARG	2.8
1	H	312	VAL	2.8
1	F	301	ALA	2.8
1	H	302	ILE	2.8
1	H	234	ASP	2.8
1	B	260	GLN	2.8
1	G	273	HIS	2.8
1	A	323	GLU	2.8
1	H	315	LEU	2.8
1	B	132	VAL	2.8
1	F	54	VAL	2.8
1	F	386	VAL	2.8
1	G	362	PHE	2.7
1	F	198	GLY	2.7
1	G	340	ILE	2.7

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Mol	Chain	Res	Type	RSRZ
1	H	321	ASP	2.7
1	F	300	PRO	2.7
1	G	318	ALA	2.7
1	F	331	PHE	2.7
1	F	215	ASP	2.7
1	B	209	PRO	2.7
1	D	102	PRO	2.7
1	C	95	PHE	2.7
1	G	310	PHE	2.7
1	E	89	ARG	2.7
1	D	100	PRO	2.7
1	F	253	PRO	2.7
1	G	44	SER	2.7
1	H	348	LEU	2.7
1	F	18	VAL	2.7
1	A	98	ALA	2.6
1	F	320	MET	2.6
1	B	322	PHE	2.6
1	F	212	THR	2.6
1	H	326	LYS	2.6
1	F	142	GLY	2.6
1	F	405	VAL	2.6
1	H	277	ASP	2.6
1	C	85	LEU	2.6
1	B	16	ILE	2.6
1	B	52	GLY	2.6
1	D	52	GLY	2.6
1	C	54	VAL	2.6
1	F	279	ALA	2.6
1	G	34	ALA	2.6
1	G	309	ALA	2.6
1	D	45	ASN	2.6
1	B	252	TYR	2.6
1	B	140	PHE	2.6
1	G	404	LEU	2.6
1	B	133	GLY	2.6
1	G	172	GLY	2.6
1	A	56	VAL	2.6
1	G	312	VAL	2.6
1	G	209	PRO	2.5
1	H	89	ARG	2.5
1	H	174	PHE	2.5

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Mol	Chain	Res	Type	RSRZ
1	G	313	ASP	2.5
1	F	387	GLY	2.5
1	G	302	ILE	2.5
1	H	114	LYS	2.5
1	B	224	ALA	2.5
1	G	40	ALA	2.5
1	G	207	ALA	2.5
1	H	279	ALA	2.5
1	F	153	VAL	2.5
1	H	255	ASP	2.5
1	H	313	ASP	2.5
1	G	241	LEU	2.5
1	G	350	LEU	2.5
1	G	237	ILE	2.5
1	F	269	ALA	2.5
1	G	311	ALA	2.5
1	G	351	ALA	2.5
1	E	56	VAL	2.5
1	G	299	VAL	2.5
1	H	88	ILE	2.5
1	H	202	SER	2.5
1	F	356	ALA	2.5
1	G	169	ALA	2.5
1	H	229	ALA	2.5
1	C	59	THR	2.5
1	G	177	THR	2.5
1	G	36	GLY	2.4
1	F	363	LEU	2.4
1	G	270	MET	2.4
1	A	97	ILE	2.4
1	G	112	ILE	2.4
1	G	114	LYS	2.4
1	G	203	ALA	2.4
1	H	33	THR	2.4
1	H	304	LYS	2.4
1	C	102	PRO	2.4
1	E	51	GLU	2.4
1	G	174	PHE	2.4
1	H	228	ILE	2.4
1	H	86	THR	2.4
1	B	386	VAL	2.4
1	A	55	GLN	2.4

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Mol	Chain	Res	Type	RSRZ
1	H	36	GLY	2.4
1	G	243	SER	2.4
1	A	49	ASP	2.4
1	B	87	ASP	2.4
1	B	277	ASP	2.4
1	E	95	PHE	2.4
1	G	37	PHE	2.4
1	F	376	ILE	2.4
1	F	390	ILE	2.4
1	F	207	ALA	2.4
1	F	379	ALA	2.4
1	F	131	VAL	2.4
1	G	387	GLY	2.4
1	H	320	MET	2.4
1	F	205	TRP	2.4
1	H	275	LEU	2.3
1	A	95	PHE	2.3
1	H	64	PHE	2.3
1	A	59	THR	2.3
1	H	281	THR	2.3
1	H	347	GLU	2.3
1	E	97	ILE	2.3
1	H	72	ALA	2.3
1	H	401	ALA	2.3
1	B	94	ASN	2.3
1	B	135	GLY	2.3
1	B	341	VAL	2.3
1	F	221	LEU	2.3
1	G	43	LEU	2.3
1	H	110	PHE	2.3
1	H	362	PHE	2.3
1	B	105	ALA	2.3
1	H	332	ALA	2.3
1	E	7	PRO	2.3
1	H	349	GLY	2.3
1	H	387	GLY	2.3
1	G	24	VAL	2.3
1	G	144	LEU	2.3
1	G	274	LEU	2.3
1	E	6	HIS	2.3
1	F	6	HIS	2.3
1	F	385	THR	2.3

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Mol	Chain	Res	Type	RSRZ
1	B	15	PHE	2.3
1	F	140	PHE	2.3
1	B	146	ALA	2.3
1	D	98	ALA	2.3
1	G	116	PRO	2.3
1	F	197	HIS	2.3
1	E	85	LEU	2.3
1	G	212	THR	2.3
1	H	66	LYS	2.3
1	A	89	ARG	2.2
1	B	173	TRP	2.2
1	F	305	ARG	2.2
1	F	316	ARG	2.2
1	G	284	TRP	2.2
1	C	98	ALA	2.2
1	D	328	ALA	2.2
1	F	21	ALA	2.2
1	G	57	TYR	2.2
1	G	91	GLY	2.2
1	H	25	PRO	2.2
1	H	336	GLY	2.2
1	H	398	GLY	2.2
1	G	303	ILE	2.2
1	D	55	GLN	2.2
1	G	405	VAL	2.2
1	A	94	ASN	2.2
1	G	59	THR	2.2
1	A	85	LEU	2.2
1	D	230	GLU	2.2
1	H	363	LEU	2.2
1	A	100	PRO	2.2
1	B	349	GLY	2.2
1	E	55	GLN	2.2
1	G	202	SER	2.2
1	G	238	SER	2.2
1	B	332	ALA	2.2
1	G	325	ASP	2.2
1	B	6	HIS	2.2
1	F	94	ASN	2.2
1	H	58	LYS	2.2
1	F	308	ARG	2.2
1	H	39	ARG	2.2

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Mol	Chain	Res	Type	RSRZ
1	B	257	LEU	2.2
1	G	30	LEU	2.2
1	E	103	ASP	2.2
1	G	9	SER	2.2
1	H	223	SER	2.2
1	H	366	GLY	2.2
1	F	190	PHE	2.2
1	A	28	ILE	2.2
1	B	28	ILE	2.2
1	G	343	HIS	2.2
1	B	143	THR	2.2
1	H	325	ASP	2.2
1	F	250	SER	2.2
1	A	6	HIS	2.1
1	F	310	PHE	2.1
1	F	322	PHE	2.1
1	G	94	ASN	2.1
1	F	380	TYR	2.1
1	G	97	ILE	2.1
1	H	333	ILE	2.1
1	F	281	THR	2.1
1	H	65	ASP	2.1
1	G	56	VAL	2.1
1	G	251	VAL	2.1
1	F	172	GLY	2.1
1	H	268	LEU	2.1
1	H	6	HIS	2.1
1	B	68	ALA	2.1
1	G	8	ASN	2.1
1	B	303	ILE	2.1
1	G	70	SER	2.1
1	H	70	SER	2.1
1	B	80	VAL	2.1
1	E	52	GLY	2.1
1	E	316	ARG	2.1
1	D	101	GLU	2.1
1	E	102	PRO	2.1
1	G	289	HIS	2.1
1	H	186	CYS	2.1
1	F	315	LEU	2.1
1	H	298	LEU	2.1
1	H	404	LEU	2.1

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Mol	Chain	Res	Type	RSRZ
1	B	309	ALA	2.1
1	G	201	ALA	2.1
1	G	332	ALA	2.1
1	F	395	PHE	2.1
1	B	249	TYR	2.1
1	H	97	ILE	2.1
1	H	308	ARG	2.1
1	H	388	THR	2.1
1	H	403	GLY	2.1
1	F	251	VAL	2.1
1	F	164	ALA	2.1
1	H	87	ASP	2.1
1	G	324	ARG	2.1
1	B	174	PHE	2.0
1	C	51	GLU	2.0
1	F	70	SER	2.0
1	B	86	THR	2.0
1	H	177	THR	2.0
1	B	355	VAL	2.0
1	F	17	PRO	2.0
1	B	200	LEU	2.0
1	B	262	LEU	2.0
1	G	329	LEU	2.0
1	H	200	LEU	2.0
1	B	318	ALA	2.0
1	G	92	ASP	2.0
1	G	339	LYS	2.0
1	D	95	PHE	2.0
1	F	16	ILE	2.0
1	H	227	ASN	2.0
1	B	324	ARG	2.0
1	H	386	VAL	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](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
3	PG4	F	502	13/13	0.74	0.15	56,60,63,64	0
3	PG4	B	502	13/13	0.77	0.13	54,62,67,68	0
3	PG4	D	502	13/13	0.85	0.11	51,56,59,60	0
3	PG4	E	502	13/13	0.86	0.10	45,49,54,55	0
3	PG4	C	502	13/13	0.86	0.11	45,49,59,60	0
3	PG4	G	502	13/13	0.86	0.11	51,56,63,65	0
3	PG4	A	502	13/13	0.88	0.10	43,45,49,49	0
3	PG4	H	502	13/13	0.88	0.10	49,55,57,58	0
2	NA	F	501	1/1	0.91	0.06	35,35,35,35	0
2	NA	H	501	1/1	0.92	0.07	32,32,32,32	0
2	NA	G	501	1/1	0.93	0.07	27,27,27,27	0
2	NA	B	501	1/1	0.93	0.04	29,29,29,29	0
2	NA	D	501	1/1	0.98	0.03	25,25,25,25	0
2	NA	A	501	1/1	0.98	0.06	19,19,19,19	0
2	NA	E	501	1/1	0.99	0.02	21,21,21,21	0
2	NA	C	501	1/1	0.99	0.01	23,23,23,23	0

6.5 Other polymers [i](#)

There are no such residues in this entry.