



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 28, 2026 – 07:23 PM UTC

PDB ID : 1FZW / pdb_00001fzw
Title : THE STRUCTURAL BASIS OF THE CATALYTIC MECHANISM AND
REGULATION OF GLUCOSE-1-PHOSPHATE THYMIDYLYLTRANSFERASE (RMLA). APO ENZYME.
Authors : Blankenfeldt, W.; Asuncion, M.; Lam, J.S.; Naismith, J.H.
Deposited on : 2000-10-04
Resolution : 1.90 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

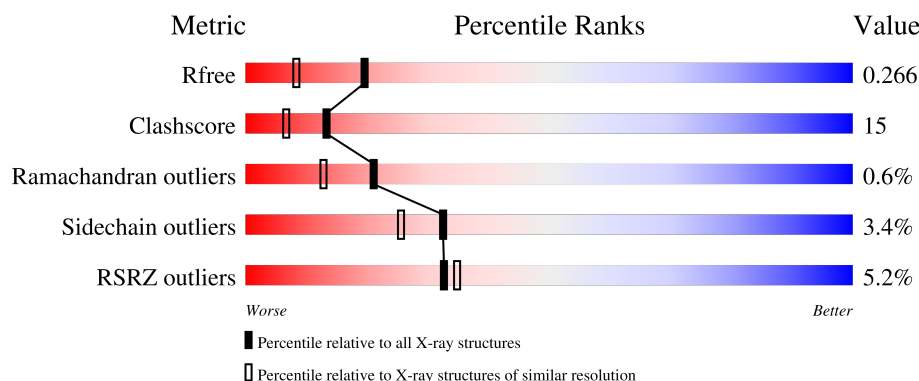
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.90 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	7789 (1.90-1.90)
Clashscore	190562	8410 (1.90-1.90)
Ramachandran outliers	187476	8333 (1.90-1.90)
Sidechain outliers	187428	8333 (1.90-1.90)
RSRZ outliers	180081	7790 (1.90-1.90)

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	293	4% 63% 32% .
1	B	293	4% 63% 31% 6%
1	C	293	5% 62% 32% 5%
1	D	293	6% 66% 28% 5% .
1	E	293	9% 65% 28% 6%

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Mol	Chain	Length	Quality of chain
1	F	293	
1	G	293	
1	H	293	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	SO4	C	5000	-	-	X	-
2	SO4	H	6101	-	-	X	-

2 Entry composition

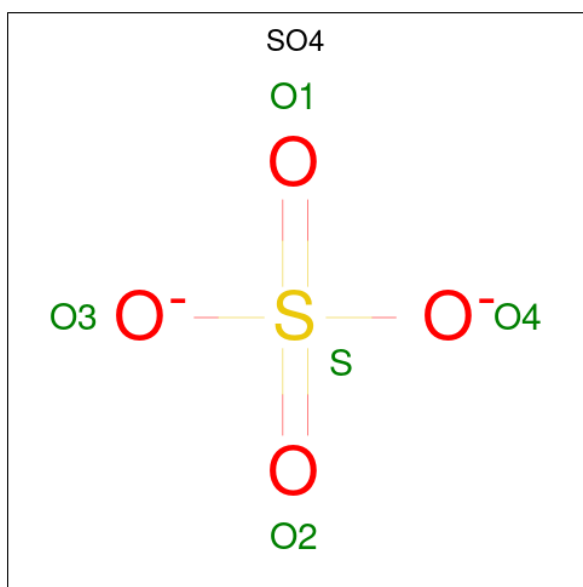
There are 3 unique types of molecules in this entry. The entry contains 21094 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 GLUCOSE-1-PHOSPHATE THYMIDYLYLTRANSFERASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	292	Total	C	N	O	S	0	2	0
			2302	1472	388	437	5			
1	B	292	Total	C	N	O	S	0	5	0
			2322	1484	391	442	5			
1	C	293	Total	C	N	O	S	0	6	0
			2340	1494	394	446	6			
1	D	292	Total	C	N	O	S	0	1	0
			2294	1467	387	436	4			
1	E	292	Total	C	N	O	S	0	7	0
			2339	1491	396	447	5			
1	F	293	Total	C	N	O	S	0	3	0
			2316	1480	389	441	6			
1	G	292	Total	C	N	O	S	0	4	0
			2318	1480	392	441	5			
1	H	292	Total	C	N	O	S	0	0	0
			2285	1462	385	434	4			

- Molecule 2 is SULFATE ION (CCD ID: SO4) (formula: O₄S).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	O	S	0	0
			5	4	1		
2	A	1	Total	O	S	0	0
			5	4	1		
2	B	1	Total	O	S	0	0
			5	4	1		
2	B	1	Total	O	S	0	0
			5	4	1		
2	C	1	Total	O	S	0	0
			5	4	1		
2	C	1	Total	O	S	0	0
			5	4	1		
2	C	1	Total	O	S	0	0
			5	4	1		
2	D	1	Total	O	S	0	0
			5	4	1		
2	D	1	Total	O	S	0	0
			5	4	1		
2	D	1	Total	O	S	0	0
			5	4	1		
2	E	1	Total	O	S	0	0
			5	4	1		
2	E	1	Total	O	S	0	0
			5	4	1		
2	E	1	Total	O	S	0	0
			5	4	1		
2	F	1	Total	O	S	0	0
			5	4	1		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	F	1	Total	O	S	0	0
			5	4	1		
2	G	1	Total	O	S	0	0
			5	4	1		
2	G	1	Total	O	S	0	0
			5	4	1		
2	G	1	Total	O	S	0	0
			5	4	1		
2	H	1	Total	O	S	0	0
			5	4	1		
2	H	1	Total	O	S	0	0
			5	4	1		

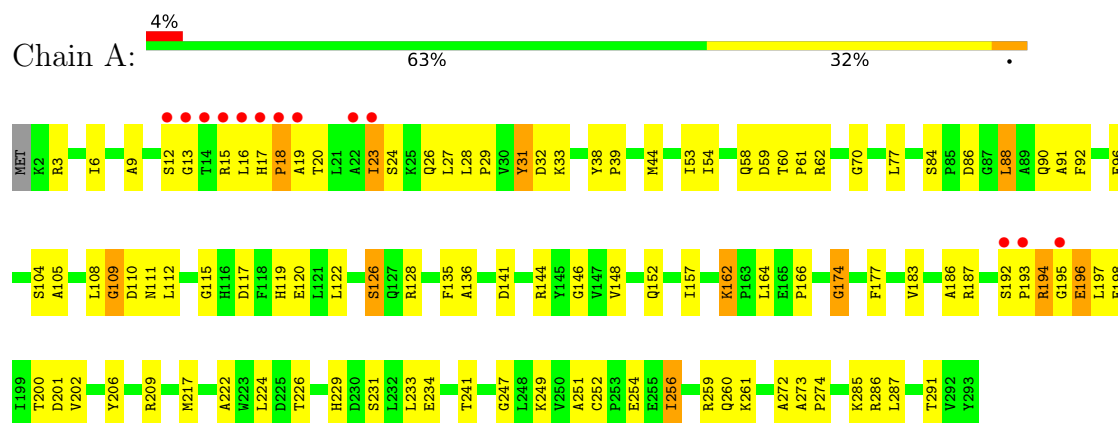
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	325	Total	O	0	0
			325	325		
3	B	335	Total	O	0	0
			335	335		
3	C	286	Total	O	0	0
			286	286		
3	D	259	Total	O	0	0
			259	259		
3	E	282	Total	O	0	0
			282	282		
3	F	321	Total	O	0	0
			321	321		
3	G	367	Total	O	0	0
			367	367		
3	H	303	Total	O	0	0
			303	303		

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.

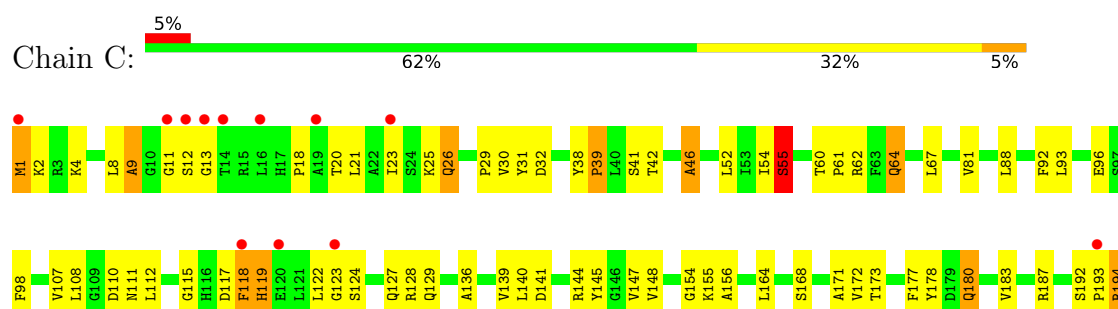
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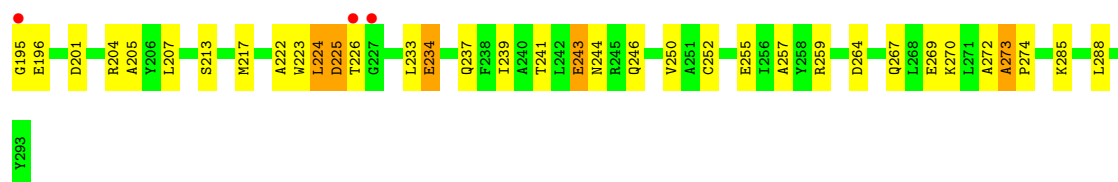


• Molecule 1: GLUCOSE-1-PHOSPHATE THYMIDYLYLTRANSFERASE

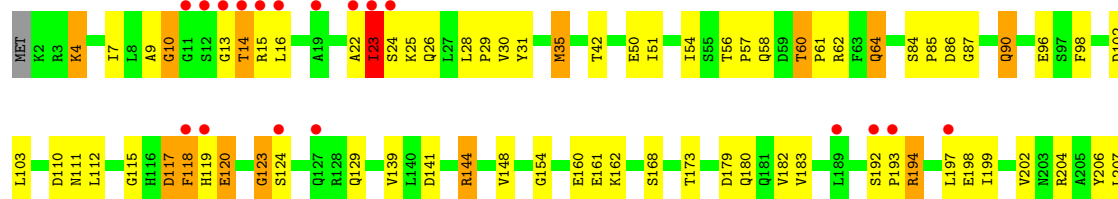


• Molecule 1: GLUCOSE-1-PHOSPHATE THYMIDYLYLTRANSFERASE

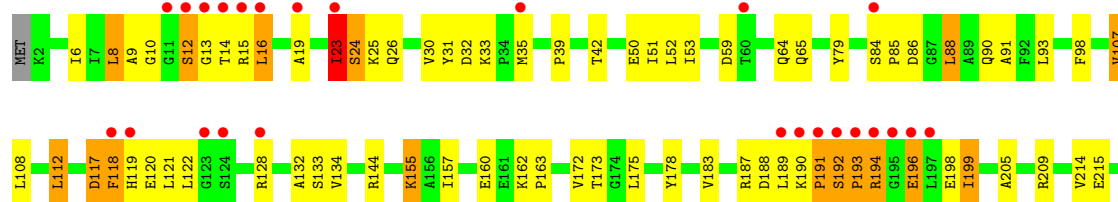




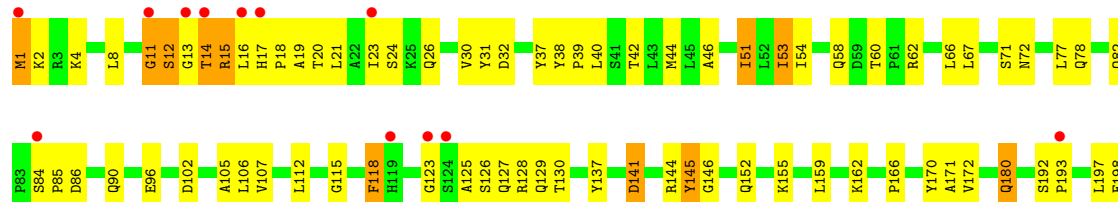
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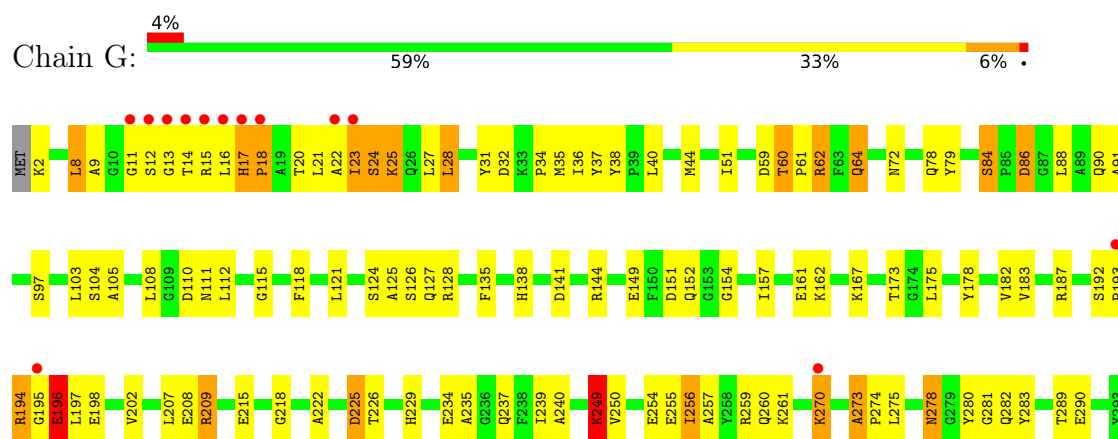
• Molecule 1: GLUCOSE-1-PHOSPHATE THYMIDYLYLTRANSFERASE



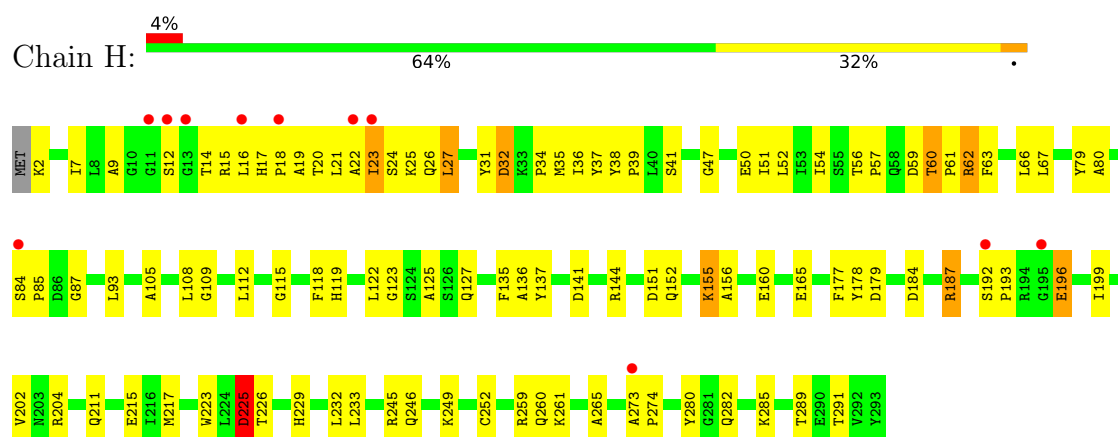
• Molecule 1: GLUCOSE-1-PHOSPHATE THYMIDYLYLTRANSFERASE



• Molecule 1: GLUCOSE-1-PHOSPHATE THYMIDYLYLTRANSFERASE



• Molecule 1: GLUCOSE-1-PHOSPHATE THYMIDYLYLTRANSFERASE



4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	71.66Å 73.66Å 134.47Å 89.98° 80.91° 80.91°	Depositor
Resolution (Å)	73.00 – 1.90 73.00 – 1.90	Depositor EDS
% Data completeness (in resolution range)	95.8 (73.00-1.90) 95.1 (73.00-1.90)	Depositor EDS
R_{merge}	0.05	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.94 (at 1.89Å)	Xtriage
Refinement program	REFMAC	Depositor
R, R_{free}	0.176 , 0.251 0.196 , 0.266	Depositor DCC
R_{free} test set	10141 reflections (5.05%)	wwPDB-VP
Wilson B-factor (Å ²)	21.7	Xtriage
Anisotropy	0.030	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 56.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	21094	wwPDB-VP
Average B, all atoms (Å ²)	25.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.49% of the height of the origin peak. No significant pseudotranslation is detected.*

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 ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: SO4

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	1.98	45/2352 (1.9%)	1.49	17/3190 (0.5%)
1	B	1.93	42/2372 (1.8%)	1.54	22/3217 (0.7%)
1	C	1.91	51/2390 (2.1%)	1.54	26/3239 (0.8%)
1	D	1.90	47/2344 (2.0%)	1.50	17/3180 (0.5%)
1	E	1.79	28/2389 (1.2%)	1.49	13/3240 (0.4%)
1	F	2.04	56/2366 (2.4%)	1.56	18/3208 (0.6%)
1	G	2.12	62/2368 (2.6%)	1.54	16/3212 (0.5%)
1	H	1.89	35/2335 (1.5%)	1.54	19/3168 (0.6%)
All	All	1.95	366/18916 (1.9%)	1.52	148/25654 (0.6%)

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	C	0	1
1	G	0	2
1	H	0	1
All	All	0	4

All (366) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	217	MET	SD-CE	-11.16	1.51	1.79
1	G	44	MET	SD-CE	-10.98	1.52	1.79
1	F	251	ALA	CA-CB	10.56	1.69	1.53
1	F	51	ILE	N-CA	-10.44	1.33	1.46
1	A	128	ARG	CZ-NH2	-10.41	1.20	1.33
1	B	38	TYR	N-CA	-10.35	1.39	1.46
1	A	44	MET	SD-CE	-10.31	1.53	1.79

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	222	ALA	CA-CB	-10.27	1.39	1.53
1	F	146	GLY	C-O	-9.96	1.15	1.24
1	A	217	MET	SD-CE	-9.81	1.55	1.79
1	D	35	MET	CG-SD	-9.75	1.56	1.80
1	B	6	ILE	C-O	9.71	1.34	1.24
1	A	136	ALA	CA-CB	-8.98	1.39	1.53
1	C	257	ALA	CA-CB	-8.83	1.38	1.53
1	H	9	ALA	CA-C	-8.82	1.41	1.52
1	G	157	ILE	N-CA	-8.78	1.37	1.46
1	A	256	ILE	C-O	8.73	1.33	1.24
1	C	64	GLN	C-O	-8.54	1.14	1.24
1	B	162	LYS	C-O	-8.51	1.19	1.23
1	A	9	ALA	CA-C	-8.37	1.41	1.52
1	D	7	ILE	CA-CB	8.35	1.64	1.54
1	C	207	LEU	CA-C	8.15	1.63	1.52
1	G	125	ALA	CA-CB	-8.13	1.40	1.53
1	D	228	THR	CA-CB	-8.12	1.40	1.53
1	H	217	MET	SD-CE	-8.11	1.59	1.79
1	A	162	LYS	C-O	8.11	1.27	1.23
1	C	168	SER	C-O	-8.10	1.15	1.23
1	F	249	LYS	CA-CB	8.09	1.66	1.53
1	D	217	MET	SD-CE	-8.01	1.59	1.79
1	G	222	ALA	CA-CB	-8.01	1.42	1.53
1	G	239	ILE	N-CA	-7.97	1.37	1.46
1	G	105	ALA	CA-CB	-7.91	1.38	1.53
1	B	44	MET	SD-CE	-7.88	1.59	1.79
1	F	53	ILE	C-O	7.84	1.32	1.24
1	F	166	PRO	CA-C	-7.78	1.42	1.52
1	F	202	VAL	C-O	-7.76	1.15	1.24
1	A	6	ILE	C-O	7.69	1.32	1.24
1	C	244	ASN	N-CA	-7.58	1.36	1.46
1	B	291	THR	CA-CB	-7.55	1.43	1.53
1	C	204	ARG	C-O	-7.55	1.14	1.24
1	A	202	VAL	CA-C	7.45	1.62	1.52
1	G	162	LYS	CA-CB	7.44	1.59	1.52
1	G	111	ASN	N-CA	7.40	1.55	1.46
1	C	54	ILE	CA-CB	-7.38	1.45	1.54
1	A	33	LYS	C-O	-7.28	1.16	1.24
1	A	110	ASP	C-O	-7.25	1.13	1.24
1	G	125	ALA	C-O	-7.23	1.15	1.24
1	F	26	GLN	C-O	7.22	1.33	1.24
1	H	137	TYR	C-O	7.21	1.31	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	E	292	VAL	C-O	-7.17	1.16	1.24
1	G	202	VAL	CA-C	7.16	1.61	1.52
1	D	202	VAL	C-O	-7.13	1.16	1.24
1	A	148	VAL	CA-CB	7.08	1.62	1.54
1	C	8	LEU	CA-C	-7.05	1.44	1.52
1	A	241	THR	C-O	-7.04	1.15	1.24
1	F	172	VAL	C-O	-7.04	1.16	1.24
1	G	105	ALA	C-O	7.00	1.32	1.23
1	G	9	ALA	CA-C	-7.00	1.43	1.52
1	D	273	ALA	CA-CB	-6.99	1.42	1.53
1	G	40	LEU	CA-CB	-6.92	1.42	1.53
1	D	30	VAL	CA-CB	-6.92	1.45	1.53
1	F	53	ILE	CG1-CD1	-6.88	1.25	1.51
1	A	206	TYR	N-CA	-6.86	1.38	1.46
1	F	224	LEU	C-O	6.86	1.32	1.23
1	E	163	PRO	C-O	-6.85	1.16	1.23
1	F	137	TYR	C-O	-6.85	1.16	1.23
1	C	41	SER	C-O	6.84	1.32	1.24
1	F	107	VAL	C-O	6.84	1.30	1.24
1	F	106	LEU	C-O	6.82	1.32	1.24
1	E	157	ILE	CA-CB	6.79	1.63	1.54
1	G	38	TYR	N-CA	-6.79	1.41	1.46
1	G	280	TYR	C-O	-6.76	1.16	1.24
1	D	115	GLY	CA-C	-6.76	1.45	1.51
1	D	244	ASN	N-CA	-6.73	1.37	1.46
1	H	249	LYS	C-O	-6.70	1.15	1.23
1	C	226	THR	N-CA	-6.69	1.39	1.46
1	F	257	ALA	CA-C	6.69	1.61	1.52
1	F	199	ILE	N-CA	6.68	1.55	1.46
1	B	40	LEU	C-O	6.68	1.31	1.24
1	G	208	GLU	C-O	6.67	1.32	1.24
1	C	9	ALA	CA-C	-6.67	1.43	1.52
1	A	148	VAL	C-O	-6.66	1.16	1.24
1	E	53	ILE	CA-CB	-6.66	1.46	1.53
1	D	162	LYS	C-O	-6.65	1.20	1.23
1	C	148	VAL	CA-C	-6.62	1.44	1.52
1	F	112	LEU	N-CA	-6.62	1.37	1.46
1	G	104	SER	C-O	6.60	1.32	1.23
1	G	128	ARG	NE-CZ	-6.60	1.25	1.33
1	B	53	ILE	CA-CB	-6.60	1.46	1.53
1	G	51	ILE	C-O	-6.56	1.17	1.24
1	B	242	LEU	C-O	6.54	1.31	1.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	F	30	VAL	CA-CB	-6.53	1.46	1.53
1	H	105	ALA	CA-CB	-6.51	1.42	1.53
1	A	122	LEU	C-O	6.51	1.31	1.24
1	H	112	LEU	CB-CG	-6.48	1.40	1.53
1	E	249	LYS	CD-CE	6.47	1.71	1.52
1	B	30	VAL	C-O	-6.45	1.16	1.24
1	A	177	PHE	CA-C	6.45	1.60	1.52
1	G	37	TYR	CA-C	6.39	1.61	1.52
1	G	256	ILE	N-CA	-6.37	1.38	1.46
1	E	272	ALA	CA-CB	-6.35	1.43	1.53
1	D	214	VAL	CA-CB	-6.35	1.45	1.53
1	A	135	PHE	C-O	6.33	1.32	1.24
1	G	234	GLU	CA-CB	6.33	1.63	1.53
1	C	183	VAL	CA-C	6.33	1.60	1.52
1	D	112	LEU	CA-C	6.30	1.60	1.52
1	G	8	LEU	C-O	6.30	1.31	1.24
1	F	8	LEU	CA-C	-6.29	1.44	1.52
1	G	182	VAL	C-O	-6.28	1.16	1.24
1	F	105	ALA	CA-CB	-6.25	1.41	1.53
1	F	240	ALA	CA-CB	-6.25	1.43	1.53
1	D	219	ARG	CA-CB	-6.21	1.42	1.53
1	H	52	LEU	N-CA	6.21	1.53	1.46
1	D	224	LEU	C-O	6.20	1.31	1.24
1	B	88	LEU	N-CA	-6.19	1.38	1.46
1	B	191	PRO	CA-C	-6.18	1.45	1.52
1	F	222	ALA	N-CA	-6.15	1.38	1.46
1	E	199	ILE	CA-C	6.14	1.61	1.52
1	A	200	THR	C-O	-6.12	1.17	1.24
1	C	117	ASP	C-O	-6.12	1.15	1.23
1	A	196	GLU	CA-C	6.11	1.59	1.52
1	C	124	SER	CA-C	6.10	1.60	1.52
1	G	282	GLN	CB-CG	6.09	1.70	1.52
1	D	236	GLY	CA-C	6.08	1.58	1.52
1	C	81	VAL	C-O	-6.08	1.17	1.24
1	G	202	VAL	CA-CB	-6.08	1.47	1.54
1	E	250	VAL	C-O	-6.07	1.17	1.24
1	D	282	GLN	CA-C	6.06	1.60	1.52
1	A	54	ILE	CA-CB	-6.06	1.47	1.54
1	G	249	LYS	CD-CE	6.06	1.70	1.52
1	F	235	ALA	N-CA	-6.06	1.39	1.46
1	F	54	ILE	N-CA	-6.05	1.38	1.46
1	F	145	TYR	CA-CB	-6.05	1.45	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	144	ARG	NE-CZ	6.05	1.39	1.33
1	F	171	ALA	CA-CB	-6.05	1.44	1.53
1	G	178	TYR	C-O	-6.04	1.16	1.23
1	D	54	ILE	C-O	6.03	1.30	1.24
1	C	246	GLN	CA-CB	-6.03	1.44	1.53
1	B	105	ALA	C-O	6.02	1.31	1.23
1	E	134	VAL	C-O	6.01	1.30	1.23
1	B	247	GLY	C-O	-6.00	1.15	1.23
1	H	249	LYS	CD-CE	6.00	1.70	1.52
1	E	243	GLU	C-O	6.00	1.31	1.24
1	F	199	ILE	C-O	-6.00	1.16	1.24
1	B	246	GLN	C-O	-5.98	1.16	1.24
1	F	290	GLU	C-O	-5.97	1.16	1.24
1	A	91	ALA	CA-CB	5.97	1.63	1.53
1	B	146	GLY	C-O	5.97	1.29	1.23
1	H	291	THR	CA-CB	-5.96	1.44	1.53
1	A	166	PRO	CA-C	-5.96	1.45	1.52
1	F	180	GLN	CD-OE1	5.96	1.34	1.23
1	D	257	ALA	CA-CB	-5.96	1.43	1.53
1	D	225	ASP	CA-CB	5.95	1.62	1.53
1	A	222	ALA	C-O	5.93	1.31	1.24
1	G	218	GLY	C-N	-5.93	1.26	1.34
1	H	137	TYR	N-CA	5.93	1.53	1.46
1	H	41	SER	C-O	-5.92	1.16	1.24
1	G	273	ALA	C-O	-5.91	1.18	1.24
1	E	243	GLU	N-CA	5.91	1.53	1.46
1	B	38	TYR	CA-C	5.90	1.58	1.52
1	C	243	GLU	C-O	5.90	1.31	1.24
1	H	62	ARG	CA-C	5.90	1.60	1.52
1	H	51	ILE	CA-CB	-5.88	1.47	1.54
1	D	226	THR	CA-C	-5.88	1.45	1.53
1	C	96	GLU	C-N	-5.87	1.26	1.33
1	B	254	GLU	C-O	-5.87	1.17	1.24
1	G	60	THR	C-O	-5.86	1.18	1.24
1	C	136	ALA	N-CA	-5.86	1.38	1.46
1	G	86	ASP	N-CA	-5.86	1.39	1.46
1	C	233	LEU	CA-C	5.85	1.60	1.52
1	G	235	ALA	CA-CB	-5.82	1.43	1.53
1	H	245	ARG	C-O	5.82	1.30	1.24
1	B	180	GLN	CG-CD	5.81	1.66	1.52
1	H	177	PHE	CA-C	5.81	1.59	1.52
1	F	82	GLN	N-CA	-5.81	1.41	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	E	132	ALA	CA-C	5.80	1.59	1.52
1	B	92	PHE	CA-C	5.80	1.60	1.52
1	C	39	PRO	CA-C	-5.79	1.43	1.52
1	C	180	GLN	CD-OE1	5.79	1.34	1.23
1	G	249	LYS	N-CA	-5.79	1.39	1.45
1	B	242	LEU	CA-C	5.79	1.60	1.52
1	C	98	PHE	N-CA	-5.79	1.39	1.46
1	A	206	TYR	CA-C	5.78	1.60	1.52
1	G	2	LYS	N-CA	5.78	1.57	1.46
1	G	198	GLU	C-O	5.78	1.31	1.24
1	D	272	ALA	CA-C	5.77	1.60	1.52
1	F	250	VAL	CA-CB	-5.77	1.47	1.54
1	H	39	PRO	C-O	-5.76	1.17	1.24
1	B	245	ARG	CG-CD	-5.74	1.35	1.52
1	H	223	TRP	N-CA	-5.74	1.39	1.46
1	C	250	VAL	CA-C	-5.73	1.45	1.52
1	H	156	ALA	CA-C	-5.71	1.44	1.52
1	E	118	PHE	CA-CB	5.71	1.62	1.53
1	C	118	PHE	CA-CB	5.70	1.63	1.53
1	D	224	LEU	CA-C	5.69	1.59	1.52
1	D	148	VAL	CA-C	-5.68	1.45	1.52
1	D	233	LEU	CA-C	5.68	1.60	1.52
1	G	290	GLU	CA-C	-5.68	1.45	1.52
1	A	53	ILE	CA-CB	5.66	1.60	1.54
1	C	67	LEU	C-O	-5.65	1.16	1.23
1	G	196	GLU	C-O	-5.64	1.17	1.23
1	D	51	ILE	N-CA	-5.64	1.39	1.46
1	F	71	SER	C-O	-5.63	1.17	1.24
1	C	107	VAL	C-O	5.63	1.29	1.24
1	G	250	VAL	CA-CB	-5.62	1.47	1.54
1	B	241	THR	N-CA	-5.62	1.39	1.46
1	D	245	ARG	CD-NE	-5.61	1.38	1.46
1	E	257	ALA	CA-C	5.61	1.60	1.52
1	F	46	ALA	C-O	-5.61	1.16	1.24
1	H	179	ASP	CA-C	5.59	1.60	1.53
1	D	168	SER	CA-C	-5.59	1.46	1.52
1	B	182	VAL	C-O	-5.58	1.17	1.24
1	D	54	ILE	CA-C	-5.57	1.45	1.52
1	C	255	GLU	C-O	-5.57	1.17	1.24
1	B	177	PHE	CA-C	5.57	1.59	1.52
1	C	136	ALA	C-O	-5.57	1.17	1.24
1	B	69	ASP	C-O	-5.56	1.16	1.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	166	PRO	CA-CB	5.56	1.61	1.53
1	C	46	ALA	CA-C	5.55	1.60	1.52
1	D	64	GLN	C-O	-5.55	1.17	1.24
1	D	222	ALA	CA-CB	-5.54	1.45	1.53
1	F	67	LEU	C-O	-5.54	1.16	1.24
1	D	207	LEU	C-O	-5.53	1.17	1.24
1	F	234	GLU	N-CA	5.53	1.53	1.46
1	D	90	GLN	C-O	-5.53	1.17	1.24
1	F	245	ARG	CA-C	5.53	1.59	1.52
1	C	252	CYS	C-O	-5.53	1.17	1.24
1	D	220	GLY	N-CA	5.52	1.54	1.45
1	G	28	LEU	C-O	-5.52	1.16	1.23
1	D	139	VAL	CA-C	-5.51	1.46	1.52
1	G	173	THR	C-O	-5.51	1.16	1.23
1	C	168	SER	CA-C	-5.50	1.46	1.52
1	G	128	ARG	CB-CG	-5.50	1.35	1.52
1	C	201	ASP	CA-C	5.49	1.59	1.52
1	G	62	ARG	N-CA	-5.49	1.39	1.46
1	E	23	ILE	CA-CB	-5.48	1.47	1.54
1	C	156	ALA	C-O	5.48	1.30	1.23
1	B	160	GLU	C-O	5.48	1.30	1.23
1	B	171	ALA	CA-CB	5.46	1.61	1.53
1	F	38	TYR	CA-C	5.45	1.58	1.52
1	A	92	PHE	C-O	-5.45	1.17	1.24
1	B	98	PHE	C-O	-5.44	1.17	1.24
1	A	249	LYS	CE-NZ	5.44	1.65	1.49
1	C	233	LEU	CB-CG	-5.43	1.42	1.53
1	F	159	LEU	N-CA	-5.43	1.39	1.46
1	A	174	GLY	N-CA	5.43	1.53	1.45
1	B	234	GLU	CA-CB	5.43	1.61	1.53
1	A	157	ILE	N-CA	-5.43	1.41	1.46
1	A	105	ALA	CA-CB	-5.43	1.44	1.53
1	E	9	ALA	CA-C	-5.42	1.44	1.52
1	F	96	GLU	CA-C	5.42	1.60	1.52
1	D	247	GLY	CA-C	5.41	1.58	1.51
1	A	249	LYS	C-O	-5.41	1.17	1.23
1	F	211	GLN	CA-CB	-5.40	1.46	1.53
1	H	199	ILE	C-O	-5.39	1.17	1.24
1	G	128	ARG	CZ-NH2	-5.39	1.26	1.33
1	F	170	TYR	CA-C	5.38	1.59	1.52
1	C	112	LEU	CA-C	5.38	1.59	1.52
1	D	225	ASP	CA-C	5.38	1.59	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	66	LEU	C-O	-5.37	1.17	1.24
1	A	146	GLY	C-O	5.37	1.29	1.23
1	F	286	ARG	CG-CD	5.36	1.68	1.52
1	G	78	GLN	N-CA	5.36	1.52	1.45
1	F	62	ARG	C-O	-5.36	1.17	1.24
1	D	225	ASP	N-CA	5.35	1.52	1.46
1	E	173	THR	C-O	-5.34	1.16	1.23
1	G	118	PHE	CG-CD1	-5.34	1.27	1.38
1	A	256	ILE	N-CA	-5.34	1.40	1.46
1	A	186	ALA	CA-CB	-5.34	1.44	1.53
1	F	265	ALA	CA-CB	-5.33	1.45	1.53
1	G	25	LYS	C-O	-5.33	1.17	1.24
1	H	37	TYR	CA-C	5.33	1.60	1.52
1	F	54	ILE	CA-C	5.32	1.59	1.52
1	D	245	ARG	C-O	-5.32	1.18	1.24
1	E	112	LEU	N-CA	-5.31	1.40	1.46
1	H	136	ALA	N-CA	-5.31	1.39	1.46
1	B	156	ALA	CA-C	-5.31	1.45	1.52
1	C	52	LEU	C-O	5.30	1.30	1.24
1	E	33	LYS	C-O	-5.30	1.17	1.24
1	H	165	GLU	CA-C	5.30	1.58	1.52
1	F	130	THR	CB-CG2	5.30	1.70	1.52
1	F	223	TRP	C-O	-5.29	1.18	1.24
1	B	130	THR	C-O	5.28	1.30	1.23
1	E	162	LYS	C-O	-5.28	1.21	1.23
1	F	235	ALA	CA-CB	-5.28	1.45	1.53
1	G	175	LEU	C-O	-5.28	1.18	1.24
1	G	261	LYS	CE-NZ	5.28	1.65	1.49
1	C	234	GLU	CA-CB	5.28	1.61	1.53
1	D	4	LYS	C-O	-5.27	1.17	1.23
1	B	257	ALA	CA-CB	5.26	1.61	1.53
1	C	29	PRO	CG-CD	-5.26	1.32	1.50
1	D	249	LYS	CA-CB	5.26	1.61	1.53
1	G	226	THR	N-CA	-5.26	1.40	1.46
1	G	36	ILE	CG1-CD1	-5.25	1.31	1.51
1	H	259	ARG	CA-C	5.25	1.59	1.52
1	A	201	ASP	C-O	-5.25	1.17	1.24
1	B	243	GLU	CA-C	-5.25	1.46	1.52
1	A	3	ARG	CA-C	-5.25	1.46	1.52
1	G	290	GLU	C-N	-5.24	1.26	1.33
1	G	283	TYR	N-CA	-5.21	1.40	1.46
1	G	24	SER	N-CA	5.21	1.52	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	109	GLY	C-O	-5.21	1.17	1.24
1	C	172	VAL	N-CA	-5.20	1.40	1.46
1	A	112	LEU	C-O	5.20	1.30	1.23
1	H	155	LYS	CA-C	5.19	1.59	1.52
1	B	135	PHE	CA-C	5.19	1.58	1.52
1	B	141	ASP	CG-OD1	5.19	1.35	1.25
1	G	24	SER	C-O	-5.19	1.16	1.23
1	F	217	MET	C-O	-5.19	1.17	1.23
1	G	121	LEU	CA-C	5.18	1.59	1.52
1	A	251	ALA	CA-CB	5.18	1.61	1.53
1	F	237	GLN	CA-CB	-5.18	1.45	1.53
1	B	217	MET	N-CA	-5.17	1.39	1.46
1	F	30	VAL	C-O	5.17	1.30	1.23
1	F	268	LEU	CA-C	-5.17	1.46	1.52
1	F	141	ASP	CA-C	5.17	1.58	1.53
1	G	257	ALA	CA-C	5.17	1.59	1.52
1	C	239	ILE	CA-CB	-5.16	1.47	1.54
1	A	128	ARG	NE-CZ	-5.16	1.27	1.33
1	B	9	ALA	CA-C	-5.16	1.45	1.52
1	C	177	PHE	CA-C	5.16	1.58	1.52
1	G	86	ASP	CA-CB	-5.15	1.46	1.53
1	C	147	VAL	N-CA	-5.15	1.40	1.46
1	E	121	LEU	CA-C	5.15	1.59	1.52
1	D	257	ALA	CA-C	5.15	1.59	1.52
1	A	115	GLY	C-O	-5.15	1.16	1.23
1	G	254	GLU	N-CA	-5.15	1.40	1.46
1	B	89	ALA	CA-C	5.15	1.59	1.52
1	A	108	LEU	C-N	-5.13	1.27	1.33
1	G	38	TYR	CA-C	5.13	1.58	1.52
1	E	244	ASN	N-CA	-5.12	1.39	1.46
1	B	24	SER	CA-C	5.12	1.59	1.52
1	C	30	VAL	C-O	5.12	1.30	1.24
1	C	273	ALA	CA-CB	-5.11	1.45	1.53
1	C	171	ALA	CA-CB	-5.10	1.45	1.53
1	G	64	GLN	CB-CG	-5.10	1.37	1.52
1	A	291	THR	N-CA	-5.09	1.39	1.46
1	F	60	THR	C-O	-5.09	1.19	1.24
1	D	9	ALA	CA-C	-5.09	1.46	1.52
1	H	204	ARG	CZ-NH2	-5.09	1.26	1.33
1	H	226	THR	CA-CB	-5.09	1.46	1.53
1	H	196	GLU	C-O	-5.08	1.17	1.23
1	F	199	ILE	CA-CB	-5.08	1.47	1.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	E	205	ALA	CA-CB	-5.08	1.45	1.53
1	H	125	ALA	CA-CB	-5.08	1.45	1.53
1	C	183	VAL	CA-CB	-5.07	1.48	1.54
1	G	240	ALA	N-CA	-5.07	1.40	1.46
1	H	226	THR	N-CA	-5.06	1.40	1.46
1	B	58	GLN	CD-OE1	5.06	1.33	1.23
1	E	242	LEU	C-O	5.06	1.30	1.24
1	D	120	GLU	N-CA	-5.05	1.40	1.46
1	E	24	SER	CA-C	5.05	1.59	1.52
1	E	107	VAL	C-O	5.05	1.29	1.24
1	H	211	GLN	C-O	-5.04	1.16	1.24
1	E	214	VAL	CA-C	5.03	1.59	1.52
1	D	102	ASP	C-O	-5.03	1.17	1.23
1	E	175	LEU	N-CA	-5.03	1.40	1.46
1	C	92	PHE	CE1-CZ	-5.03	1.23	1.38
1	D	207	LEU	CA-CB	5.03	1.61	1.53
1	H	35	MET	CG-SD	-5.03	1.68	1.80
1	H	109	GLY	N-CA	5.02	1.52	1.45
1	H	32	ASP	C-O	-5.02	1.17	1.24
1	F	239	ILE	CA-C	5.01	1.59	1.52
1	B	172	VAL	CA-CB	-5.01	1.48	1.54
1	D	206	TYR	CA-C	5.01	1.59	1.52
1	H	225	ASP	CA-C	5.01	1.58	1.52

All (148) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	118	PHE	N-CA-C	-11.85	98.44	111.36
1	D	118	PHE	N-CA-C	-11.79	98.15	111.71
1	C	154	GLY	N-CA-C	10.15	128.87	115.36
1	C	118	PHE	N-CA-C	-10.11	100.21	112.54
1	B	118	PHE	N-CA-C	-10.01	100.45	111.36
1	C	226	THR	CB-CA-C	9.46	124.29	111.14
1	E	118	PHE	CA-C-O	8.71	129.65	120.42
1	A	162	LYS	CB-CA-C	-8.06	105.48	111.20
1	B	157	ILE	N-CA-C	7.89	121.26	113.53
1	F	118	PHE	N-CA-C	-7.71	103.13	112.54
1	F	115	GLY	N-CA-C	7.70	120.12	110.96
1	G	118	PHE	N-CA-C	-7.49	103.09	111.71
1	F	66	LEU	N-CA-C	7.46	119.20	111.14
1	H	289	THR	CB-CA-C	-7.39	99.61	111.28
1	H	246	GLN	N-CA-C	7.38	121.53	112.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	H	118	PHE	N-CA-C	-7.32	103.30	111.71
1	G	115	GLY	N-CA-C	7.24	119.57	110.96
1	A	252	CYS	CA-C-O	7.23	123.99	119.29
1	D	182	VAL	N-CA-C	7.22	117.35	110.42
1	D	194	ARG	N-CA-C	-7.15	104.56	113.28
1	C	226	THR	OG1-CB-CG2	-7.08	95.15	109.30
1	H	226	THR	OG1-CB-CG2	-7.07	95.16	109.30
1	F	145	TYR	CA-C-N	7.07	127.34	120.98
1	F	145	TYR	C-N-CA	7.07	127.34	120.98
1	F	125	ALA	N-CA-C	-6.98	103.73	111.82
1	G	34	PRO	CA-C-O	-6.94	112.98	121.31
1	C	11	GLY	N-CA-C	6.87	119.98	112.29
1	D	198	GLU	N-CA-C	6.82	120.78	109.46
1	G	226	THR	OG1-CB-CG2	-6.75	95.81	109.30
1	C	93	LEU	N-CA-C	-6.69	103.78	112.68
1	D	23	ILE	N-CA-C	6.68	117.92	108.17
1	A	224	LEU	CA-C-N	-6.68	112.33	122.81
1	A	224	LEU	C-N-CA	-6.68	112.33	122.81
1	B	24	SER	N-CA-C	6.62	118.84	110.24
1	D	29	PRO	CB-CA-C	-6.58	102.46	111.21
1	E	198	GLU	N-CA-C	6.57	119.30	109.25
1	G	110	ASP	CA-C-N	-6.57	112.87	122.65
1	G	110	ASP	C-N-CA	-6.57	112.87	122.65
1	C	145	TYR	N-CA-C	6.46	118.99	109.69
1	F	249	LYS	CB-CG-CD	6.45	126.14	111.30
1	H	115	GLY	N-CA-C	6.45	118.64	110.96
1	A	198	GLU	N-CA-C	6.41	119.94	109.76
1	B	209	ARG	NE-CZ-NH2	-6.40	113.44	119.20
1	H	23	ILE	N-CA-C	6.37	116.66	107.88
1	F	198	GLU	N-CA-C	6.35	118.97	109.25
1	F	37	TYR	N-CA-C	-6.30	104.86	112.54
1	D	180	GLN	N-CA-C	6.27	120.40	112.87
1	E	189	LEU	N-CA-C	6.25	118.10	110.41
1	H	66	LEU	N-CA-C	6.24	118.08	111.28
1	C	118	PHE	CB-CA-C	6.22	123.31	110.31
1	A	104	SER	N-CA-C	6.20	118.38	109.14
1	C	139	VAL	N-CA-C	6.16	118.33	108.85
1	A	128	ARG	NE-CZ-NH2	-6.15	113.67	119.20
1	D	173	THR	OG1-CB-CG2	-6.13	97.04	109.30
1	G	126	SER	N-CA-C	6.13	118.04	111.36
1	B	124	SER	N-CA-C	6.09	118.41	111.11
1	H	60	THR	CA-C-O	6.06	124.67	118.73

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	81	VAL	N-CA-C	6.06	117.32	108.53
1	F	230	ASP	N-CA-C	6.06	117.56	111.07
1	G	289	THR	CB-CA-C	-6.05	100.92	110.85
1	G	128	ARG	NE-CZ-NH1	-6.05	115.45	121.50
1	B	137	TYR	CA-CB-CG	6.05	124.79	113.90
1	H	7	ILE	CA-C-N	-6.04	114.99	122.84
1	H	7	ILE	C-N-CA	-6.04	114.99	122.84
1	H	202	VAL	N-CA-C	-6.03	104.45	110.30
1	B	220	GLY	N-CA-C	6.03	121.09	114.40
1	B	247	GLY	N-CA-C	-6.02	105.62	114.90
1	C	173	THR	OG1-CB-CG2	-5.98	97.33	109.30
1	D	223	TRP	N-CA-CB	5.97	120.08	110.65
1	G	124	SER	N-CA-C	5.97	118.30	111.02
1	C	205	ALA	N-CA-C	-5.94	104.89	111.36
1	G	11	GLY	N-CA-C	-5.88	102.83	112.83
1	C	4	LYS	CA-C-N	-5.87	118.13	122.18
1	C	4	LYS	C-N-CA	-5.87	118.13	122.18
1	D	282	GLN	N-CA-C	-5.87	104.88	111.28
1	B	131	GLY	CA-C-N	5.86	131.74	122.94
1	B	131	GLY	C-N-CA	5.86	131.74	122.94
1	E	199	ILE	N-CA-C	-5.86	103.72	111.05
1	B	226	THR	OG1-CB-CG2	-5.85	97.61	109.30
1	C	55	SER	N-CA-C	5.84	116.00	108.34
1	H	184	ASP	N-CA-C	5.84	117.64	111.28
1	A	38	TYR	O-C-N	5.83	124.29	120.27
1	E	237	GLN	N-CA-C	-5.82	104.93	111.28
1	H	252	CYS	CA-C-O	5.82	123.07	119.29
1	F	53	ILE	CA-CB-CG1	5.82	120.29	110.40
1	G	154	GLY	CA-C-O	5.80	125.73	119.06
1	A	126	SER	N-CA-C	5.77	118.34	111.71
1	D	123	GLY	CA-C-O	5.76	126.45	120.80
1	G	103	LEU	N-CA-C	-5.73	102.97	110.53
1	E	9	ALA	N-CA-C	5.72	117.30	110.44
1	F	51	ILE	N-CA-C	5.68	116.31	108.12
1	G	225	ASP	N-CA-CB	5.68	119.93	110.85
1	E	173	THR	OG1-CB-CG2	-5.65	98.00	109.30
1	B	146	GLY	N-CA-C	-5.64	103.86	111.54
1	F	20	THR	CB-CA-C	-5.64	102.31	111.06
1	G	207	LEU	N-CA-C	-5.64	105.21	111.36
1	F	247	GLY	N-CA-C	-5.64	105.58	114.10
1	B	225	ASP	CB-CA-C	5.63	120.43	109.33
1	D	289	THR	N-CA-C	5.62	122.04	113.61

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	115	GLY	N-CA-C	5.62	118.66	110.63
1	A	247	GLY	N-CA-C	-5.61	106.27	114.90
1	B	37	TYR	CA-C-N	5.61	126.05	119.83
1	B	37	TYR	C-N-CA	5.61	126.05	119.83
1	D	10	GLY	N-CA-C	-5.57	104.67	112.13
1	A	197	LEU	N-CA-C	-5.56	100.05	108.67
1	C	124	SER	N-CA-CB	-5.56	101.95	110.01
1	E	88	LEU	CA-CB-CG	5.54	135.68	116.30
1	F	180	GLN	N-CA-C	5.53	119.77	113.19
1	B	16	LEU	N-CA-C	5.51	119.86	113.20
1	A	202	VAL	N-CA-C	-5.46	105.40	110.53
1	H	122	LEU	N-CA-C	5.42	116.87	111.07
1	C	2	LYS	N-CA-C	5.41	118.16	110.10
1	G	209	ARG	NE-CZ-NH2	-5.38	114.36	119.20
1	B	117	ASP	CA-C-N	5.38	127.93	120.29
1	B	117	ASP	C-N-CA	5.38	127.93	120.29
1	H	199	ILE	N-CA-C	-5.38	105.13	110.62
1	A	115	GLY	N-CA-C	5.37	118.30	111.37
1	C	224	LEU	CA-C-N	-5.37	114.16	122.59
1	C	224	LEU	C-N-CA	-5.37	114.16	122.59
1	A	183	VAL	N-CA-C	-5.37	105.27	110.42
1	A	254	GLU	N-CA-C	-5.37	105.43	111.28
1	F	11	GLY	O-C-N	5.36	128.93	122.98
1	B	70	GLY	N-CA-C	5.32	122.43	115.40
1	B	122	LEU	CB-CA-C	-5.31	102.78	110.96
1	C	140	LEU	N-CA-C	5.30	117.06	111.28
1	E	223	TRP	N-CA-C	-5.30	98.75	108.02
1	D	13	GLY	N-CA-C	5.29	118.89	112.49
1	B	60	THR	OG1-CB-CG2	-5.28	98.73	109.30
1	D	154	GLY	N-CA-C	5.28	122.64	115.30
1	E	172	VAL	O-C-N	-5.26	116.94	122.83
1	E	163	PRO	CB-CA-C	-5.26	105.10	111.46
1	C	164	LEU	N-CA-C	-5.23	105.69	111.71
1	A	194	ARG	CB-CA-C	-5.22	100.02	110.42
1	A	226	THR	OG1-CB-CG2	-5.19	98.92	109.30
1	E	193	PRO	N-CA-C	-5.18	106.33	113.53
1	H	178	TYR	N-CA-C	5.17	117.67	109.50
1	C	178	TYR	N-CA-C	5.17	117.67	109.50
1	H	27	LEU	N-CA-C	-5.15	106.84	113.23
1	D	225	ASP	CB-CA-C	5.14	118.62	109.72
1	H	38	TYR	O-C-N	5.13	124.43	120.38
1	C	1	MET	CA-C-N	5.10	128.00	120.82

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	1	MET	C-N-CA	5.10	128.00	120.82
1	F	224	LEU	CA-C-N	-5.08	114.69	122.62
1	F	224	LEU	C-N-CA	-5.08	114.69	122.62
1	D	223	TRP	N-CA-C	-5.08	99.13	108.02
1	H	34	PRO	CA-C-O	-5.07	115.57	121.34
1	C	225	ASP	N-CA-CB	5.04	120.33	111.55
1	B	76	ASP	CB-CA-C	5.02	118.91	111.17

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	C	119	HIS	Sidechain
1	G	138	HIS	Sidechain
1	G	17	HIS	Sidechain
1	H	17	HIS	Sidechain

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	2302	0	2287	89	0
1	B	2322	0	2305	91	0
1	C	2340	0	2324	68	0
1	D	2294	0	2279	67	0
1	E	2339	0	2316	94	0
1	F	2316	0	2301	69	0
1	G	2318	0	2300	61	1
1	H	2285	0	2272	58	0
2	A	10	0	0	0	0
2	B	10	0	0	1	0
2	C	15	0	0	2	0
2	D	15	0	0	0	0
2	E	15	0	0	0	0
2	F	10	0	0	0	0
2	G	15	0	0	1	0
2	H	10	0	0	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	A	325	0	0	35	1
3	B	335	0	0	24	0
3	C	286	0	0	14	0
3	D	259	0	0	17	0
3	E	282	0	0	33	0
3	F	321	0	0	22	4
3	G	367	0	0	22	3
3	H	303	0	0	15	1
All	All	21094	0	18384	550	5

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 15.

All (550) 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:A:23:ILE:HG23	1:A:28:LEU:HD21	1.33	1.09
1:E:23:ILE:HG21	1:F:23:ILE:HG12	1.22	1.09
1:C:23:ILE:HG12	1:D:23:ILE:HG21	1.14	1.07
1:A:23:ILE:HB	1:B:23:ILE:HD12	1.11	1.06
1:A:23:ILE:CB	1:B:23:ILE:HD12	1.86	1.06
1:G:14:THR:HA	3:G:4997:HOH:O	1.56	1.04
1:E:23:ILE:HD13	1:F:23:ILE:HD13	1.04	1.04
1:B:23:ILE:HG13	3:B:4009:HOH:O	1.55	1.03
1:F:273:ALA:HB3	1:F:274:PRO:HD3	1.37	1.02
1:C:119:HIS:CD2	3:C:5244:HOH:O	2.13	1.01
1:B:192:SER:HB2	1:B:193:PRO:HD2	1.41	0.99
1:G:141[A]:ASP:OD2	1:G:144:ARG:HD3	1.59	0.99
1:G:141[B]:ASP:OD2	1:G:144:ARG:HD3	1.59	0.99
1:A:23:ILE:CG2	1:A:28:LEU:HD21	1.93	0.99
1:A:23:ILE:HG23	1:A:28:LEU:CD2	1.93	0.98
1:A:23:ILE:HD13	1:B:23:ILE:HB	1.43	0.97
1:A:162:LYS:NZ	1:A:194:ARG:HH21	1.61	0.97
1:C:23:ILE:CG1	1:D:23:ILE:HG21	1.95	0.96
1:E:23:ILE:CD1	1:F:23:ILE:HD13	1.96	0.95
1:A:162:LYS:HZ3	1:A:194:ARG:HH21	1.11	0.94
1:F:17:HIS:NE2	1:F:21:LEU:HD23	1.83	0.94
1:A:23:ILE:HB	1:B:23:ILE:CD1	1.98	0.93
1:C:119:HIS:HB2	3:C:5275:HOH:O	1.71	0.91
1:B:192:SER:HB2	1:B:193:PRO:CD	2.01	0.91
1:E:23:ILE:HD13	1:F:23:ILE:CD1	1.98	0.91

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:23:ILE:CG2	1:A:28:LEU:CD2	2.49	0.90
1:C:23:ILE:HG21	1:D:23:ILE:HG12	1.52	0.90
1:C:192:SER:HB2	1:C:193:PRO:HD2	1.54	0.89
1:G:90:GLN:HG2	1:G:197:LEU:HD12	1.55	0.88
1:E:273:ALA:HB3	1:E:274:PRO:HD3	1.57	0.87
1:C:13:GLY:O	3:C:5196:HOH:O	1.92	0.87
1:E:227:GLY:N	3:E:6150:HOH:O	2.04	0.84
1:E:190:LYS:HD2	1:E:190:LYS:C	2.02	0.84
1:H:2:LYS:N	3:H:6268:HOH:O	2.09	0.84
1:D:23:ILE:HD13	1:D:28:LEU:HD21	1.59	0.84
1:F:123:GLY:O	1:F:127:GLN:HG3	1.78	0.84
1:H:60:THR:HG23	3:H:6390:HOH:O	1.78	0.84
1:H:60:THR:HB	1:H:61:PRO:HD3	1.60	0.83
1:F:141:ASP:OD2	1:F:144:ARG:NH2	2.12	0.83
1:F:15:ARG:NH2	3:F:4951:HOH:O	2.12	0.83
1:A:162:LYS:NZ	1:A:194:ARG:NH2	2.25	0.83
1:E:23:ILE:CD1	1:F:23:ILE:HG21	2.08	0.82
1:D:160:GLU:HG2	3:D:3996:HOH:O	1.80	0.82
1:H:25:LYS:HE3	1:H:26:GLN:HE22	1.45	0.82
1:F:269:GLU:OE2	3:F:4984:HOH:O	1.97	0.81
1:H:260:GLN:CD	3:H:6392:HOH:O	2.24	0.80
1:E:128:ARG:NH2	1:E:215:GLU:OE2	2.15	0.79
1:G:209:ARG:HD3	3:G:5132:HOH:O	1.80	0.79
1:A:31:TYR:CD1	1:B:233[B]:LEU:HD11	2.18	0.79
1:B:17:HIS:NE2	3:B:3873:HOH:O	2.14	0.79
1:E:128:ARG:NH1	1:E:133:SER:OG	2.16	0.79
1:G:270:LYS:HG2	3:G:5175:HOH:O	1.80	0.79
1:B:141:ASP:HB2	3:B:3773:HOH:O	1.83	0.79
1:E:190:LYS:HD2	1:E:191:PRO:N	1.97	0.79
1:G:16:LEU:HD12	1:G:25:LYS:HB2	1.65	0.78
1:H:273:ALA:HB3	1:H:274:PRO:HD3	1.65	0.78
1:F:23:ILE:HA	3:F:4846:HOH:O	1.84	0.78
1:F:287:LEU:HD23	3:F:5016:HOH:O	1.83	0.78
1:A:31:TYR:HD1	1:B:233[B]:LEU:HD11	1.49	0.77
1:F:152:GLN:HB2	3:F:4947:HOH:O	1.84	0.77
1:H:260:GLN:NE2	3:H:6392:HOH:O	2.17	0.77
1:A:12:SER:HB3	3:A:3800:HOH:O	1.83	0.77
1:C:55:SER:OG	3:C:5263:HOH:O	2.00	0.77
1:D:161:GLU:HG3	1:D:194:ARG:HH21	1.49	0.76
1:B:16:LEU:HA	1:B:229:HIS:CE1	2.20	0.76
1:A:194:ARG:HB2	1:A:196:GLU:HG3	1.66	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:161:GLU:HG3	1:D:194:ARG:NH2	2.00	0.76
1:A:119:HIS:HB3	3:A:3841:HOH:O	1.85	0.76
1:F:234:GLU:CD	3:F:4818:HOH:O	2.29	0.76
1:E:119:HIS:HE1	3:E:6270:HOH:O	1.67	0.75
1:D:161:GLU:CG	1:D:194:ARG:HH21	1.99	0.75
1:E:23:ILE:HG21	1:F:23:ILE:CG1	2.12	0.75
1:F:32:ASP:OD2	1:F:249:LYS:HE3	1.87	0.75
1:A:162:LYS:HZ3	1:A:194:ARG:NH2	1.81	0.75
1:A:31:TYR:CD1	1:B:233[A]:LEU:HD11	2.22	0.74
1:B:155:LYS:HD3	3:B:3982:HOH:O	1.86	0.74
1:E:119:HIS:CE1	3:E:6270:HOH:O	2.40	0.74
1:B:192:SER:CB	1:B:193:PRO:CD	2.62	0.74
1:B:119:HIS:C	1:B:119:HIS:CD2	2.65	0.74
1:E:26:GLN:NE2	3:E:6286:HOH:O	2.09	0.74
1:B:23:ILE:HD11	1:B:27:LEU:HB3	1.69	0.74
1:E:86:ASP:HB2	3:E:6335:HOH:O	1.86	0.73
1:B:84:SER:OG	1:B:85:PRO:HD2	1.89	0.73
1:B:141:ASP:OD1	3:B:3954:HOH:O	2.07	0.73
1:B:273:ALA:HB3	1:B:274:PRO:HD3	1.69	0.73
1:G:60:THR:HG23	3:G:4915:HOH:O	1.87	0.73
1:G:273:ALA:HB3	1:G:274:PRO:HD3	1.71	0.73
1:D:64:GLN:NE2	3:D:3933:HOH:O	2.22	0.73
1:A:259:ARG:HD2	3:A:3728:HOH:O	1.89	0.72
1:E:188:ASP:HB2	3:E:6209:HOH:O	1.87	0.72
1:B:86:ASP:HB3	3:B:3977:HOH:O	1.90	0.72
3:A:3921:HOH:O	1:C:241:THR:HG23	1.90	0.71
1:G:127:GLN:OE1	3:G:5199:HOH:O	2.09	0.71
1:A:31:TYR:HD1	1:B:233[A]:LEU:HD11	1.53	0.71
1:F:234:GLU:CG	3:F:4818:HOH:O	2.39	0.71
1:A:96:GLU:OE1	1:A:187:ARG:NH1	2.24	0.71
1:F:273:ALA:HB3	1:F:274:PRO:CD	2.18	0.71
1:F:141:ASP:OD2	1:F:144:ARG:NE	2.24	0.70
1:F:273:ALA:CB	1:F:274:PRO:HD3	2.19	0.70
1:H:225:ASP:OD1	1:H:225:ASP:C	2.33	0.70
1:B:192:SER:CB	1:B:193:PRO:HD2	2.21	0.70
1:D:273:ALA:HB3	1:D:274:PRO:CD	2.20	0.70
1:F:123:GLY:O	1:F:126:SER:HB3	1.92	0.70
1:E:98:PHE:N	3:E:6239:HOH:O	2.02	0.70
1:E:23:ILE:HD13	1:F:23:ILE:HG21	1.74	0.70
1:G:152:GLN:OE1	3:G:5042:HOH:O	2.09	0.70
1:H:282:GLN:HG2	3:H:6351:HOH:O	1.91	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:119:HIS:CD2	1:C:119:HIS:C	2.69	0.69
1:E:190:LYS:HD3	3:E:6294:HOH:O	1.92	0.69
1:A:194:ARG:CB	1:A:196:GLU:HG3	2.22	0.69
1:F:282:GLN:O	1:F:286:ARG:HG3	1.92	0.69
1:F:16:LEU:HD22	3:F:4861:HOH:O	1.91	0.69
1:C:234:GLU:OE2	3:C:5256:HOH:O	2.11	0.68
1:G:35[B]:MET:HE3	1:G:35[B]:MET:O	1.93	0.68
1:B:149:GLU:OE2	3:B:3960:HOH:O	2.09	0.68
1:A:234:GLU:CG	3:A:3904:HOH:O	2.41	0.68
1:A:194:ARG:CD	1:A:196:GLU:HG3	2.24	0.68
1:G:16:LEU:HA	1:G:229:HIS:CE1	2.29	0.68
1:B:12:SER:HB2	3:B:3895:HOH:O	1.95	0.67
1:A:141:ASP:OD1	3:A:3913:HOH:O	2.12	0.67
1:A:209:ARG:HD3	3:A:3863:HOH:O	1.95	0.67
1:H:141:ASP:OD2	1:H:144:ARG:NH1	2.23	0.67
1:B:245:ARG:HG2	3:D:3974:HOH:O	1.93	0.67
1:G:195:GLY:C	1:G:196:GLU:HG2	2.18	0.67
1:E:260[A]:GLN:NE2	3:E:6211:HOH:O	2.16	0.67
1:F:4:LYS:HE2	3:F:4786:HOH:O	1.93	0.67
1:E:26:GLN:O	3:E:6299:HOH:O	2.11	0.67
1:G:16:LEU:HD22	3:G:4952:HOH:O	1.94	0.67
1:G:24:SER:HB2	1:G:59:ASP:OD2	1.95	0.67
1:A:194:ARG:HD3	1:A:196:GLU:HG3	1.77	0.66
1:E:260[B]:GLN:NE2	3:E:6211:HOH:O	2.15	0.66
1:D:117:ASP:CG	1:D:120:GLU:OE1	2.39	0.66
1:B:23:ILE:HD11	1:B:27:LEU:CB	2.24	0.66
1:E:144:ARG:NH2	1:E:225:ASP:OD2	2.29	0.66
1:G:18:PRO:HD3	1:H:280:TYR:CD1	2.31	0.66
1:D:124:SER:HB2	3:D:3948:HOH:O	1.96	0.65
1:G:16:LEU:HD11	3:G:4989:HOH:O	1.96	0.65
1:C:23:ILE:HG12	1:D:23:ILE:CG2	2.09	0.65
1:H:23:ILE:HD11	1:H:27:LEU:HD12	1.79	0.65
1:D:60:THR:HG22	1:D:61:PRO:HD3	1.79	0.65
1:C:23:ILE:CG2	1:D:23:ILE:HG12	2.24	0.65
1:E:244:ASN:HB3	3:E:6338:HOH:O	1.95	0.65
1:G:152:GLN:CD	3:G:5235:HOH:O	2.39	0.65
1:D:199:ILE:HG22	3:D:3978:HOH:O	1.96	0.65
1:D:10:GLY:O	1:D:26:GLN:NE2	2.28	0.64
1:H:23:ILE:HD12	1:H:62:ARG:HH11	1.62	0.64
1:F:1:MET:HE1	1:F:180:GLN:HE22	1.62	0.64
1:B:16:LEU:HD22	3:B:3752:HOH:O	1.96	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:12:SER:HB2	3:F:4976:HOH:O	1.97	0.64
1:H:160:GLU:CD	3:H:6286:HOH:O	2.40	0.64
1:B:194:ARG:HD2	3:B:3798:HOH:O	1.98	0.64
1:B:273:ALA:HB3	1:B:274:PRO:CD	2.27	0.64
1:E:42:THR:HG23	1:E:118:PHE:CE2	2.32	0.64
1:H:141:ASP:OD2	1:H:144:ARG:HD3	1.98	0.64
1:A:152:GLN:HG3	3:A:3846:HOH:O	1.96	0.64
1:E:10:GLY:HA3	3:E:6180:HOH:O	1.98	0.64
1:H:232:LEU:HD22	3:H:6319:HOH:O	1.98	0.64
1:A:164:LEU:HD22	3:A:4009:HOH:O	1.97	0.63
1:B:16:LEU:O	1:B:19:ALA:HB3	1.98	0.63
1:A:90:GLN:OE1	3:A:3877:HOH:O	2.15	0.63
1:G:88:LEU:HG	3:G:4993:HOH:O	1.98	0.63
1:F:17:HIS:CD2	1:F:21:LEU:HD23	2.33	0.63
1:G:72:ASN:ND2	3:G:5085:HOH:O	2.31	0.63
1:C:234:GLU:HA	1:C:237[B]:GLN:HE21	1.64	0.62
1:C:123:GLY:O	1:C:127:GLN:HG2	1.99	0.62
1:E:178:TYR:OH	1:E:199:ILE:HD11	1.99	0.62
1:A:26:GLN:HB3	3:A:3866:HOH:O	1.98	0.62
1:A:23:ILE:HD13	1:B:23:ILE:CB	2.22	0.62
1:A:162:LYS:HZ2	1:A:194:ARG:NH2	1.97	0.62
1:E:190:LYS:HA	3:E:6240:HOH:O	1.99	0.62
1:E:30:VAL:HG21	1:E:35[B]:MET:SD	2.40	0.62
1:A:18:PRO:HD3	1:B:280:TYR:CD1	2.35	0.62
3:A:3745:HOH:O	1:B:233[B]:LEU:HD23	1.99	0.61
1:E:155:LYS:NZ	3:E:6237:HOH:O	2.33	0.61
1:C:223:TRP:O	1:C:224:LEU:HD23	2.00	0.61
1:A:16:LEU:HA	1:A:229:HIS:CE1	2.34	0.61
1:B:16:LEU:O	1:B:229:HIS:HE1	1.83	0.61
1:E:23:ILE:HD11	1:F:23:ILE:HG21	1.84	0.60
1:G:149:GLU:OE2	3:G:5106:HOH:O	2.17	0.60
1:A:285:LYS:HE2	3:A:3865:HOH:O	2.01	0.60
1:B:209:ARG:HD3	3:B:3830:HOH:O	2.01	0.60
1:C:273:ALA:HB3	1:C:274:PRO:CD	2.32	0.60
1:E:15:ARG:HB3	3:E:6280:HOH:O	2.02	0.60
1:E:286:ARG:HG3	3:E:6382:HOH:O	2.01	0.60
1:B:65:GLN:HB2	3:B:4022:HOH:O	2.01	0.59
1:H:25:LYS:HE3	1:H:26:GLN:NE2	2.17	0.59
1:H:87:GLY:N	1:H:196:GLU:OE1	2.35	0.59
1:E:30:VAL:HG21	1:E:35[A]:MET:SD	2.42	0.59
3:A:3745:HOH:O	1:B:233[A]:LEU:HD23	2.02	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:144:ARG:NH1	1:F:145:TYR:OH	2.36	0.59
1:A:23:ILE:CG2	1:A:28:LEU:HD23	2.30	0.59
1:D:60:THR:HG22	1:D:61:PRO:CD	2.32	0.58
1:D:192:SER:HB2	1:D:193:PRO:HD2	1.85	0.58
1:D:50:GLU:HB2	3:D:4038:HOH:O	2.02	0.58
1:E:183:VAL:O	1:E:187:ARG:HG3	2.03	0.58
1:E:191:PRO:HD2	3:E:6240:HOH:O	2.04	0.58
1:A:109:GLY:O	3:A:3866:HOH:O	2.17	0.58
1:B:155:LYS:HE3	3:B:3950:HOH:O	2.03	0.58
1:C:234:GLU:HA	1:C:237[A]:GLN:HE21	1.67	0.58
1:G:18:PRO:HD2	1:H:32:ASP:O	2.02	0.58
1:A:273:ALA:HB3	1:A:274:PRO:HD3	1.85	0.58
1:B:88:LEU:HD12	1:B:199:ILE:HG21	1.85	0.58
1:F:58:GLN:HG3	3:F:4922:HOH:O	2.04	0.58
1:F:152:GLN:CB	3:F:4947:HOH:O	2.48	0.58
1:C:237[A]:GLN:HG3	1:D:233:LEU:HD11	1.85	0.57
1:C:237[B]:GLN:HG3	1:D:233:LEU:HD11	1.86	0.57
1:A:194:ARG:HD3	1:A:196:GLU:CD	2.29	0.57
1:G:23:ILE:HG12	1:G:28:LEU:HD23	1.87	0.57
1:F:21:LEU:O	3:F:5001:HOH:O	2.18	0.57
1:H:232:LEU:HB2	3:H:6319:HOH:O	2.04	0.57
1:C:1:MET:N	1:C:129:GLN:NE2	2.52	0.57
1:F:234:GLU:HG3	3:F:4818:HOH:O	2.03	0.57
1:G:24:SER:HB2	1:G:59:ASP:CG	2.30	0.57
1:G:60:THR:HG22	1:G:64:GLN:HE21	1.70	0.57
1:F:16:LEU:O	1:F:19:ALA:HB3	2.04	0.57
1:B:194:ARG:HB2	1:B:194:ARG:HH11	1.69	0.57
1:D:60:THR:HG22	1:D:61:PRO:N	2.20	0.57
1:D:282:GLN:HG3	3:D:3970:HOH:O	2.03	0.57
1:B:60:THR:HB	1:B:61:PRO:HD3	1.87	0.56
1:E:42:THR:HG23	1:E:118:PHE:HE2	1.67	0.56
1:F:141:ASP:OD2	1:F:144:ARG:CZ	2.54	0.56
1:C:23:ILE:HD13	1:D:23:ILE:HG12	1.87	0.56
1:F:1:MET:HE1	1:F:180:GLN:NE2	2.21	0.56
1:F:13:GLY:O	1:F:16:LEU:N	2.38	0.56
1:E:88:LEU:HD12	1:E:199:ILE:CG2	2.36	0.56
1:C:128:ARG:NE	3:C:5286:HOH:O	2.38	0.56
1:D:96:GLU:HG3	1:D:183:VAL:HG11	1.88	0.56
1:E:118:PHE:O	1:E:119:HIS:C	2.45	0.56
1:B:119:HIS:C	1:B:119:HIS:HD2	2.10	0.56
1:G:183:VAL:O	1:G:187:ARG:HG3	2.06	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:128:ARG:NE	3:F:5021:HOH:O	2.30	0.56
1:A:32:ASP:O	1:B:18:PRO:HD2	2.05	0.55
1:E:12:SER:OG	1:E:13:GLY:N	2.35	0.55
1:E:65:GLN:HB2	3:E:6217:HOH:O	2.05	0.55
1:G:195:GLY:O	1:G:196:GLU:HG2	2.06	0.55
1:F:141:ASP:CG	1:F:144:ARG:HH21	2.13	0.55
1:G:13:GLY:O	1:G:16:LEU:N	2.37	0.55
1:B:197:LEU:HD11	3:B:3801:HOH:O	2.07	0.55
1:A:192:SER:HB2	1:A:193:PRO:HD2	1.88	0.55
1:C:119:HIS:CB	3:C:5275:HOH:O	2.40	0.55
1:H:285:LYS:NZ	3:H:6347:HOH:O	2.39	0.55
1:C:264:ASP:N	1:C:267:GLN:OE1	2.37	0.55
1:E:118:PHE:CZ	1:E:122:LEU:HD21	2.41	0.55
1:A:287:LEU:HD22	3:A:3750:HOH:O	2.08	0.54
1:E:25:LYS:NZ	3:E:6374:HOH:O	2.39	0.54
1:E:273:ALA:CB	1:E:274:PRO:HD3	2.34	0.54
1:E:84:SER:OG	1:E:85:PRO:HD2	2.07	0.54
1:G:256:ILE:O	1:G:260:GLN:HG2	2.08	0.54
1:A:194:ARG:HD3	1:A:196:GLU:CG	2.37	0.54
3:A:3987:HOH:O	1:B:29:PRO:HG3	2.07	0.54
1:A:234:GLU:CD	3:A:3904:HOH:O	2.51	0.53
1:D:90:GLN:HG2	1:D:197:LEU:HD12	1.90	0.53
1:E:274:PRO:HD2	3:E:6255:HOH:O	2.07	0.53
1:E:30:VAL:CG2	1:E:35[B]:MET:SD	2.96	0.53
1:H:12:SER:OG	2:H:6101:SO4:O2	2.27	0.53
1:E:190:LYS:C	1:E:190:LYS:CD	2.75	0.53
1:A:23:ILE:HG21	1:A:28:LEU:CD2	2.36	0.53
1:D:35:MET:HE2	1:D:110:ASP:HA	1.90	0.53
1:G:144:ARG:NH2	3:G:5144:HOH:O	2.41	0.53
1:G:278:ASN:HB3	3:G:5127:HOH:O	2.07	0.53
1:D:42:THR:HG23	1:D:118:PHE:CE2	2.44	0.52
1:C:193:PRO:C	1:C:195:GLY:H	2.17	0.52
1:E:8:LEU:HD22	1:E:91:ALA:HB2	1.92	0.52
1:F:1:MET:CE	1:F:180:GLN:HE22	2.21	0.52
1:D:23:ILE:HD12	1:D:23:ILE:H	1.73	0.52
1:E:269:GLU:HG3	3:E:6254:HOH:O	2.07	0.52
1:C:1:MET:CE	1:C:180:GLN:HE22	2.22	0.52
1:D:103:LEU:HD11	1:D:129:GLN:HG2	1.91	0.52
1:A:286:ARG:HG3	3:A:3812:HOH:O	2.08	0.52
1:C:234:GLU:CD	3:C:5256:HOH:O	2.52	0.52
1:D:90:GLN:NE2	3:D:3989:HOH:O	2.41	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:119:HIS:CE1	3:B:3794:HOH:O	2.63	0.52
1:F:162:LYS:HE3	3:F:4895:HOH:O	2.10	0.52
1:C:60:THR:HG22	1:C:64:GLN:HE21	1.75	0.52
1:C:128:ARG:CD	3:C:5286:HOH:O	2.58	0.52
1:D:23:ILE:HD13	1:D:28:LEU:CD2	2.37	0.52
1:E:193:PRO:O	1:E:194:ARG:C	2.53	0.52
1:H:15:ARG:HG3	1:H:15:ARG:HH11	1.75	0.51
1:A:174:GLY:O	3:A:3902:HOH:O	2.19	0.51
1:E:30:VAL:CG2	1:E:35[A]:MET:SD	2.98	0.51
1:A:58:GLN:NE2	3:A:3963:HOH:O	2.29	0.51
1:G:23:ILE:HG12	1:G:28:LEU:CD2	2.40	0.51
1:D:273:ALA:HB3	1:D:274:PRO:HD2	1.91	0.51
1:B:269:GLU:CD	3:B:3940:HOH:O	2.54	0.51
1:C:60:THR:N	1:C:61:PRO:CD	2.73	0.51
1:F:11:GLY:HA2	1:F:85:PRO:HB3	1.93	0.51
1:H:108:LEU:HD22	3:H:6398:HOH:O	2.09	0.51
1:G:249:LYS:NZ	3:G:5022:HOH:O	2.42	0.51
1:B:16:LEU:CD1	1:B:25:LYS:HD3	2.41	0.51
1:C:119:HIS:CD2	1:C:119:HIS:O	2.63	0.51
1:F:261:LYS:HE2	3:F:4971:HOH:O	2.10	0.51
1:F:4:LYS:NZ	1:F:102:ASP:OD2	2.44	0.51
1:B:88:LEU:HG	3:B:3959:HOH:O	2.11	0.50
1:H:16:LEU:HA	1:H:229:HIS:CE1	2.46	0.50
1:C:60:THR:HB	1:C:61:PRO:HD3	1.93	0.50
1:E:227:GLY:CA	3:E:6150:HOH:O	2.52	0.50
1:A:152:GLN:HG2	3:A:3725:HOH:O	2.11	0.50
1:C:119:HIS:NE2	3:C:5244:HOH:O	2.35	0.50
1:E:16:LEU:HD13	1:E:229:HIS:CD2	2.46	0.50
1:G:152:GLN:NE2	3:G:5054:HOH:O	2.44	0.50
1:B:13:GLY:O	1:B:14:THR:C	2.55	0.50
1:B:119:HIS:ND1	3:B:3937:HOH:O	2.34	0.50
3:B:3997:HOH:O	1:E:155:LYS:HE2	2.12	0.50
1:D:14:THR:O	1:D:15:ARG:C	2.54	0.50
1:G:15:ARG:NH2	3:G:5168:HOH:O	2.44	0.50
1:C:194:ARG:HD2	1:C:196:GLU:HG3	1.94	0.50
1:C:270:LYS:HE2	3:C:5169:HOH:O	2.10	0.50
1:H:23:ILE:HG13	1:H:24:SER:N	2.25	0.50
1:A:234:GLU:HG3	3:A:3904:HOH:O	2.07	0.49
1:C:119:HIS:CD2	3:C:5250:HOH:O	2.65	0.49
1:D:42:THR:HG23	1:D:118:PHE:CZ	2.47	0.49
1:C:26:GLN:H	1:C:26:GLN:NE2	2.10	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:5000:SO4:O4	1:D:62:ARG:NH2	2.26	0.49
1:C:1:MET:SD	1:C:180:GLN:NE2	2.86	0.49
1:C:32:ASP:OD2	1:C:243:GLU:OE1	2.30	0.49
1:D:269:GLU:HG3	3:D:3871:HOH:O	2.12	0.49
1:D:22:ALA:HA	3:D:3920:HOH:O	2.11	0.49
1:G:88:LEU:HD13	1:G:108:LEU:HD21	1.95	0.49
1:D:56:THR:HB	1:D:58:GLN:NE2	2.28	0.49
1:G:60:THR:HB	1:G:61:PRO:HD3	1.95	0.49
1:D:86:ASP:HB2	1:D:90:GLN:NE2	2.28	0.48
1:G:8:LEU:HD22	1:G:91:ALA:HB2	1.94	0.48
1:G:278:ASN:CG	3:G:5127:HOH:O	2.56	0.48
1:H:260:GLN:O	1:H:261:LYS:HB2	2.13	0.48
1:A:15:ARG:HH11	1:A:15:ARG:HG3	1.78	0.48
1:B:60:THR:HG23	3:B:3717:HOH:O	2.13	0.48
1:B:286:ARG:HG3	3:B:3875:HOH:O	2.13	0.48
1:B:117:ASP:HA	1:B:120:GLU:OE1	2.13	0.48
1:C:60:THR:N	1:C:61:PRO:HD2	2.29	0.48
1:G:20:THR:O	1:G:21:LEU:C	2.57	0.48
1:H:60:THR:CB	1:H:61:PRO:HD3	2.39	0.48
1:B:49:ARG:HD2	1:B:262:TRP:CE2	2.49	0.48
1:B:97:SER:OG	3:B:3956:HOH:O	2.19	0.48
1:B:128:ARG:NH2	2:B:3701:SO4:O4	2.47	0.48
1:B:256:ILE:O	1:B:260:GLN:HG2	2.14	0.48
1:D:35:MET:HE3	1:D:35:MET:O	2.14	0.48
1:H:2:LYS:NZ	1:H:50:GLU:OE1	2.42	0.48
1:C:141:ASP:OD2	1:C:144:ARG:HD3	2.14	0.48
1:E:117:ASP:CG	1:E:120:GLU:OE1	2.57	0.48
1:G:167:LYS:NZ	3:G:5153:HOH:O	2.46	0.48
1:A:233:LEU:HD21	1:B:237[B]:GLN:HA	1.96	0.47
1:D:56:THR:HB	1:D:58:GLN:HE21	1.79	0.47
1:H:123:GLY:O	1:H:127:GLN:HB2	2.14	0.47
1:B:16:LEU:C	1:B:229:HIS:CE1	2.92	0.47
1:C:18:PRO:HA	1:C:21:LEU:HG	1.96	0.47
1:E:155:LYS:CE	3:E:6237:HOH:O	2.61	0.47
1:F:273:ALA:CB	1:F:274:PRO:CD	2.83	0.47
1:G:255:GLU:O	1:G:259:ARG:HG3	2.14	0.47
1:A:88:LEU:HG	3:A:3758:HOH:O	2.14	0.47
1:B:152:GLN:HA	1:B:152:GLN:NE2	2.29	0.47
1:E:32:ASP:OD2	1:E:249:LYS:HE3	2.14	0.47
1:G:161:GLU:O	1:G:194[A]:ARG:NH2	2.47	0.47
1:D:60:THR:O	1:D:64:GLN:HG3	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:141:ASP:OD1	3:F:4873:HOH:O	2.20	0.47
1:A:23:ILE:CB	1:B:23:ILE:CD1	2.74	0.47
1:A:60:THR:HB	1:A:61:PRO:HD3	1.96	0.47
3:A:3911:HOH:O	1:B:14:THR:HA	2.15	0.47
1:B:88:LEU:HD12	1:B:199:ILE:CG2	2.44	0.47
1:H:84:SER:OG	1:H:85:PRO:HD2	2.15	0.47
1:H:192:SER:HB2	1:H:193:PRO:HD2	1.97	0.47
1:C:1:MET:H2	1:C:129:GLN:NE2	2.13	0.47
1:C:187:ARG:HG2	1:C:187:ARG:NH1	2.30	0.47
1:A:23:ILE:HG23	1:A:28:LEU:HD23	1.85	0.47
1:A:23:ILE:CD1	1:B:23:ILE:HB	2.30	0.47
1:A:231:SER:HA	3:A:3904:HOH:O	2.15	0.47
1:D:60:THR:N	1:D:61:PRO:HD2	2.30	0.47
1:A:23:ILE:CG2	1:B:23:ILE:CD1	2.93	0.46
1:A:234:GLU:CD	3:A:3921:HOH:O	2.58	0.46
1:A:233:LEU:HD21	1:B:237[A]:GLN:HA	1.96	0.46
1:B:23:ILE:CD1	1:B:27:LEU:HB2	2.46	0.46
1:C:25:LYS:HE3	1:C:110:ASP:HB3	1.97	0.46
1:E:15:ARG:HG2	1:E:16:LEU:HD23	1.96	0.46
1:E:268:LEU:HD23	1:E:288:LEU:CD2	2.44	0.46
1:H:19:ALA:O	3:H:6271:HOH:O	2.20	0.46
1:E:160:GLU:HG2	3:E:6247:HOH:O	2.15	0.46
1:E:191:PRO:CD	3:E:6240:HOH:O	2.60	0.46
1:B:25:LYS:NZ	1:B:110:ASP:OD2	2.43	0.46
1:G:192:SER:HB2	1:G:193:PRO:HD2	1.98	0.46
1:G:270:LYS:HE3	3:G:5175:HOH:O	2.15	0.46
1:H:36:ILE:HD12	1:H:63:PHE:CE2	2.51	0.46
1:C:42:THR:HG23	1:C:118:PHE:CE2	2.51	0.46
1:D:4:LYS:HB3	1:D:98:PHE:CE2	2.51	0.46
1:C:237[A]:GLN:CG	1:D:233:LEU:HD11	2.46	0.46
1:C:237[A]:GLN:HA	1:D:233:LEU:HD21	1.97	0.46
1:E:23:ILE:HG12	1:F:23:ILE:HG23	1.97	0.46
1:H:151:ASP:OD2	1:H:155:LYS:HB3	2.16	0.46
1:A:19:ALA:HB1	1:B:29:PRO:HB3	1.96	0.46
1:C:237[B]:GLN:HA	1:D:233:LEU:HD21	1.97	0.46
1:D:16:LEU:HD22	1:D:229:HIS:CE1	2.51	0.46
1:E:23:ILE:CG2	1:F:23:ILE:HG12	2.16	0.46
1:E:191:PRO:O	1:E:192:SER:O	2.33	0.46
1:G:237:GLN:HA	1:H:233:LEU:HD21	1.97	0.46
1:C:1:MET:H3	1:C:129:GLN:NE2	2.14	0.45
1:E:90:GLN:O	1:E:93:LEU:N	2.42	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:268:LEU:HD23	1:E:288:LEU:HD21	1.98	0.45
1:B:23:ILE:HG23	1:B:23:ILE:O	2.16	0.45
1:H:93:LEU:CD2	1:H:187:ARG:HG2	2.46	0.45
1:E:190:LYS:HD2	1:E:191:PRO:CD	2.46	0.45
1:E:209:ARG:CZ	3:E:6168:HOH:O	2.65	0.45
1:G:275:LEU:O	1:G:281:GLY:HA3	2.16	0.45
1:A:164:LEU:HB3	3:A:4009:HOH:O	2.16	0.45
1:E:35[A]:MET:HE1	1:E:112:LEU:HD12	1.97	0.45
1:H:56:THR:HB	1:H:57:PRO:HD2	1.97	0.45
1:A:13:GLY:HA2	3:A:3851:HOH:O	2.15	0.45
1:B:24:SER:HB2	1:B:59:ASP:CG	2.42	0.45
1:C:273:ALA:HB3	1:C:274:PRO:HD3	1.98	0.45
1:E:64:GLN:HA	1:E:79:TYR:CZ	2.52	0.45
1:F:86:ASP:HB2	1:F:90:GLN:NE2	2.32	0.45
1:C:194:ARG:CD	1:C:196:GLU:HG3	2.47	0.45
1:D:123:GLY:O	1:D:124:SER:C	2.59	0.45
1:D:225:ASP:HB3	3:D:3975:HOH:O	2.16	0.45
1:B:16:LEU:CD2	3:B:3980:HOH:O	2.65	0.45
1:A:23:ILE:HG21	1:A:28:LEU:HD23	1.98	0.45
1:F:78:GLN:NE2	3:F:4781:HOH:O	2.39	0.45
1:H:18:PRO:O	1:H:21:LEU:HB2	2.17	0.45
1:D:273:ALA:HB3	1:D:274:PRO:HD3	1.98	0.45
1:E:278:ASN:HB3	3:E:6363:HOH:O	2.16	0.45
1:F:51:ILE:HB	1:F:77:LEU:HD23	1.99	0.45
1:H:16:LEU:HB3	1:H:20:THR:HG23	1.99	0.45
1:A:111:ASN:HB2	3:A:3902:HOH:O	2.16	0.44
1:B:16:LEU:C	1:B:229:HIS:HE1	2.24	0.44
1:B:24:SER:HB3	1:B:27:LEU:HD12	1.97	0.44
1:C:88:LEU:HD13	1:C:108:LEU:HD21	1.99	0.44
1:C:23:ILE:CD1	1:D:23:ILE:HG21	2.47	0.44
1:D:123:GLY:HA3	3:D:3912:HOH:O	2.16	0.44
1:F:192:SER:HB2	1:F:193:PRO:CD	2.47	0.44
1:F:192:SER:HB2	1:F:193:PRO:HD2	1.99	0.44
1:H:23:ILE:O	1:H:23:ILE:HG23	2.17	0.44
1:H:135:PHE:HA	1:H:215:GLU:O	2.18	0.44
1:A:234:GLU:HB2	3:A:3904:HOH:O	2.18	0.44
1:F:21:LEU:HD23	1:F:21:LEU:HA	1.85	0.44
1:G:141[B]:ASP:OD1	3:G:5077:HOH:O	2.21	0.44
1:H:24:SER:HB2	1:H:59:ASP:OD2	2.17	0.44
1:A:59:ASP:O	1:A:60:THR:C	2.58	0.44
1:A:193:PRO:C	1:A:195:GLY:N	2.68	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:59:ASP:HA	1:A:62:ARG:HD2	1.99	0.44
1:D:87:GLY:HA2	3:D:3990:HOH:O	2.17	0.44
1:H:119:HIS:CD2	3:H:6299:HOH:O	2.69	0.44
1:E:88:LEU:HD12	1:E:199:ILE:HG21	1.99	0.44
1:E:191:PRO:HA	1:E:196:GLU:O	2.18	0.44
1:H:60:THR:HB	1:H:61:PRO:CD	2.38	0.44
1:D:118:PHE:HB2	3:D:3916:HOH:O	2.18	0.43
1:F:256:ILE:O	1:F:260:GLN:HG2	2.18	0.43
1:A:39:PRO:HA	3:A:3791:HOH:O	2.17	0.43
1:D:119:HIS:HE1	3:D:4030:HOH:O	2.01	0.43
1:A:272:ALA:HB1	1:A:285:LYS:HG3	2.00	0.43
1:G:86:ASP:HB2	1:G:90:GLN:NE2	2.33	0.43
1:H:25:LYS:CE	1:H:26:GLN:HE22	2.25	0.43
1:C:269:GLU:HG2	3:C:5162:HOH:O	2.18	0.43
1:E:23:ILE:CD1	1:F:23:ILE:CG2	2.89	0.43
1:G:62:ARG:NE	2:G:4900:SO4:O3	2.51	0.43
1:G:135:PHE:HA	1:G:215:GLU:O	2.18	0.43
1:H:265:ALA:HB3	3:H:6161:HOH:O	2.17	0.43
1:F:42:THR:HG23	1:F:118:PHE:CE2	2.54	0.43
1:G:84:SER:HA	3:G:5000:HOH:O	2.18	0.43
1:D:273:ALA:CB	1:D:274:PRO:CD	2.88	0.43
1:E:191:PRO:O	1:E:192:SER:C	2.61	0.43
1:B:13:GLY:O	1:B:16:LEU:N	2.49	0.43
1:G:23:ILE:HD11	1:G:27:LEU:C	2.44	0.43
1:G:32:ASP:O	1:H:18:PRO:HD2	2.18	0.43
1:F:17:HIS:HB3	1:F:18:PRO:HA	2.00	0.43
1:G:22:ALA:HB1	1:H:27:LEU:HD22	2.00	0.43
1:G:64:GLN:HG2	1:G:79:TYR:CD1	2.54	0.43
1:A:16:LEU:HB3	1:A:20:THR:HG23	2.01	0.43
1:B:23:ILE:HD11	1:B:27:LEU:HB2	2.00	0.43
1:B:273:ALA:CB	1:B:274:PRO:CD	2.92	0.43
1:C:128:ARG:NH1	1:C:213[B]:SER:OG	2.51	0.43
1:C:264:ASP:C	1:C:264:ASP:OD1	2.61	0.43
1:E:16:LEU:O	1:E:19:ALA:HB3	2.19	0.43
1:E:277:LYS:C	3:E:6363:HOH:O	2.62	0.43
1:H:27:LEU:HA	1:H:27:LEU:HD23	1.71	0.43
1:A:84:SER:O	1:A:86:ASP:N	2.52	0.43
1:C:259:ARG:NH2	3:C:5019:HOH:O	2.51	0.43
1:A:29:PRO:HD2	3:A:3898:HOH:O	2.19	0.42
1:A:117:ASP:HA	1:A:120:GLU:OE1	2.19	0.42
1:F:40:LEU:O	1:F:44:MET:HG3	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:16:LEU:HD22	3:A:3909:HOH:O	2.19	0.42
1:A:24:SER:HB2	1:A:59:ASP:OD2	2.19	0.42
1:A:119:HIS:CE1	3:A:3875:HOH:O	2.72	0.42
1:A:141:ASP:OD2	1:A:144:ARG:NH1	2.38	0.42
1:D:56:THR:HB	1:D:57:PRO:HD2	2.01	0.42
1:H:16:LEU:HD23	1:H:229:HIS:ND1	2.34	0.42
1:E:35[B]:MET:O	1:E:39:PRO:HD2	2.19	0.42
1:G:151:ASP:C	1:G:151:ASP:OD1	2.61	0.42
1:H:15:ARG:HG3	2:H:6101:SO4:O1	2.19	0.42
1:B:88:LEU:HB2	1:B:199:ILE:HB	2.01	0.42
1:E:107:VAL:HG22	1:E:108:LEU:N	2.35	0.42
1:A:23:ILE:CG2	1:B:23:ILE:HD12	2.43	0.42
1:B:67:LEU:HB2	1:B:79:TYR:OH	2.19	0.42
1:B:112:LEU:HD23	1:B:112:LEU:C	2.45	0.42
1:C:128:ARG:NH1	1:C:213[A]:SER:OG	2.51	0.42
1:F:2:LYS:HD3	1:F:4:LYS:HE3	2.01	0.42
1:B:16:LEU:CA	1:B:229:HIS:CE1	2.98	0.42
1:D:204:ARG:HH11	1:D:204:ARG:HD2	1.59	0.42
1:E:259[A]:ARG:NH2	3:E:6119:HOH:O	2.52	0.42
1:E:259[B]:ARG:NH2	3:E:6119:HOH:O	2.52	0.42
1:H:273:ALA:HB3	1:H:274:PRO:CD	2.45	0.42
1:A:18:PRO:HD2	1:B:32:ASP:O	2.19	0.42
1:B:23:ILE:HG12	1:B:27:LEU:HB2	2.01	0.42
1:C:9:ALA:O	1:C:55:SER:OG	2.38	0.42
1:E:278:ASN:OD1	1:E:280:TYR:N	2.51	0.42
1:F:4:LYS:HZ2	1:F:102:ASP:CG	2.28	0.42
1:C:46:ALA:HB2	1:C:122:LEU:HD13	2.01	0.42
1:C:223:TRP:C	1:C:224:LEU:HD23	2.45	0.42
1:D:209:ARG:HG2	1:D:209:ARG:HH11	1.85	0.42
1:F:72:ASN:OD1	3:F:4813:HOH:O	2.22	0.42
1:G:192:SER:OG	1:G:194[A]:ARG:HB2	2.19	0.42
1:H:22:ALA:HB3	3:H:6188:HOH:O	2.18	0.42
1:A:23:ILE:HG13	1:A:24:SER:N	2.35	0.42
1:A:256:ILE:O	1:A:260:GLN:CG	2.68	0.42
1:C:234:GLU:HA	1:C:237[B]:GLN:NE2	2.32	0.41
1:C:272:ALA:HB1	1:C:285:LYS:HG2	2.02	0.41
1:E:6:ILE:HA	1:E:52:LEU:O	2.20	0.41
1:H:54:ILE:HA	1:H:80:ALA:O	2.20	0.41
1:H:67:LEU:HB2	1:H:79:TYR:OH	2.20	0.41
1:A:70:GLY:HA3	1:A:77:LEU:HG	2.02	0.41
1:E:35[B]:MET:HE1	1:E:112:LEU:HD12	2.01	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:50:GLU:C	1:E:51:ILE:HG13	2.44	0.41
1:E:288:LEU:HA	1:E:288:LEU:HD23	1.85	0.41
1:D:84:SER:OG	1:D:85:PRO:HD2	2.21	0.41
1:B:16:LEU:HD11	1:B:25:LYS:HD3	2.03	0.41
1:D:141:ASP:OD2	1:D:144:ARG:HD3	2.21	0.41
1:E:118:PHE:CE2	1:E:122:LEU:HD11	2.56	0.41
1:B:116:HIS:O	1:B:117:ASP:HB2	2.20	0.41
1:D:199:ILE:CG2	3:D:3978:HOH:O	2.60	0.41
1:E:190:LYS:CD	3:E:6294:HOH:O	2.60	0.41
1:E:24:SER:HB2	1:E:59:ASP:OD2	2.20	0.41
1:F:32:ASP:OD1	1:F:32:ASP:N	2.54	0.41
1:C:1:MET:N	1:C:129:GLN:HE22	2.19	0.41
1:E:227:GLY:C	3:E:6150:HOH:O	2.64	0.41
1:G:90:GLN:O	1:G:91:ALA:C	2.63	0.41
1:B:180:GLN:NE2	3:B:3887:HOH:O	2.53	0.40
1:C:38:TYR:HB2	1:C:39:PRO:CD	2.52	0.40
1:E:35[A]:MET:O	1:E:39:PRO:HD2	2.20	0.40
1:E:264:ASP:OD1	1:E:264:ASP:C	2.64	0.40
1:G:14:THR:C	1:G:16:LEU:N	2.78	0.40
1:B:113:TYR:CB	1:B:118:PHE:CZ	3.04	0.40
1:C:62:ARG:NE	2:C:5000:SO4:O1	2.54	0.40
1:F:129:GLN:NE2	3:F:5005:HOH:O	2.55	0.40
1:A:15:ARG:HG3	1:A:15:ARG:NH1	2.35	0.40
1:A:27:LEU:HA	1:A:27:LEU:HD23	1.86	0.40
1:D:179:ASP:OD1	1:D:179:ASP:C	2.64	0.40
1:F:84:SER:HB3	1:F:86:ASP:OD2	2.21	0.40
1:H:47:GLY:HA3	3:H:6318:HOH:O	2.21	0.40
1:D:287:LEU:HD22	3:D:4025:HOH:O	2.20	0.40
1:F:17:HIS:CB	1:F:18:PRO:HA	2.52	0.40
1:F:39:PRO:HA	3:F:4943:HOH:O	2.22	0.40
1:H:187:ARG:HH11	1:H:187:ARG:HD2	1.64	0.40
1:A:260:GLN:O	1:A:261:LYS:HB2	2.21	0.40
1:B:50:GLU:C	1:B:51:ILE:HG13	2.46	0.40

All (5) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:84:SER:OG	3:F:4852:HOH:O[1_655]	1.25	0.95
3:A:3776:HOH:O	3:F:4954:HOH:O[1_566]	1.99	0.21

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:F:4955:HOH:O	3:G:5148:HOH:O[1_455]	2.06	0.14
3:G:5209:HOH:O	3:H:6340:HOH:O[1_565]	2.09	0.11
3:F:4950:HOH:O	3:G:4974:HOH:O[1_455]	2.18	0.02

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	292/293 (100%)	284 (97%)	7 (2%)	1 (0%)	36	29
1	B	295/293 (101%)	285 (97%)	9 (3%)	1 (0%)	36	29
1	C	297/293 (101%)	290 (98%)	5 (2%)	2 (1%)	18	10
1	D	291/293 (99%)	282 (97%)	7 (2%)	2 (1%)	18	10
1	E	297/293 (101%)	286 (96%)	7 (2%)	4 (1%)	9	3
1	F	294/293 (100%)	285 (97%)	6 (2%)	3 (1%)	12	5
1	G	294/293 (100%)	287 (98%)	6 (2%)	1 (0%)	36	29
1	H	290/293 (99%)	284 (98%)	5 (2%)	1 (0%)	36	29
All	All	2350/2344 (100%)	2283 (97%)	52 (2%)	15 (1%)	21	13

All (15) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	E	14	THR
1	D	14	THR
1	E	31	TYR
1	F	15	ARG
1	F	31	TYR
1	H	31	TYR
1	A	31	TYR
1	B	31	TYR
1	D	31	TYR

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Mol	Chain	Res	Type
1	E	192	SER
1	F	14	THR
1	G	31	TYR
1	C	31	TYR
1	C	194	ARG
1	E	191	PRO

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	241/240 (100%)	236 (98%)	5 (2%)	47	44
1	B	244/240 (102%)	235 (96%)	9 (4%)	30	22
1	C	246/240 (102%)	237 (96%)	9 (4%)	30	22
1	D	240/240 (100%)	232 (97%)	8 (3%)	33	26
1	E	246/240 (102%)	235 (96%)	11 (4%)	24	17
1	F	243/240 (101%)	235 (97%)	8 (3%)	33	26
1	G	243/240 (101%)	229 (94%)	14 (6%)	18	10
1	H	239/240 (100%)	235 (98%)	4 (2%)	53	52
All	All	1942/1920 (101%)	1874 (96%)	68 (4%)	32	24

All (68) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	17	HIS
1	A	18	PRO
1	A	23	ILE
1	A	88	LEU
1	A	126	SER
1	B	25	LYS
1	B	53	ILE
1	B	112	LEU
1	B	119	HIS

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Mol	Chain	Res	Type
1	B	152	GLN
1	B	194	ARG
1	B	196	GLU
1	B	225	ASP
1	B	287	LEU
1	C	12	SER
1	C	20	THR
1	C	26	GLN
1	C	55	SER
1	C	111	ASN
1	C	155[A]	LYS
1	C	155[B]	LYS
1	C	225	ASP
1	C	288	LEU
1	D	23	ILE
1	D	24	SER
1	D	25	LYS
1	D	60	THR
1	D	111	ASN
1	D	117	ASP
1	D	282	GLN
1	D	286	ARG
1	E	8	LEU
1	E	12	SER
1	E	16	LEU
1	E	23	ILE
1	E	117	ASP
1	E	155	LYS
1	E	194	ARG
1	E	196	GLU
1	E	233	LEU
1	E	269	GLU
1	E	270	LYS
1	F	1	MET
1	F	12	SER
1	F	14	THR
1	F	24	SER
1	F	53	ILE
1	F	155	LYS
1	F	197	LEU
1	F	286	ARG
1	G	12	SER

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Mol	Chain	Res	Type
1	G	17	HIS
1	G	18	PRO
1	G	23	ILE
1	G	84	SER
1	G	97	SER
1	G	112	LEU
1	G	194[A]	ARG
1	G	194[B]	ARG
1	G	196	GLU
1	G	225	ASP
1	G	249	LYS
1	G	270	LYS
1	G	278	ASN
1	H	14	THR
1	H	152	GLN
1	H	187	ARG
1	H	225	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (47) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	65	GLN
1	A	119	HIS
1	A	229	HIS
1	B	65	GLN
1	B	82	GLN
1	B	90	GLN
1	B	119	HIS
1	B	152	GLN
1	B	229	HIS
1	B	246	GLN
1	C	26	GLN
1	C	64	GLN
1	C	82	GLN
1	C	119	HIS
1	C	129	GLN
1	C	180	GLN
1	C	246	GLN
1	C	260	GLN
1	D	58	GLN
1	D	65	GLN
1	D	82	GLN

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Mol	Chain	Res	Type
1	D	90	GLN
1	D	181	GLN
1	D	211	GLN
1	D	229	HIS
1	D	246	GLN
1	E	17	HIS
1	E	229	HIS
1	F	65	GLN
1	F	78	GLN
1	F	82	GLN
1	F	90	GLN
1	F	181	GLN
1	F	211	GLN
1	F	244	ASN
1	G	17	HIS
1	G	64	GLN
1	G	65	GLN
1	G	78	GLN
1	G	82	GLN
1	G	90	GLN
1	H	17	HIS
1	H	26	GLN
1	H	82	GLN
1	H	90	GLN
1	H	111	ASN
1	H	278	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 oligosaccharides in this entry.

5.6 Ligand geometry

20 ligands are modelled in this entry.

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	$\# Z > 2$
2	SO4	C	3600	-	4,4,4	1.04	0	6,6,6	0.79	0
2	SO4	C	5000	-	4,4,4	0.90	0	6,6,6	0.73	0
2	SO4	E	3607	-	4,4,4	0.80	0	6,6,6	0.74	0
2	SO4	H	6101	-	4,4,4	0.51	0	6,6,6	0.72	0
2	SO4	D	3800	-	4,4,4	0.32	0	6,6,6	1.17	0
2	SO4	C	3702	-	4,4,4	0.32	0	6,6,6	0.66	0
2	SO4	B	3603	-	4,4,4	0.87	0	6,6,6	0.65	0
2	SO4	D	3601	-	4,4,4	1.06	0	6,6,6	0.71	0
2	SO4	D	3703	-	4,4,4	0.52	0	6,6,6	0.61	0
2	SO4	G	3605	-	4,4,4	0.75	0	6,6,6	0.88	0
2	SO4	A	3602	-	4,4,4	0.70	0	6,6,6	0.63	0
2	SO4	H	3604	-	4,4,4	0.88	0	6,6,6	0.59	0
2	SO4	G	3704	-	4,4,4	0.50	0	6,6,6	1.04	0
2	SO4	F	3606	-	4,4,4	0.79	0	6,6,6	0.73	0
2	SO4	A	3700	-	4,4,4	0.28	0	6,6,6	0.60	0
2	SO4	B	3701	-	4,4,4	0.44	0	6,6,6	1.03	0
2	SO4	E	6100	-	4,4,4	0.75	0	6,6,6	0.78	0
2	SO4	F	4700	-	4,4,4	0.51	0	6,6,6	0.84	0
2	SO4	E	5001	-	4,4,4	0.36	0	6,6,6	0.55	0
2	SO4	G	4900	-	4,4,4	0.34	0	6,6,6	0.85	0

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

4 monomers are involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	C	5000	SO4	2	0
2	H	6101	SO4	2	0
2	B	3701	SO4	1	0
2	G	4900	SO4	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	292/293 (99%)	0.15	13 (4%)	38	40	8, 20, 41, 60	2 (0%)
1	B	292/293 (99%)	0.06	13 (4%)	38	40	7, 19, 44, 63	5 (1%)
1	C	293/293 (100%)	0.18	15 (5%)	33	36	7, 20, 43, 65	6 (2%)
1	D	292/293 (99%)	0.29	18 (6%)	26	28	7, 21, 47, 72	1 (0%)
1	E	292/293 (99%)	0.44	26 (8%)	15	16	7, 22, 45, 67	7 (2%)
1	F	293/293 (100%)	0.03	13 (4%)	39	41	5, 16, 43, 69	3 (1%)
1	G	292/293 (99%)	-0.02	13 (4%)	38	40	5, 16, 38, 66	4 (1%)
1	H	292/293 (99%)	0.17	11 (3%)	44	47	10, 20, 42, 52	0
All	All	2338/2344 (99%)	0.16	122 (5%)	33	35	5, 19, 43, 72	28 (1%)

All (122) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	13	GLY	8.5
1	F	13	GLY	8.0
1	A	13	GLY	6.5
1	B	13	GLY	6.3
1	B	16	LEU	6.2
1	E	193	PRO	6.1
1	H	23	ILE	5.9
1	G	195	GLY	5.6
1	H	11	GLY	5.5
1	E	195	GLY	5.4
1	G	16	LEU	5.3
1	D	16	LEU	5.2
1	A	16	LEU	5.1
1	H	22	ALA	4.9
1	D	23	ILE	4.8
1	C	13	GLY	4.6

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Mol	Chain	Res	Type	RSRZ
1	E	13	GLY	4.5
1	G	18	PRO	4.4
1	F	23	ILE	4.3
1	G	23	ILE	4.0
1	E	12	SER	4.0
1	F	14	THR	4.0
1	D	19	ALA	4.0
1	B	193	PRO	3.9
1	E	14	THR	3.8
1	B	17	HIS	3.8
1	H	195	GLY	3.6
1	E	194	ARG	3.6
1	C	11	GLY	3.5
1	E	191	PRO	3.5
1	B	23	ILE	3.5
1	B	14	THR	3.4
1	A	23	ILE	3.4
1	C	14	THR	3.4
1	H	16	LEU	3.4
1	A	195	GLY	3.3
1	E	11	GLY	3.3
1	F	11	GLY	3.3
1	G	17	HIS	3.3
1	D	22	ALA	3.2
1	C	195	GLY	3.2
1	H	12	SER	3.2
1	A	14	THR	3.1
1	G	22	ALA	3.1
1	G	13	GLY	3.1
1	E	190	LYS	3.1
1	E	84	SER	3.0
1	D	193	PRO	3.0
1	H	13	GLY	2.9
1	D	189	LEU	2.9
1	E	16	LEU	2.9
1	D	24	SER	2.9
1	D	197	LEU	2.9
1	G	14	THR	2.9
1	F	123	GLY	2.9
1	B	22	ALA	2.8
1	E	196	GLU	2.8
1	A	192	SER	2.8

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Mol	Chain	Res	Type	RSRZ
1	E	192	SER	2.8
1	C	16	LEU	2.8
1	E	35[A]	MET	2.8
1	D	192	SER	2.8
1	E	119	HIS	2.8
1	D	15	ARG	2.7
1	E	118	PHE	2.7
1	E	23	ILE	2.7
1	H	84	SER	2.7
1	F	17	HIS	2.7
1	A	18	PRO	2.7
1	G	11	GLY	2.6
1	G	12	SER	2.6
1	F	1	MET	2.6
1	H	192	SER	2.6
1	D	119	HIS	2.5
1	C	120	GLU	2.5
1	D	118	PHE	2.5
1	G	15	ARG	2.4
1	E	189	LEU	2.4
1	H	273	ALA	2.4
1	B	195	GLY	2.4
1	B	192	SER	2.4
1	D	12	SER	2.4
1	C	23	ILE	2.4
1	D	14	THR	2.4
1	A	22	ALA	2.4
1	C	193	PRO	2.4
1	F	193	PRO	2.4
1	A	17	HIS	2.4
1	F	119	HIS	2.3
1	B	194	ARG	2.3
1	C	118	PHE	2.3
1	E	124	SER	2.3
1	B	277	LYS	2.3
1	E	19	ALA	2.2
1	E	123	GLY	2.2
1	A	15	ARG	2.2
1	E	226	THR	2.2
1	B	275	LEU	2.2
1	F	124	SER	2.2
1	H	18	PRO	2.2

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Mol	Chain	Res	Type	RSRZ
1	B	15	ARG	2.2
1	C	1	MET	2.2
1	F	84	SER	2.2
1	E	197	LEU	2.2
1	C	12	SER	2.1
1	C	227	GLY	2.1
1	A	193	PRO	2.1
1	D	127	GLN	2.1
1	D	11	GLY	2.1
1	G	193	PRO	2.1
1	F	16	LEU	2.1
1	C	19	ALA	2.1
1	F	286	ARG	2.1
1	D	124	SER	2.0
1	A	19	ALA	2.0
1	E	15	ARG	2.0
1	E	128	ARG	2.0
1	G	270	LYS	2.0
1	A	12	SER	2.0
1	C	123	GLY	2.0
1	C	226	THR	2.0
1	E	60	THR	2.0

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

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

6.3 Carbohydrates [i](#)

There are no 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($\text{\AA}^2$)	Q<0.9
2	SO4	H	6101	5/5	0.79	0.11	50,58,59,65	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	SO4	C	5000	5/5	0.82	0.11	41,48,52,53	0
2	SO4	G	4900	5/5	0.86	0.10	59,60,61,63	0
2	SO4	D	3703	5/5	0.87	0.12	52,59,62,64	0
2	SO4	E	5001	5/5	0.87	0.10	45,46,50,50	0
2	SO4	F	4700	5/5	0.89	0.10	42,52,58,59	0
2	SO4	B	3701	5/5	0.91	0.10	55,57,58,59	0
2	SO4	E	6100	5/5	0.92	0.09	45,47,49,51	0
2	SO4	C	3702	5/5	0.92	0.09	53,58,58,59	0
2	SO4	G	3704	5/5	0.93	0.09	47,50,52,56	0
2	SO4	D	3800	5/5	0.93	0.10	48,52,56,56	0
2	SO4	A	3700	5/5	0.94	0.08	45,47,52,55	0
2	SO4	F	3606	5/5	0.98	0.07	22,28,31,32	0
2	SO4	C	3600	5/5	0.98	0.08	27,31,35,37	0
2	SO4	E	3607	5/5	0.98	0.06	25,27,31,32	0
2	SO4	D	3601	5/5	0.98	0.07	25,28,30,34	0
2	SO4	H	3604	5/5	0.98	0.07	29,30,30,31	0
2	SO4	A	3602	5/5	0.98	0.07	25,26,29,29	0
2	SO4	B	3603	5/5	0.99	0.06	28,30,32,33	0
2	SO4	G	3605	5/5	0.99	0.07	27,28,31,31	0

6.5 Other polymers [i](#)

There are no such residues in this entry.