



Full wwPDB X-ray Structure Validation Report ⓘ

Jan 31, 2016 – 10:44 PM GMT

PDB ID : 1UYP
Title : THE THREE-DIMENSIONAL STRUCTURE OF BETA-FRUCTOSIDASE
(INVERTASE) FROM THERMOTOGA MARITIMA
Authors : Alberto, F.; Bignon, C.; Sulzenbacher, G.; Henrissat, B.; Czjzek, M.
Deposited on : 2004-03-02
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
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467
Mogul : 1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix) : 1.9-1692
EDS : rb-20026688
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac : 5.8.0135
CCP4 : 6.5.0
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : trunk26865

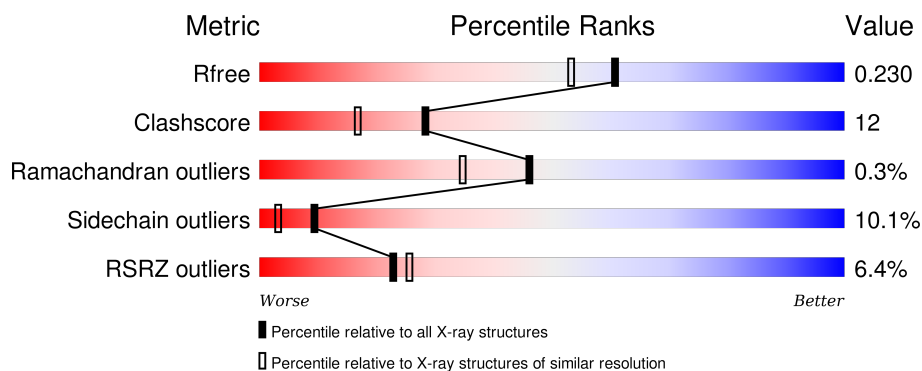
1 Overall quality at a glance

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}	91344	4755 (1.90-1.90)
Clashscore	102246	5398 (1.90-1.90)
Ramachandran outliers	100387	5338 (1.90-1.90)
Sidechain outliers	100360	5339 (1.90-1.90)
RSRZ outliers	91569	4766 (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 on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. 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	432	<div> <div>4%</div> <div>77% 17% 5%</div> </div>
1	B	432	<div> <div>6%</div> <div>74% 22%</div> </div>
1	C	432	<div> <div>8%</div> <div>73% 22%</div> </div>
1	D	432	<div> <div>7%</div> <div>74% 19% 6%</div> </div>
1	E	432	<div> <div>7%</div> <div>72% 22% 5%</div> </div>

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Mol	Chain	Length	Quality of chain
1	F	432	

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	A	1433	-	-	-	X
2	SO4	A	1435	-	-	-	X
2	SO4	B	1435	-	-	X	-
2	SO4	C	1435	-	-	X	-
2	SO4	F	1433	-	-	X	-
4	GOL	A	1437	-	-	-	X
4	GOL	C	1436	-	-	-	X

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 22996 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 BETA-FRUCTOSIDASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	432	Total	C	N	O	S	0	0	0
			3520	2253	589	665	13			
1	B	432	Total	C	N	O	S	0	0	0
			3520	2253	589	665	13			
1	C	432	Total	C	N	O	S	0	0	0
			3520	2253	589	665	13			
1	D	432	Total	C	N	O	S	0	0	0
			3520	2253	589	665	13			
1	E	432	Total	C	N	O	S	0	0	0
			3520	2253	589	665	13			
1	F	432	Total	C	N	O	S	0	0	0
			3520	2253	589	665	13			

There are 18 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1	LEU	MET	CONFLICT	UNP O33833
B	1	LEU	MET	CONFLICT	UNP O33833
C	1	LEU	MET	CONFLICT	UNP O33833
D	1	LEU	MET	CONFLICT	UNP O33833
E	1	LEU	MET	CONFLICT	UNP O33833
F	1	LEU	MET	CONFLICT	UNP O33833
A	108	VAL	ALA	CONFLICT	UNP O33833
B	108	VAL	ALA	CONFLICT	UNP O33833
C	108	VAL	ALA	CONFLICT	UNP O33833
D	108	VAL	ALA	CONFLICT	UNP O33833
E	108	VAL	ALA	CONFLICT	UNP O33833
F	108	VAL	ALA	CONFLICT	UNP O33833
A	179	ALA	VAL	CONFLICT	UNP O33833
B	179	ALA	VAL	CONFLICT	UNP O33833
C	179	ALA	VAL	CONFLICT	UNP O33833
D	179	ALA	VAL	CONFLICT	UNP O33833
E	179	ALA	VAL	CONFLICT	UNP O33833

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Chain	Residue	Modelled	Actual	Comment	Reference
F	179	ALA	VAL	CONFLICT	UNP O33833

- Molecule 2 is SULFATE ION (three-letter code: SO4) (formula: O₄S).



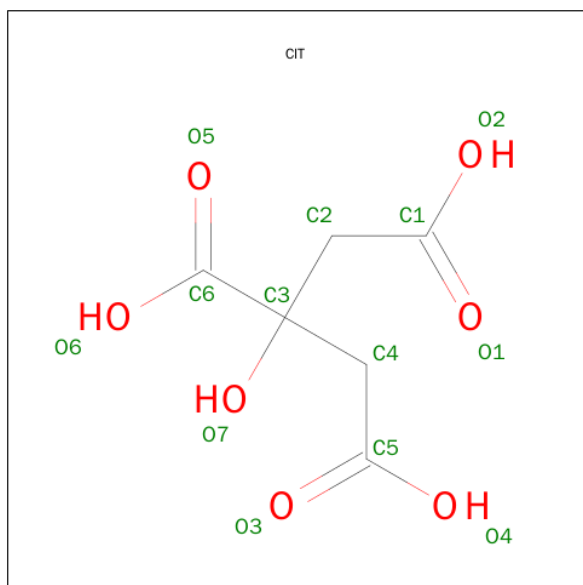
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	O	S	0	0
			5	4	1		
2	A	1	Total	O	S	0	0
			5	4	1		
2	A	1	Total	O	S	0	0
			5	4	1		
2	B	1	Total	O	S	0	0
			5	4	1		
2	B	1	Total	O	S	0	0
			5	4	1		
2	B	1	Total	O	S	0	0
			5	4	1		
2	B	1	Total	O	S	0	0
			5	4	1		
2	C	1	Total	O	S	0	0
			5	4	1		
2	C	1	Total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

- Molecule 3 is CITRIC ACID (three-letter code: CIT) (formula: $C_6H_8O_7$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			13	6	7		

- Molecule 4 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total C O 6 3 3	0	0
4	B	1	Total C O 6 3 3	0	0
4	C	1	Total C O 6 3 3	0	0
4	D	1	Total C O 6 3 3	0	0
4	E	1	Total C O 6 3 3	0	0
4	F	1	Total C O 6 3 3	0	0

- Molecule 5 is SODIUM ION (three-letter code: NA) (formula: Na).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	1	Total Na 1 1	0	0

- Molecule 6 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	289	Total O 289 289	0	0
6	B	312	Total O 312 312	0	0

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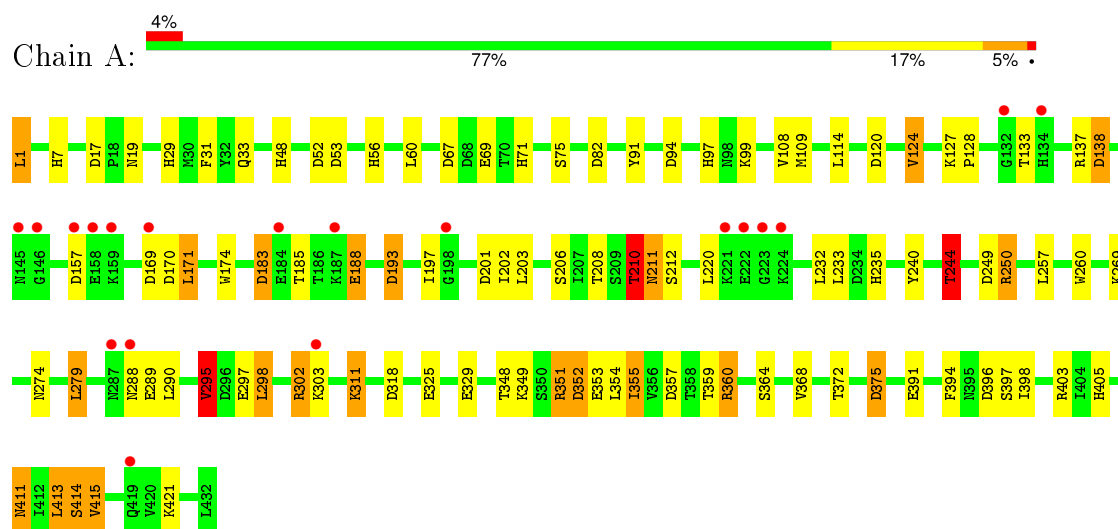
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	C	298	Total 298	O 298	0	0
6	D	286	Total 286	O 286	0	0
6	E	294	Total 294	O 294	0	0
6	F	277	Total 277	O 277	0	0

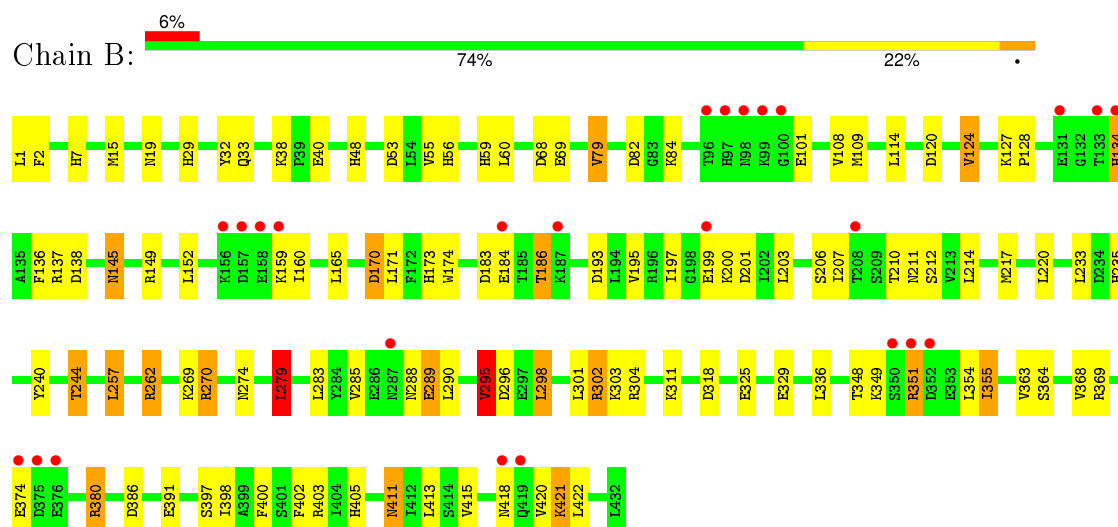
3 Residue-property plots

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

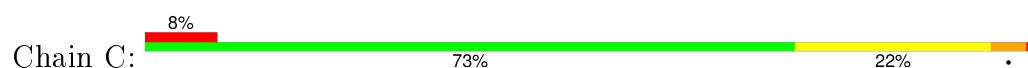
• Molecule 1: BETA-FRUCTOSIDASE

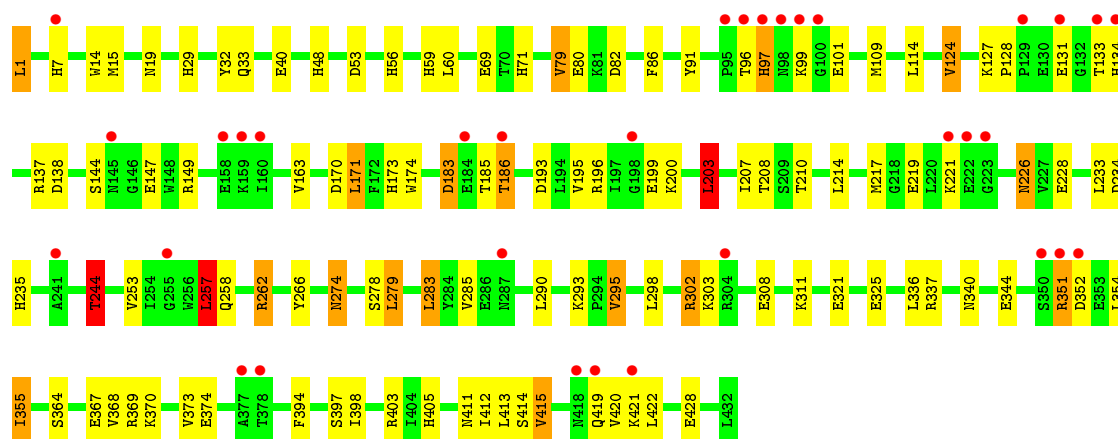


• Molecule 1: BETA-FRUCTOSIDASE

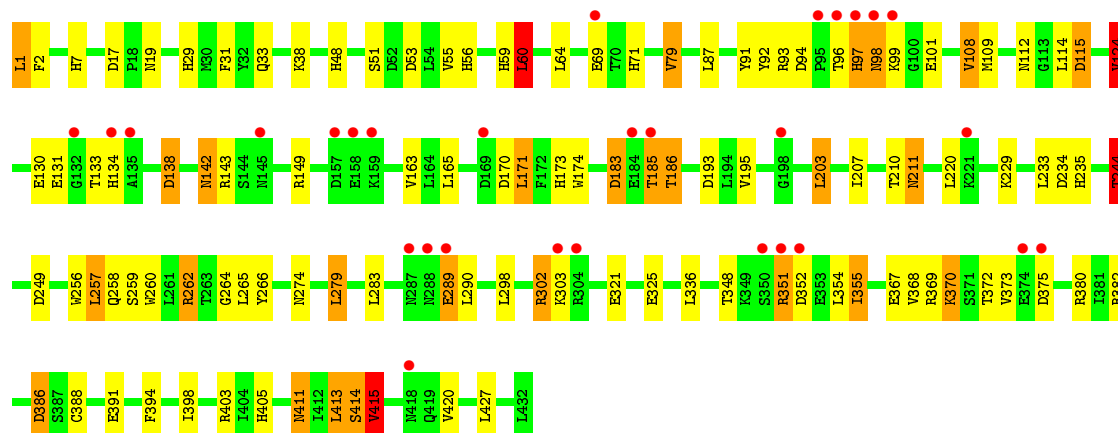
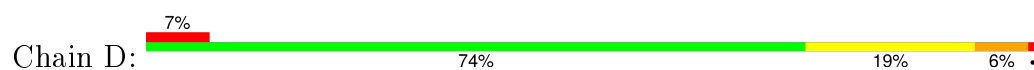


• Molecule 1: BETA-FRUCTOSIDASE

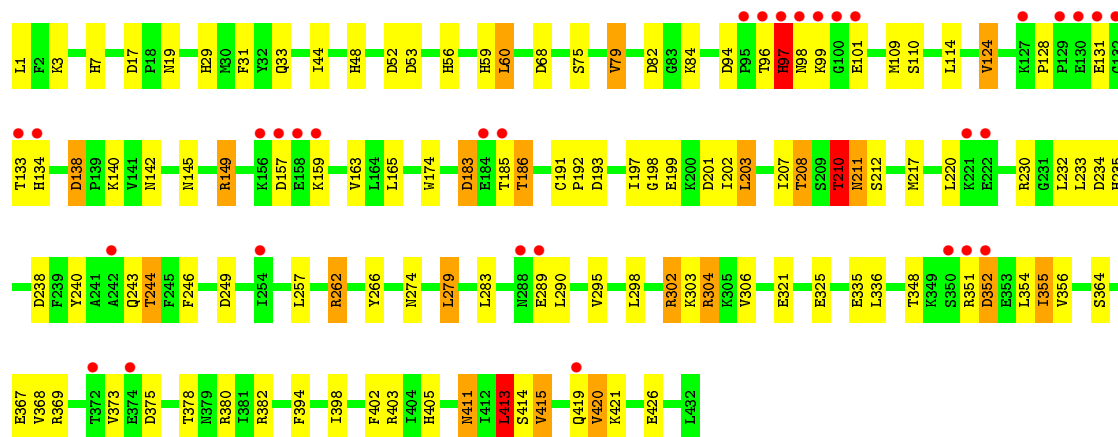




• Molecule 1: BETA-FRUCTOSIDASE

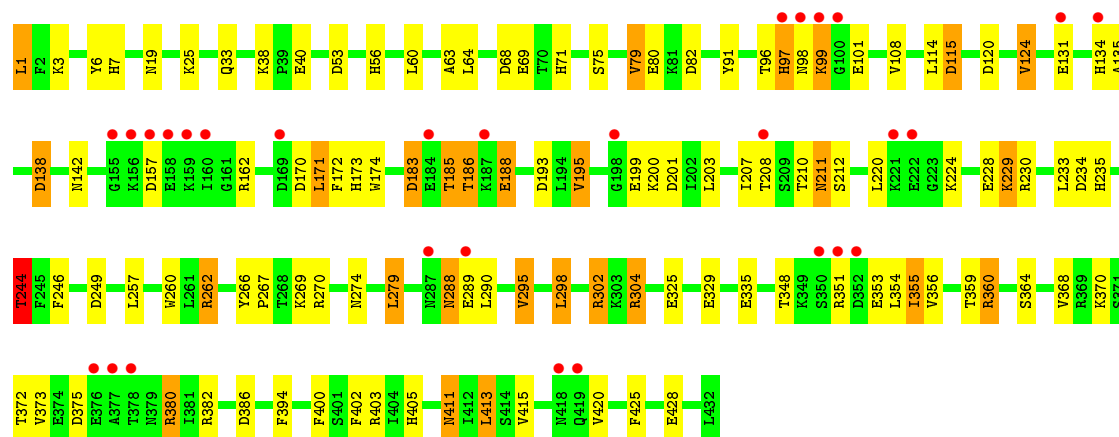


• Molecule 1: BETA-FRUCTOSIDASE



• Molecule 1: BETA-FRUCTOSIDASE





4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	94.48Å 114.67Å 130.03Å 90.00° 98.96° 90.00°	Depositor
Resolution (Å)	129.10 – 1.90 39.29 – 1.90	Depositor EDS
% Data completeness (in resolution range)	99.1 (129.10-1.90) 99.1 (39.29-1.90)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.61 (at 1.89Å)	Xtriage
Refinement program	REFMAC 5.1.24	Depositor
R, R_{free}	0.177 , 0.220 0.189 , 0.230	Depositor DCC
R_{free} test set	10694 reflections (5.28%)	DCC
Wilson B-factor (Å ²)	21.2	Xtriage
Anisotropy	0.317	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.41 , 65.8	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Outliers	0 of 213214 reflections	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	22996	wwPDB-VP
Average B, all atoms (Å ²)	27.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.55% 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, 0.375 respectively for untwinned datasets, and 0.333, 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: GOL, CIT, SO4, NA

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	A	0.78	1/3611 (0.0%)	1.03	26/4886 (0.5%)
1	B	0.78	0/3611	0.99	14/4886 (0.3%)
1	C	0.77	0/3611	0.98	18/4886 (0.4%)
1	D	0.75	0/3611	1.07	21/4886 (0.4%)
1	E	0.75	0/3611	1.01	21/4886 (0.4%)
1	F	0.75	0/3611	1.02	21/4886 (0.4%)
All	All	0.76	1/21666 (0.0%)	1.02	121/29316 (0.4%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	244	THR	CB-CG2	-5.77	1.33	1.52

All (121) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	262	ARG	NE-CZ-NH2	-18.66	110.97	120.30
1	D	302	ARG	NE-CZ-NH1	14.50	127.55	120.30
1	F	262	ARG	NE-CZ-NH2	-14.20	113.20	120.30
1	E	262	ARG	NE-CZ-NH2	-12.67	113.97	120.30
1	D	262	ARG	NE-CZ-NH1	12.40	126.50	120.30
1	D	302	ARG	NE-CZ-NH2	-11.82	114.39	120.30
1	F	262	ARG	NE-CZ-NH1	11.54	126.07	120.30
1	C	302	ARG	NE-CZ-NH1	10.99	125.80	120.30
1	A	302	ARG	NE-CZ-NH1	10.89	125.75	120.30
1	B	302	ARG	NE-CZ-NH1	10.29	125.44	120.30
1	E	302	ARG	NE-CZ-NH1	9.79	125.19	120.30
1	E	262	ARG	NE-CZ-NH1	9.70	125.15	120.30
1	F	115	ASP	CB-CG-OD2	9.39	126.75	118.30
1	A	17	ASP	CB-CG-OD1	9.19	126.57	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	138	ASP	CB-CG-OD2	9.07	126.46	118.30
1	F	302	ARG	NE-CZ-NH1	8.68	124.64	120.30
1	A	250	ARG	NE-CZ-NH1	-8.65	115.98	120.30
1	E	17	ASP	CB-CG-OD1	8.44	125.90	118.30
1	C	262	ARG	NE-CZ-NH2	-8.44	116.08	120.30
1	A	302	ARG	NE-CZ-NH2	-8.27	116.17	120.30
1	E	302	ARG	NE-CZ-NH2	-8.15	116.23	120.30
1	C	302	ARG	NE-CZ-NH2	-8.00	116.30	120.30
1	A	352	ASP	CB-CG-OD2	7.92	125.42	118.30
1	A	250	ARG	NE-CZ-NH2	7.54	124.07	120.30
1	E	183	ASP	CB-CG-OD2	7.47	125.03	118.30
1	B	302	ARG	NE-CZ-NH2	-7.43	116.59	120.30
1	B	183	ASP	CB-CG-OD2	7.15	124.74	118.30
1	D	415	VAL	CB-CA-C	-7.12	97.87	111.40
1	D	115	ASP	CB-CG-OD2	7.11	124.69	118.30
1	B	257	LEU	CA-CB-CG	7.01	131.43	115.30
1	C	183	ASP	CB-CG-OD2	6.98	124.58	118.30
1	D	262	ARG	CG-CD-NE	-6.92	97.26	111.80
1	F	82	ASP	CB-CG-OD2	6.86	124.47	118.30
1	A	138	ASP	CB-CG-OD2	6.81	124.43	118.30
1	F	234	ASP	CB-CG-OD2	6.69	124.32	118.30
1	D	382	ARG	NE-CZ-NH2	-6.63	116.98	120.30
1	C	138	ASP	CB-CG-OD2	6.62	124.26	118.30
1	F	38	LYS	CA-CB-CG	6.42	127.53	113.40
1	A	183	ASP	CB-CG-OD2	6.41	124.07	118.30
1	C	262	ARG	NE-CZ-NH1	6.40	123.50	120.30
1	F	413	LEU	CA-CB-CG	6.34	129.89	115.30
1	D	60	LEU	CB-CG-CD1	6.33	121.77	111.00
1	B	79	VAL	CG1-CB-CG2	6.31	120.99	110.90
1	C	344	GLU	CB-CA-C	-6.24	97.92	110.40
1	B	296	ASP	CB-CG-OD2	6.23	123.91	118.30
1	F	138	ASP	CB-CG-OD2	6.21	123.89	118.30
1	F	38	LYS	N-CA-CB	-6.20	99.44	110.60
1	C	415	VAL	CB-CA-C	-6.16	99.70	111.40
1	C	295	VAL	CG1-CB-CG2	6.15	120.75	110.90
1	E	415	VAL	CB-CA-C	-6.15	99.71	111.40
1	A	82	ASP	CB-CG-OD2	6.14	123.83	118.30
1	C	244	THR	N-CA-CB	-6.11	98.69	110.30
1	C	352	ASP	CB-CG-OD2	6.10	123.79	118.30
1	E	149	ARG	NE-CZ-NH2	-6.08	117.26	120.30
1	F	302	ARG	NE-CZ-NH2	-6.08	117.26	120.30
1	D	386	ASP	CB-CG-OD2	6.04	123.73	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	120	ASP	CB-CG-OD2	6.00	123.70	118.30
1	E	238	ASP	CB-CG-OD2	5.99	123.69	118.30
1	B	201	ASP	CB-CG-OD2	5.97	123.67	118.30
1	E	201	ASP	CB-CG-OD2	5.97	123.67	118.30
1	D	183	ASP	CB-CG-OD2	5.96	123.67	118.30
1	C	79	VAL	CG1-CB-CG2	5.95	120.42	110.90
1	E	157	ASP	CB-CG-OD2	5.94	123.64	118.30
1	D	234	ASP	CB-CG-OD2	5.92	123.63	118.30
1	A	415	VAL	CB-CA-C	-5.87	100.25	111.40
1	B	68	ASP	CB-CG-OD2	5.85	123.57	118.30
1	A	157	ASP	CB-CG-OD2	5.85	123.56	118.30
1	D	17	ASP	CB-CG-OD1	5.85	123.56	118.30
1	D	138	ASP	CB-CG-OD2	5.81	123.53	118.30
1	E	375	ASP	CB-CG-OD2	5.80	123.52	118.30
1	C	257	LEU	CB-CG-CD2	5.79	120.84	111.00
1	A	137	ARG	NE-CZ-NH2	-5.69	117.45	120.30
1	E	210	THR	OG1-CB-CG2	-5.65	97.01	110.00
1	E	52	ASP	CB-CG-OD2	5.61	123.34	118.30
1	F	249	ASP	CB-CG-OD2	5.60	123.34	118.30
1	F	183	ASP	CB-CG-OD2	5.54	123.28	118.30
1	A	169	ASP	CB-CG-OD2	5.52	123.27	118.30
1	C	147	GLU	CB-CA-C	-5.50	99.39	110.40
1	F	68	ASP	CB-CG-OD2	5.50	123.25	118.30
1	B	170	ASP	CB-CG-OD2	5.47	123.22	118.30
1	C	82	ASP	CB-CG-OD2	5.46	123.21	118.30
1	D	257	LEU	CA-CB-CG	5.44	127.81	115.30
1	B	82	ASP	CB-CG-OD2	5.44	123.19	118.30
1	A	52	ASP	CB-CG-OD2	5.43	123.19	118.30
1	A	396	ASP	CB-CG-OD2	5.42	123.18	118.30
1	A	193	ASP	CB-CG-OD1	5.42	123.18	118.30
1	A	357	ASP	CB-CG-OD1	5.42	123.18	118.30
1	B	262	ARG	NE-CZ-NH1	5.41	123.01	120.30
1	F	298	LEU	CB-CG-CD1	5.37	120.12	111.00
1	F	279	LEU	CB-CG-CD1	5.35	120.09	111.00
1	E	234	ASP	CB-CG-OD2	5.33	123.09	118.30
1	C	234	ASP	CB-CG-OD2	5.31	123.08	118.30
1	F	295	VAL	CG1-CB-CG2	5.31	119.39	110.90
1	C	257	LEU	CA-CB-CG	5.30	127.49	115.30
1	A	298	LEU	CB-CG-CD1	5.28	119.97	111.00
1	F	244	THR	N-CA-CB	-5.28	100.27	110.30
1	A	210	THR	N-CA-CB	-5.25	100.33	110.30
1	A	67	ASP	CB-CG-OD2	5.25	123.02	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	203	LEU	CA-CB-CG	5.24	127.36	115.30
1	D	244	THR	N-CA-CB	-5.24	100.34	110.30
1	E	82	ASP	CB-CG-OD2	5.23	123.01	118.30
1	D	262	ARG	CD-NE-CZ	5.21	130.90	123.60
1	D	352	ASP	CB-CG-OD2	5.21	122.99	118.30
1	B	295	VAL	N-CA-CB	-5.19	100.08	111.50
1	B	145	ASN	CB-CA-C	-5.19	100.03	110.40
1	E	413	LEU	CA-CB-CG	5.17	127.19	115.30
1	D	302	ARG	CD-NE-CZ	5.17	130.83	123.60
1	D	124	VAL	CG1-CB-CG2	5.16	119.15	110.90
1	F	201	ASP	CB-CG-OD2	5.16	122.94	118.30
1	A	318	ASP	CB-CG-OD2	5.13	122.92	118.30
1	D	94	ASP	CB-CA-C	-5.13	100.14	110.40
1	B	279	LEU	CB-CG-CD1	5.12	119.69	111.00
1	A	295	VAL	CG1-CB-CG2	5.09	119.04	110.90
1	A	352	ASP	CB-CG-OD1	-5.08	113.72	118.30
1	A	94	ASP	CB-CG-OD1	5.08	122.87	118.30
1	E	94	ASP	CB-CA-C	-5.06	100.28	110.40
1	F	157	ASP	CB-CG-OD2	5.05	122.85	118.30
1	E	68	ASP	CB-CG-OD2	5.03	122.83	118.30
1	A	17	ASP	CB-CG-OD2	-5.02	113.78	118.30
1	E	420	VAL	CB-CA-C	-5.01	101.88	111.40
1	A	201	ASP	CB-CG-OD2	5.00	122.80	118.30

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts ⓘ

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	3520	0	3413	61	0
1	B	3520	0	3413	72	0
1	C	3520	0	3413	81	0
1	D	3520	0	3413	82	0
1	E	3520	0	3413	101	0
1	F	3520	0	3413	97	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	A	15	0	0	1	0
2	B	20	0	0	3	0
2	C	15	0	0	2	0
2	E	5	0	0	0	0
2	F	15	0	0	4	0
3	A	13	0	5	1	0
4	A	6	0	8	0	0
4	B	6	0	8	0	0
4	C	6	0	8	0	0
4	D	6	0	8	0	0
4	E	6	0	8	0	0
4	F	6	0	8	0	0
5	A	1	0	0	0	0
6	A	289	0	0	10	0
6	B	312	0	0	22	0
6	C	298	0	0	16	0
6	D	286	0	0	17	0
6	E	294	0	0	30	0
6	F	277	0	0	27	0
All	All	22996	0	20531	485	0

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 12.

All (485) 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:109:MET:SD	1:A:109:MET:CE	2.03	1.46
1:F:7:HIS:CE1	6:F:2010:HOH:O	1.90	1.23
1:E:48:HIS:CE1	1:E:60:LEU:HD23	1.81	1.15
1:F:96:THR:HB	1:F:99:LYS:HZ2	1.00	1.09
1:D:96:THR:O	1:D:98:ASN:N	1.86	1.07
1:F:96:THR:CB	1:F:99:LYS:NZ	2.18	1.06
1:F:7:HIS:CG	6:F:2010:HOH:O	2.12	1.03
1:F:96:THR:HB	1:F:99:LYS:NZ	1.71	1.03
1:E:235:HIS:ND1	1:E:398:ILE:HD11	1.73	1.02
1:D:97:HIS:C	1:D:98:ASN:HD22	1.65	1.00
1:F:96:THR:CB	1:F:99:LYS:HZ2	1.76	0.94
1:A:7:HIS:CD2	1:A:279:LEU:HD13	2.03	0.93
1:D:1:LEU:HD22	6:D:2268:HOH:O	1.65	0.93
1:E:193:ASP:OD2	1:E:244:THR:HB	1.69	0.93

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:7:HIS:CD2	6:F:2010:HOH:O	2.22	0.92
1:F:96:THR:O	1:F:98:ASN:N	2.02	0.92
1:E:31:PHE:CE2	1:E:48:HIS:CD2	2.58	0.91
1:B:134:HIS:ND1	2:B:1435:SO4:O2	2.08	0.87
1:D:193:ASP:OD2	1:D:244:THR:HB	1.75	0.86
1:F:193:ASP:OD2	1:F:244:THR:HB	1.76	0.85
1:C:302:ARG:HD3	1:C:325:GLU:OE1	1.76	0.84
1:D:31:PHE:CE2	1:D:48:HIS:CD2	2.67	0.83
1:D:235:HIS:ND1	1:D:398:ILE:HD11	1.94	0.82
1:B:193:ASP:OD2	1:B:244:THR:HB	1.79	0.82
1:E:149:ARG:HD2	6:E:2116:HOH:O	1.80	0.82
1:F:142:ASN:HB3	6:F:2122:HOH:O	1.81	0.80
1:F:115:ASP:HB2	6:F:2101:HOH:O	1.80	0.80
1:F:96:THR:OG1	1:F:99:LYS:NZ	2.09	0.80
1:E:211:ASN:OD1	6:E:2161:HOH:O	1.99	0.80
1:E:48:HIS:ND1	1:E:60:LEU:HD23	1.97	0.79
1:B:235:HIS:ND1	1:B:398:ILE:HD11	1.98	0.79
1:D:48:HIS:CE1	1:D:60:LEU:HD23	2.17	0.79
1:D:302:ARG:HD3	1:D:325:GLU:OE1	1.82	0.79
1:F:134:HIS:CD2	1:F:135:ALA:H	2.01	0.79
1:F:96:THR:CB	1:F:99:LYS:HZ1	1.89	0.77
1:F:200:LYS:NZ	1:F:288:ASN:HD21	1.82	0.77
1:C:29:HIS:HD2	1:C:48:HIS:NE2	1.83	0.77
1:E:235:HIS:CE1	1:E:398:ILE:HD11	2.19	0.77
1:B:269:LYS:HE3	6:B:2195:HOH:O	1.86	0.75
1:D:19:ASN:HD21	1:D:33:GLN:HE21	1.34	0.75
1:F:304:ARG:HG2	6:F:2206:HOH:O	1.87	0.75
1:A:193:ASP:OD2	1:A:244:THR:HB	1.86	0.74
1:F:7:HIS:ND1	6:F:2010:HOH:O	1.96	0.74
1:D:373:VAL:HG11	1:D:394:PHE:CE2	2.23	0.74
1:C:373:VAL:HG11	1:C:394:PHE:CE2	2.22	0.74
1:E:53:ASP:OD2	1:E:56:HIS:HD2	1.71	0.73
1:D:97:HIS:C	1:D:98:ASN:ND2	2.41	0.73
1:F:186:THR:CG2	1:F:207:ILE:HG23	2.18	0.73
1:E:31:PHE:CE2	1:E:48:HIS:HD2	2.05	0.73
1:C:137:ARG:NH1	2:C:1435:SO4:O3	2.22	0.73
1:F:6:TYR:CE1	1:F:7:HIS:CE1	2.77	0.72
1:E:7:HIS:CE1	1:E:279:LEU:HD13	2.25	0.72
1:A:349:LYS:NZ	1:A:375:ASP:OD2	2.19	0.72
1:E:348:THR:HG21	6:E:2238:HOH:O	1.89	0.72
1:C:134:HIS:CE1	6:C:2119:HOH:O	2.41	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:302:ARG:HD3	1:A:325:GLU:OE1	1.88	0.72
1:B:302:ARG:HD3	1:B:325:GLU:OE1	1.90	0.72
1:A:197:ILE:HD12	1:A:202:ILE:HD13	1.72	0.71
1:B:29:HIS:HD2	1:B:48:HIS:NE2	1.89	0.71
1:A:29:HIS:HD2	1:A:48:HIS:NE2	1.89	0.71
1:F:183:ASP:OD1	1:F:185:THR:HB	1.91	0.70
1:F:1:LEU:HD13	6:F:2262:HOH:O	1.90	0.70
1:A:210:THR:HG23	1:A:212:SER:OG	1.91	0.70
1:B:7:HIS:HE1	1:B:391:GLU:OE1	1.75	0.70
6:B:2132:HOH:O	1:C:80:GLU:HG2	1.91	0.70
1:E:373:VAL:HG11	1:E:394:PHE:CE2	2.26	0.70
1:F:302:ARG:HD3	1:F:325:GLU:OE1	1.91	0.70
1:E:249:ASP:HB2	6:E:2178:HOH:O	1.90	0.69
1:E:138:ASP:HB3	6:E:2067:HOH:O	1.92	0.69
1:B:418:ASN:HA	6:B:2303:HOH:O	1.92	0.69
1:A:138:ASP:OD2	6:A:2114:HOH:O	2.10	0.69
1:D:149:ARG:CG	1:D:165:LEU:HD11	2.24	0.68
1:D:29:HIS:HD2	1:D:48:HIS:NE2	1.91	0.68
1:D:7:HIS:HE1	1:D:391:GLU:OE1	1.77	0.68
1:C:19:ASN:HD21	1:C:33:GLN:HE21	1.39	0.68
1:E:7:HIS:ND1	1:E:279:LEU:HD13	2.07	0.68
1:F:210:THR:HG21	6:F:2078:HOH:O	1.93	0.68
1:A:249:ASP:HB2	1:D:249:ASP:OD1	1.94	0.68
1:E:96:THR:O	1:E:98:ASN:N	2.26	0.68
1:D:235:HIS:CE1	1:D:398:ILE:HD11	2.27	0.68
1:B:7:HIS:HD2	1:B:386:ASP:OD2	1.77	0.68
1:C:193:ASP:OD2	1:C:244:THR:HB	1.94	0.68
1:C:69:GLU:H	1:C:69:GLU:CD	1.95	0.68
1:A:235:HIS:ND1	1:A:398:ILE:HD11	2.08	0.68
1:C:208:THR:HB	6:C:2154:HOH:O	1.92	0.67
1:D:134:HIS:HB2	6:D:2060:HOH:O	1.94	0.67
1:C:235:HIS:ND1	1:C:398:ILE:HD11	2.08	0.67
1:B:210:THR:HG23	1:B:212:SER:OG	1.93	0.67
1:F:210:THR:HG23	1:F:212:SER:OG	1.93	0.67
1:D:96:THR:O	1:D:97:HIS:C	2.32	0.67
1:F:200:LYS:HZ1	1:F:288:ASN:HD21	1.42	0.67
1:C:1:LEU:HD22	6:C:2278:HOH:O	1.93	0.67
1:E:302:ARG:HD3	1:E:325:GLU:OE1	1.95	0.67
1:F:373:VAL:HG11	1:F:394:PHE:CE2	2.30	0.67
1:F:1:LEU:N	6:F:2002:HOH:O	2.27	0.66
1:C:1:LEU:HD13	6:C:2278:HOH:O	1.93	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:19:ASN:HD21	1:B:33:GLN:HE21	1.42	0.66
1:A:413:LEU:HD12	1:A:414:SER:N	2.10	0.66
1:C:367:GLU:OE1	1:C:369:ARG:NH2	2.29	0.66
1:D:348:THR:HG23	6:D:2237:HOH:O	1.95	0.66
1:B:262:ARG:NH2	6:B:2191:HOH:O	2.27	0.66
1:F:7:HIS:NE2	6:F:2010:HOH:O	2.03	0.66
1:D:7:HIS:HD2	1:D:386:ASP:OD2	1.78	0.65
1:D:130:GLU:O	1:D:133:THR:HG23	1.97	0.65
1:D:53:ASP:OD2	1:D:56:HIS:HD2	1.80	0.65
1:E:31:PHE:CZ	1:E:48:HIS:CD2	2.84	0.65
1:C:186:THR:CG2	1:C:207:ILE:HG23	2.27	0.65
1:F:359:THR:OG1	1:F:360:ARG:HD3	1.96	0.65
1:F:96:THR:C	1:F:98:ASN:H	2.01	0.64
1:C:186:THR:HG23	1:C:207:ILE:HG23	1.79	0.64
1:E:352:ASP:CB	6:E:2244:HOH:O	2.46	0.64
1:F:360:ARG:HG2	6:F:2238:HOH:O	1.97	0.64
1:F:186:THR:HG23	1:F:207:ILE:HG23	1.77	0.64
1:E:96:THR:O	1:E:99:LYS:N	2.25	0.64
1:F:6:TYR:CE1	1:F:7:HIS:HE1	2.15	0.64
1:E:193:ASP:HB2	6:E:2152:HOH:O	1.97	0.64
1:E:210:THR:HG21	6:E:2160:HOH:O	1.98	0.64
1:E:306:VAL:HG11	1:E:426:GLU:HG3	1.80	0.64
1:F:360:ARG:CG	6:F:2238:HOH:O	2.44	0.63
1:C:53:ASP:OD2	1:C:56:HIS:HD2	1.82	0.63
1:C:7:HIS:CE1	1:C:279:LEU:HD13	2.34	0.63
1:E:19:ASN:HD21	1:E:33:GLN:HE21	1.46	0.63
1:A:19:ASN:HD21	1:A:33:GLN:HE21	1.46	0.63
1:C:97:HIS:CE1	6:C:2082:HOH:O	2.50	0.63
1:E:403:ARG:HH21	1:E:405:HIS:HE1	1.46	0.62
1:B:336:LEU:HD11	1:B:413:LEU:HD11	1.82	0.61
1:C:19:ASN:ND2	1:C:33:GLN:HE21	1.99	0.61
1:A:244:THR:CG2	6:A:2165:HOH:O	2.49	0.61
1:C:7:HIS:ND1	1:C:279:LEU:HD13	2.16	0.60
1:A:403:ARG:HH21	1:A:405:HIS:HE1	1.49	0.60
1:A:53:ASP:OD2	1:A:56:HIS:HD2	1.83	0.60
1:B:53:ASP:OD2	1:B:56:HIS:HD2	1.85	0.60
1:C:96:THR:OG1	1:C:99:LYS:NZ	2.33	0.60
1:B:270:ARG:H	1:B:270:ARG:HD2	1.67	0.60
1:D:112:ASN:ND2	1:D:115:ASP:OD2	2.23	0.59
1:A:359:THR:OG1	1:A:360:ARG:HD3	2.02	0.59
1:E:131:GLU:OE1	1:E:131:GLU:HA	2.02	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:210:THR:CG2	1:A:212:SER:OG	2.51	0.59
1:A:348:THR:HG21	6:A:2223:HOH:O	2.02	0.59
1:C:29:HIS:HE1	6:C:2018:HOH:O	1.82	0.59
1:D:124:VAL:HG13	1:D:174:TRP:CD1	2.37	0.59
1:D:262:ARG:HD3	1:D:266:TYR:OH	2.01	0.59
1:E:186:THR:CG2	1:E:207:ILE:HG23	2.33	0.59
1:E:364:SER:OG	1:E:405:HIS:HD2	1.86	0.59
1:D:96:THR:O	1:D:99:LYS:N	2.35	0.58
1:E:367:GLU:OE1	1:E:369:ARG:NH2	2.36	0.58
1:D:149:ARG:HG3	1:D:165:LEU:HD11	1.84	0.58
1:C:364:SER:OG	1:C:405:HIS:HD2	1.86	0.58
1:E:134:HIS:HB2	6:E:2130:HOH:O	2.02	0.58
1:A:31:PHE:CE2	1:A:48:HIS:CD2	2.91	0.58
1:F:3:LYS:CE	6:F:2005:HOH:O	2.50	0.58
1:D:19:ASN:ND2	1:D:33:GLN:HE21	1.99	0.58
1:F:1:LEU:HG	2:F:1433:SO4:O1	2.04	0.58
1:E:96:THR:O	1:E:97:HIS:C	2.42	0.58
1:C:86:PHE:CE2	1:C:109:MET:HG2	2.39	0.58
1:B:19:ASN:ND2	1:B:33:GLN:HE21	2.01	0.57
1:E:133:THR:O	1:E:134:HIS:ND1	2.36	0.57
1:E:84:LYS:NZ	6:E:2073:HOH:O	2.31	0.57
1:E:149:ARG:HG2	1:E:165:LEU:HD11	1.86	0.57
1:F:69:GLU:H	1:F:69:GLU:CD	2.08	0.57
1:D:133:THR:HG22	6:D:2122:HOH:O	2.03	0.57
1:C:303:LYS:NZ	6:C:2211:HOH:O	2.38	0.57
1:F:53:ASP:OD2	1:F:56:HIS:HD2	1.86	0.57
1:F:353:GLU:OE2	1:F:372:THR:HG22	2.05	0.57
1:A:170:ASP:O	1:A:171:LEU:HB2	2.05	0.57
1:B:186:THR:CG2	1:B:207:ILE:HG23	2.35	0.56
1:A:183:ASP:OD1	1:A:185:THR:HB	2.05	0.56
1:B:348:THR:HG23	6:B:2263:HOH:O	2.04	0.56
1:B:186:THR:HG23	1:B:207:ILE:HG23	1.88	0.56
1:D:31:PHE:CZ	1:D:48:HIS:CD2	2.92	0.56
1:A:7:HIS:NE2	1:A:279:LEU:HD13	2.21	0.56
1:E:352:ASP:HB3	6:E:2244:HOH:O	2.06	0.56
1:E:134:HIS:CD2	6:E:2130:HOH:O	2.59	0.56
1:B:269:LYS:HB2	6:B:2195:HOH:O	2.05	0.56
1:F:134:HIS:CG	1:F:135:ALA:H	2.24	0.56
1:B:29:HIS:HE1	6:B:2023:HOH:O	1.88	0.56
1:F:1:LEU:CG	2:F:1433:SO4:O1	2.54	0.56
1:E:243:GLN:HG3	6:E:2152:HOH:O	2.05	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:142:ASN:CB	6:F:2122:HOH:O	2.48	0.55
1:C:336:LEU:HD11	1:C:413:LEU:HD11	1.88	0.55
1:E:244:THR:CG2	6:E:2172:HOH:O	2.54	0.55
1:C:403:ARG:HH21	1:C:405:HIS:HE1	1.53	0.55
1:E:348:THR:HG23	6:E:2247:HOH:O	2.06	0.55
1:D:186:THR:HG23	1:D:207:ILE:HG23	1.88	0.55
1:F:228:GLU:HG2	1:F:229:LYS:HG2	1.89	0.55
1:D:71:HIS:CE1	1:D:93:ARG:HG3	2.41	0.55
1:F:186:THR:HG21	1:F:207:ILE:HG23	1.87	0.55
1:F:262:ARG:HD3	1:F:266:TYR:OH	2.06	0.55
1:E:249:ASP:CB	6:E:2178:HOH:O	2.52	0.55
1:F:329:GLU:HG3	1:F:380:ARG:HG2	1.89	0.55
1:B:149:ARG:HG3	1:B:165:LEU:HD11	1.89	0.55
1:E:208:THR:HG22	1:E:240:TYR:OH	2.06	0.54
1:B:355:ILE:CD1	1:B:368:VAL:HG13	2.38	0.54
1:C:253:VAL:HG21	1:C:283:LEU:HD22	1.89	0.54
1:A:1:LEU:HD12	1:A:1:LEU:H3	1.72	0.54
1:D:264:GLY:C	6:D:2177:HOH:O	2.45	0.54
1:D:170:ASP:O	1:D:171:LEU:HB2	2.08	0.54
1:D:59:HIS:HD2	6:D:2029:HOH:O	1.91	0.54
1:E:186:THR:HG23	1:E:207:ILE:HG23	1.90	0.54
1:C:244:THR:OG1	1:C:253:VAL:HG22	2.08	0.54
1:D:403:ARG:HH21	1:D:405:HIS:HE1	1.55	0.54
1:A:7:HIS:CD2	1:A:279:LEU:CD1	2.86	0.54
1:E:208:THR:HG23	6:E:2145:HOH:O	2.08	0.54
1:A:411:ASN:H	1:A:411:ASN:HD22	1.56	0.54
1:B:137:ARG:NH1	2:B:1435:SO4:O4	2.42	0.53
1:D:163:VAL:HG21	1:D:203:LEU:HD11	1.91	0.53
1:E:59:HIS:HD2	6:E:2028:HOH:O	1.90	0.53
1:B:120:ASP:HB2	6:B:2111:HOH:O	2.08	0.53
1:C:253:VAL:CG2	1:C:283:LEU:HD22	2.39	0.53
1:C:99:LYS:NZ	6:C:2084:HOH:O	2.41	0.53
1:B:170:ASP:OD2	1:B:173:HIS:HD2	1.91	0.53
1:E:124:VAL:HG13	1:E:174:TRP:CD1	2.43	0.53
1:A:250:ARG:NH1	1:A:295:VAL:HG22	2.22	0.53
1:F:101:GLU:OE2	1:F:134:HIS:NE2	2.40	0.53
1:C:7:HIS:HD1	1:C:279:LEU:HD13	1.74	0.53
1:F:230:ARG:CD	6:F:2160:HOH:O	2.56	0.53
1:C:302:ARG:CD	1:C:325:GLU:OE1	2.54	0.53
1:D:64:LEU:HD21	1:D:108:VAL:HG11	1.91	0.53
1:A:19:ASN:ND2	1:A:33:GLN:HE21	2.07	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:340:ASN:HA	1:C:412:ILE:HD12	1.91	0.52
1:C:170:ASP:OD2	1:C:173:HIS:HD2	1.92	0.52
1:D:55:VAL:C	6:D:2049:HOH:O	2.48	0.52
1:B:235:HIS:ND1	1:B:398:ILE:CD1	2.70	0.52
1:B:210:THR:HG21	6:B:2172:HOH:O	2.09	0.52
1:A:364:SER:OG	1:A:405:HIS:HD2	1.93	0.52
1:B:364:SER:OG	1:B:405:HIS:HD2	1.92	0.52
1:D:302:ARG:CD	1:D:325:GLU:OE1	2.56	0.52
1:F:3:LYS:HE2	6:F:2005:HOH:O	2.10	0.52
1:B:124:VAL:HG13	1:B:174:TRP:CD1	2.44	0.52
1:A:352:ASP:OD1	1:C:228:GLU:OE2	2.27	0.52
1:B:235:HIS:CE1	1:B:398:ILE:HD11	2.44	0.52
1:A:302:ARG:CD	1:A:325:GLU:OE1	2.55	0.52
1:A:250:ARG:HD3	2:A:1434:SO4:O3	2.09	0.52
1:B:329:GLU:HG3	1:B:380:ARG:HG2	1.91	0.52
1:C:71:HIS:HD2	1:C:91:TYR:CE2	2.28	0.52
1:E:48:HIS:HE1	1:E:60:LEU:HD23	1.60	0.52
1:F:134:HIS:CD2	1:F:135:ALA:N	2.75	0.52
1:D:289:GLU:HG2	6:D:2256:HOH:O	2.10	0.52
1:B:421:LYS:NZ	6:B:2305:HOH:O	2.43	0.51
1:E:7:HIS:CE1	1:E:279:LEU:CD1	2.94	0.51
1:F:69:GLU:HG3	6:F:2038:HOH:O	2.11	0.51
1:B:15:MET:HG3	1:B:32:TYR:CD1	2.45	0.51
1:F:138:ASP:HB3	6:F:2079:HOH:O	2.10	0.51
1:D:98:ASN:N	1:D:98:ASN:ND2	2.58	0.51
1:E:355:ILE:CD1	1:E:368:VAL:HG13	2.41	0.51
1:D:7:HIS:CE1	1:D:391:GLU:OE1	2.62	0.51
1:D:69:GLU:HG3	6:D:2031:HOH:O	2.10	0.51
1:B:101:GLU:OE2	2:B:1435:SO4:O3	2.28	0.51
1:C:19:ASN:HD21	1:C:33:GLN:NE2	2.09	0.51
1:B:403:ARG:HH21	1:B:405:HIS:HE1	1.58	0.51
1:F:355:ILE:CD1	1:F:368:VAL:HG13	2.40	0.51
1:C:355:ILE:HB	1:C:370:LYS:HG2	1.92	0.51
1:F:411:ASN:H	1:F:411:ASN:HD22	1.58	0.51
1:C:124:VAL:HG13	1:C:174:TRP:CD1	2.46	0.51
1:B:295:VAL:HG12	1:B:298:LEU:HD22	1.91	0.51
1:C:144:SER:HB3	1:C:149:ARG:HD2	1.93	0.50
1:D:336:LEU:HD13	1:D:415:VAL:HG13	1.92	0.50
1:D:71:HIS:HD2	1:D:91:TYR:CE2	2.30	0.50
1:E:335:GLU:HG3	1:E:348:THR:HG22	1.94	0.50
1:B:369:ARG:NE	6:B:2281:HOH:O	2.40	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:133:THR:O	1:D:134:HIS:ND1	2.45	0.50
1:F:329:GLU:HG3	1:F:380:ARG:CG	2.40	0.50
1:E:235:HIS:CE1	1:E:398:ILE:CD1	2.93	0.50
1:F:195:VAL:HG21	1:F:244:THR:HG21	1.94	0.50
1:B:1:LEU:HD11	1:B:2:PHE:CE1	2.47	0.50
1:E:262:ARG:NH2	6:E:2183:HOH:O	2.20	0.50
1:E:19:ASN:ND2	1:E:33:GLN:HE21	2.10	0.50
1:F:124:VAL:HG13	1:F:174:TRP:CD1	2.46	0.50
1:E:336:LEU:CD1	1:E:413:LEU:HD11	2.42	0.50
1:D:7:HIS:CE1	1:D:279:LEU:HD13	2.47	0.49
1:A:372:THR:OG1	1:C:226:ASN:OD1	2.29	0.49
1:F:25:LYS:NZ	6:F:2025:HOH:O	2.40	0.49
1:C:373:VAL:HG11	1:C:394:PHE:HE2	1.70	0.49
1:C:199:GLU:O	1:C:219:GLU:OE2	2.30	0.49
1:A:71:HIS:HD2	1:A:91:TYR:CE2	2.30	0.49
1:E:207:ILE:HG22	1:E:210:THR:HG22	1.95	0.49
1:C:373:VAL:HG12	1:C:374:GLU:N	2.28	0.49
1:A:235:HIS:CE1	1:A:398:ILE:HD11	2.47	0.49
1:B:160:ILE:HD12	1:B:184:GLU:HG3	1.93	0.49
1:E:183:ASP:OD1	1:E:185:THR:HB	2.13	0.49
1:D:235:HIS:CE1	1:D:398:ILE:CD1	2.96	0.49
1:C:134:HIS:NE2	6:C:2119:HOH:O	2.34	0.49
1:C:1:LEU:N	6:C:2003:HOH:O	2.45	0.48
1:C:96:THR:O	1:C:97:HIS:C	2.50	0.48
1:A:355:ILE:HD12	1:A:368:VAL:HG13	1.95	0.48
1:A:97:HIS:CE1	6:A:2085:HOH:O	2.66	0.48
1:D:133:THR:CG2	6:D:2122:HOH:O	2.60	0.48
1:D:97:HIS:CA	1:D:98:ASN:HD22	2.24	0.48
1:A:249:ASP:CB	1:D:249:ASP:OD1	2.61	0.48
1:B:336:LEU:CD1	1:B:413:LEU:HD11	2.43	0.48
1:B:1:LEU:HD13	6:B:2295:HOH:O	2.12	0.48
1:E:29:HIS:HD2	1:E:48:HIS:NE2	2.12	0.48
1:E:373:VAL:CG1	1:E:394:PHE:CE2	2.96	0.48
1:D:355:ILE:CD1	1:D:368:VAL:HG13	2.43	0.48
1:F:170:ASP:O	1:F:171:LEU:HB2	2.12	0.48
1:B:289:GLU:HG3	6:B:2212:HOH:O	2.14	0.48
1:F:40:GLU:OE2	1:F:269:LYS:CD	2.62	0.48
1:C:40:GLU:HG3	6:C:2031:HOH:O	2.13	0.48
1:F:230:ARG:HD2	6:F:2160:HOH:O	2.13	0.47
1:F:124:VAL:HG22	1:F:172:PHE:HA	1.96	0.47
1:B:304:ARG:HG2	6:B:2226:HOH:O	2.13	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:197:ILE:HG21	1:B:285:VAL:HG23	1.97	0.47
1:A:279:LEU:HD22	1:A:391:GLU:OE1	2.14	0.47
1:B:145:ASN:HA	1:C:80:GLU:O	2.15	0.47
1:E:193:ASP:CG	6:E:2152:HOH:O	2.52	0.47
1:B:7:HIS:CE1	1:B:391:GLU:OE1	2.61	0.47
1:D:186:THR:CG2	1:D:207:ILE:HG23	2.44	0.47
1:D:170:ASP:OD2	1:D:173:HIS:CD2	2.68	0.47
1:D:138:ASP:HB3	6:D:2063:HOH:O	2.14	0.47
1:F:356:VAL:HG11	1:F:402:PHE:CE2	2.49	0.47
1:E:411:ASN:HD22	1:E:411:ASN:H	1.62	0.47
1:A:69:GLU:H	1:A:69:GLU:CD	2.18	0.47
1:F:364:SER:OG	1:F:405:HIS:HD2	1.98	0.47
1:E:210:THR:HG1	1:E:212:SER:HG	1.46	0.47
1:C:128:PRO:HB2	1:C:133:THR:OG1	2.15	0.47
1:B:411:ASN:HD22	1:B:411:ASN:H	1.62	0.47
1:E:31:PHE:CD2	1:E:48:HIS:HD2	2.33	0.47
1:D:109:MET:HE1	6:D:2097:HOH:O	2.14	0.47
1:E:29:HIS:HE1	6:E:2022:HOH:O	1.98	0.46
1:E:75:SER:HB2	1:E:138:ASP:OD1	2.15	0.46
1:E:33:GLN:OE1	1:E:44:ILE:HG21	2.14	0.46
1:F:79:VAL:HG22	1:F:246:PHE:CE1	2.49	0.46
1:F:373:VAL:CG1	1:F:394:PHE:CE2	2.98	0.46
1:D:69:GLU:CG	6:D:2031:HOH:O	2.62	0.46
1:C:128:PRO:CB	1:C:133:THR:OG1	2.64	0.46
1:F:71:HIS:HD2	1:F:91:TYR:CE2	2.33	0.46
1:D:29:HIS:HE1	6:D:2022:HOH:O	1.98	0.46
1:E:336:LEU:HD11	1:E:413:LEU:HD11	1.97	0.46
1:D:411:ASN:H	1:D:411:ASN:HD22	1.62	0.46
1:B:138:ASP:HB3	6:B:2078:HOH:O	2.14	0.46
1:E:378:THR:HG22	6:E:2286:HOH:O	2.15	0.46
1:D:183:ASP:OD1	1:D:185:THR:HB	2.14	0.46
1:D:207:ILE:HG22	1:D:210:THR:HG22	1.97	0.46
1:C:170:ASP:O	1:C:171:LEU:HB2	2.16	0.46
1:D:355:ILE:HB	1:D:370:LYS:HG3	1.97	0.46
1:E:380:ARG:NH2	1:E:382:ARG:HD2	2.30	0.46
1:E:211:ASN:HB3	6:E:2161:HOH:O	2.16	0.46
1:F:270:ARG:HD2	2:F:1433:SO4:O4	2.16	0.46
1:C:183:ASP:OD1	1:C:185:THR:HB	2.16	0.46
1:C:214:LEU:HD12	1:C:214:LEU:N	2.30	0.46
1:E:232:LEU:CD1	1:E:235:HIS:HD2	2.29	0.46
1:A:29:HIS:HE1	6:A:2019:HOH:O	1.99	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:359:THR:OG1	1:F:360:ARG:NH1	2.49	0.46
1:C:336:LEU:CD1	1:C:413:LEU:HD11	2.45	0.46
1:C:144:SER:CB	1:C:149:ARG:HD2	2.46	0.46
1:F:403:ARG:HH21	1:F:405:HIS:HE1	1.63	0.46
1:D:142:ASN:HD22	1:D:143:ARG:N	2.14	0.46
1:B:69:GLU:CG	6:B:2034:HOH:O	2.63	0.46
1:F:19:ASN:HD21	1:F:33:GLN:HG2	1.81	0.45
1:D:413:LEU:HD12	1:D:414:SER:N	2.31	0.45
1:B:400:PHE:HB3	1:B:402:PHE:CE2	2.51	0.45
1:F:211:ASN:HD21	1:F:260:TRP:HB2	1.80	0.45
1:D:87:LEU:HB2	1:D:108:VAL:HG12	1.97	0.45
1:A:128:PRO:CB	1:A:133:THR:OG1	2.65	0.45
1:E:193:ASP:CB	6:E:2152:HOH:O	2.62	0.45
1:B:69:GLU:HG3	6:B:2034:HOH:O	2.15	0.45
1:C:15:MET:HG3	1:C:32:TYR:CD1	2.51	0.45
1:A:206:SER:HB3	1:A:240:TYR:CE1	2.51	0.45
1:E:149:ARG:CG	1:E:165:LEU:HD11	2.45	0.45
1:B:235:HIS:CE1	1:B:398:ILE:CD1	3.00	0.45
1:C:253:VAL:HG21	1:C:283:LEU:CD2	2.47	0.45
1:D:265:LEU:HD23	6:D:2177:HOH:O	2.16	0.45
1:F:235:HIS:HD2	6:F:2248:HOH:O	1.99	0.45
1:E:140:LYS:HG3	6:E:2152:HOH:O	2.17	0.45
1:F:56:HIS:HE1	1:F:428:GLU:OE1	2.00	0.45
1:A:188:GLU:CD	6:A:2139:HOH:O	2.55	0.45
1:E:142:ASN:ND2	6:E:2116:HOH:O	2.41	0.45
1:E:355:ILE:HD12	1:E:368:VAL:HG13	2.00	0.45
1:E:202:ILE:CG1	1:E:217:MET:HG3	2.47	0.45
1:E:235:HIS:ND1	1:E:398:ILE:CD1	2.62	0.44
1:A:185:THR:HG21	6:A:2063:HOH:O	2.16	0.44
1:E:262:ARG:HD3	1:E:266:TYR:OH	2.17	0.44
1:B:422:LEU:C	1:B:422:LEU:HD23	2.37	0.44
1:D:1:LEU:CD1	1:D:2:PHE:CD1	3.00	0.44
1:B:244:THR:CG2	6:B:2187:HOH:O	2.64	0.44
1:F:1:LEU:HD11	2:F:1433:SO4:O1	2.17	0.44
1:B:7:HIS:CE1	1:B:279:LEU:HD13	2.52	0.44
1:A:232:LEU:HD12	1:A:235:HIS:CD2	2.53	0.44
1:E:369:ARG:NE	6:E:2256:HOH:O	2.36	0.44
1:E:128:PRO:HB2	1:E:133:THR:OG1	2.18	0.44
1:A:394:PHE:HB3	1:A:398:ILE:CG2	2.48	0.44
1:A:250:ARG:NH1	1:A:297:GLU:OE1	2.50	0.44
1:C:59:HIS:HD2	6:C:2023:HOH:O	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:244:THR:CG2	6:F:2173:HOH:O	2.65	0.44
1:B:170:ASP:O	1:B:171:LEU:HB2	2.17	0.44
1:A:351:ARG:NE	6:A:2237:HOH:O	2.49	0.44
1:E:232:LEU:HD13	1:E:235:HIS:HD2	1.83	0.44
1:C:29:HIS:CD2	1:C:48:HIS:NE2	2.73	0.44
1:A:232:LEU:HD12	1:A:235:HIS:HD2	1.83	0.44
1:F:266:TYR:HA	1:F:267:PRO:HD3	1.92	0.44
1:B:160:ILE:HD12	1:B:184:GLU:CG	2.47	0.44
1:D:211:ASN:HD21	1:D:260:TRP:HB2	1.83	0.44
1:B:200:LYS:HD3	1:B:217:MET:HE2	2.00	0.44
1:F:69:GLU:CG	6:F:2038:HOH:O	2.65	0.43
1:A:211:ASN:HD21	1:A:260:TRP:HB2	1.81	0.43
1:B:127:LYS:CG	1:B:128:PRO:HD2	2.47	0.43
1:E:197:ILE:HD12	1:E:202:ILE:HD13	2.00	0.43
1:A:124:VAL:HG13	1:A:174:TRP:CD1	2.53	0.43
1:F:19:ASN:HD21	1:F:33:GLN:HE21	1.66	0.43
1:C:7:HIS:CE1	1:C:279:LEU:CD1	2.99	0.43
1:A:128:PRO:HB2	1:A:133:THR:OG1	2.19	0.43
1:C:337:ARG:O	1:C:413:LEU:HD12	2.18	0.43
1:F:98:ASN:OD1	6:F:2091:HOH:O	2.21	0.43
1:A:75:SER:HB2	1:A:138:ASP:OD1	2.18	0.43
1:F:162:ARG:HD3	6:F:2129:HOH:O	2.18	0.43
1:F:134:HIS:CG	1:F:135:ALA:N	2.87	0.43
1:F:359:THR:CB	1:F:360:ARG:HH11	2.32	0.43
1:E:356:VAL:HG11	1:E:402:PHE:CE2	2.53	0.43
1:D:256:TRP:CE2	1:D:258:GLN:HB3	2.54	0.43
1:A:120:ASP:CG	3:A:1436:CIT:H22	2.39	0.43
1:D:325:GLU:HB2	1:D:427:LEU:HD11	2.01	0.43
1:D:373:VAL:CG1	1:D:394:PHE:CE2	2.99	0.43
1:C:149:ARG:NH1	6:C:2131:HOH:O	2.51	0.43
1:C:163:VAL:HG21	1:C:203:LEU:HD11	2.01	0.43
1:E:97:HIS:CD2	6:E:2081:HOH:O	2.72	0.42
1:F:360:ARG:N	1:F:360:ARG:HD3	2.34	0.42
1:C:217:MET:CE	1:C:285:VAL:HG21	2.49	0.42
1:F:96:THR:O	1:F:99:LYS:N	2.51	0.42
1:F:40:GLU:OE2	1:F:269:LYS:HD3	2.19	0.42
1:B:348:THR:HG21	6:B:2254:HOH:O	2.18	0.42
1:A:353:GLU:OE2	1:C:226:ASN:ND2	2.53	0.42
1:A:329:GLU:OE1	1:E:304:ARG:CZ	2.68	0.42
1:E:191:CYS:N	1:E:192:PRO:CD	2.83	0.42
1:A:211:ASN:HB3	6:A:2151:HOH:O	2.18	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:109:MET:SD	1:E:110:SER:N	2.92	0.42
1:C:14:TRP:C	1:C:14:TRP:CD1	2.93	0.42
1:C:195:VAL:HG21	1:C:244:THR:HG21	2.00	0.42
1:D:403:ARG:HH21	1:D:405:HIS:CE1	2.37	0.42
1:D:109:MET:CE	6:D:2097:HOH:O	2.66	0.42
1:E:3:LYS:NZ	6:E:2005:HOH:O	2.52	0.42
1:B:59:HIS:HE1	6:B:2011:HOH:O	2.02	0.42
1:E:210:THR:OG1	1:E:212:SER:OG	2.18	0.42
1:F:75:SER:HB2	1:F:138:ASP:OD1	2.20	0.42
1:C:262:ARG:NH2	6:C:2183:HOH:O	2.53	0.42
1:D:388:CYS:HB2	1:D:405:HIS:CE1	2.55	0.41
1:B:55:VAL:CG1	1:B:301:LEU:HD21	2.50	0.41
1:C:210:THR:HG21	6:C:2066:HOH:O	2.19	0.41
1:D:48:HIS:ND1	1:D:60:LEU:HD23	2.33	0.41
1:E:302:ARG:CD	1:E:325:GLU:OE1	2.66	0.41
1:E:403:ARG:HH21	1:E:405:HIS:CE1	2.32	0.41
1:C:262:ARG:HD3	1:C:266:TYR:OH	2.20	0.41
1:C:355:ILE:CD1	1:C:368:VAL:HG13	2.49	0.41
1:E:1:LEU:HA	6:E:2006:HOH:O	2.20	0.41
1:E:163:VAL:HG21	1:E:203:LEU:HD11	2.02	0.41
1:B:40:GLU:HG3	6:B:2041:HOH:O	2.19	0.41
1:E:79:VAL:HG22	1:E:246:PHE:CE1	2.55	0.41
1:F:131:GLU:HA	1:F:131:GLU:OE1	2.21	0.41
1:F:7:HIS:NE2	1:F:386:ASP:HB2	2.35	0.41
1:A:421:LYS:HG2	1:E:306:VAL:HA	2.03	0.41
1:C:221:LYS:NZ	1:C:226:ASN:ND2	2.68	0.41
1:E:31:PHE:CZ	1:E:48:HIS:HD2	2.34	0.41
1:F:200:LYS:HZ2	1:F:288:ASN:HD21	1.63	0.41
1:F:335:GLU:HG3	1:F:348:THR:HG22	2.03	0.41
1:D:149:ARG:HG2	1:D:165:LEU:HD11	2.01	0.41
1:D:259:SER:HB3	1:D:262:ARG:HB2	2.01	0.41
1:D:71:HIS:HA	1:D:92:TYR:O	2.21	0.41
1:E:145:ASN:HA	1:F:80:GLU:O	2.21	0.41
1:C:422:LEU:C	1:C:422:LEU:HD23	2.41	0.41
1:B:235:HIS:ND1	1:B:398:ILE:CG1	2.83	0.41
1:F:170:ASP:OD2	1:F:173:HIS:CD2	2.73	0.41
1:A:69:GLU:CG	6:A:2030:HOH:O	2.68	0.41
1:C:257:LEU:HG	1:C:278:SER:HA	2.03	0.41
1:A:311:LYS:HE3	1:A:311:LYS:HB3	1.88	0.41
1:F:302:ARG:HD2	1:F:425:PHE:CG	2.56	0.41
1:C:56:HIS:HE1	1:C:428:GLU:OE1	2.04	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1:LEU:H3	1:B:1:LEU:HG	1.82	0.41
1:C:311:LYS:NZ	6:C:2224:HOH:O	2.54	0.41
1:B:136:PHE:CE1	1:B:152:LEU:HD13	2.55	0.41
1:B:206:SER:HB3	1:B:240:TYR:CE1	2.56	0.41
1:B:207:ILE:HD12	1:B:214:LEU:HD13	2.02	0.40
1:D:79:VAL:HG11	1:D:171:LEU:HD21	2.03	0.40
1:E:198:GLY:O	1:E:199:GLU:HB2	2.22	0.40
1:E:7:HIS:ND1	1:E:279:LEU:CD1	2.81	0.40
1:F:400:PHE:HB3	1:F:402:PHE:CE2	2.56	0.40
1:E:202:ILE:HG13	1:E:217:MET:HG3	2.02	0.40
1:B:398:ILE:HD13	1:B:398:ILE:HG21	1.88	0.40
1:D:51:SER:HB3	6:D:2049:HOH:O	2.21	0.40
1:F:63:ALA:O	1:F:64:LEU:HD23	2.22	0.40
1:C:101:GLU:OE2	2:C:1435:SO4:O1	2.40	0.40
1:C:258:GLN:HE22	1:C:274:ASN:ND2	2.20	0.40
1:E:355:ILE:CD1	1:E:368:VAL:CG1	2.99	0.40
1:F:188:GLU:OE1	6:F:2139:HOH:O	2.22	0.40
1:D:367:GLU:OE1	1:D:369:ARG:NH2	2.53	0.40
1:B:84:LYS:HD3	1:B:109:MET:SD	2.62	0.40
1:B:84:LYS:NZ	6:B:2084:HOH:O	2.55	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	430/432 (100%)	414 (96%)	16 (4%)	0	100	100
1	B	430/432 (100%)	412 (96%)	17 (4%)	1 (0%)	52	42
1	C	430/432 (100%)	411 (96%)	18 (4%)	1 (0%)	52	42
1	D	430/432 (100%)	415 (96%)	13 (3%)	2 (0%)	34	21

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	E	430/432 (100%)	412 (96%)	16 (4%)	2 (0%)	34	21
1	F	430/432 (100%)	414 (96%)	13 (3%)	3 (1%)	26	14
All	All	2580/2592 (100%)	2478 (96%)	93 (4%)	9 (0%)	46	35

All (9) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	97	HIS
1	E	97	HIS
1	F	97	HIS
1	B	351	ARG
1	C	351	ARG
1	D	351	ARG
1	E	351	ARG
1	F	304	ARG
1	F	351	ARG

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	387/387 (100%)	350 (90%)	37 (10%)	10	3
1	B	387/387 (100%)	346 (89%)	41 (11%)	8	3
1	C	387/387 (100%)	351 (91%)	36 (9%)	11	4
1	D	387/387 (100%)	345 (89%)	42 (11%)	8	2
1	E	387/387 (100%)	350 (90%)	37 (10%)	10	3
1	F	387/387 (100%)	346 (89%)	41 (11%)	8	3
All	All	2322/2322 (100%)	2088 (90%)	234 (10%)	9	3

All (234) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1	LEU

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Mol	Chain	Res	Type
1	A	60	LEU
1	A	99	LYS
1	A	108	VAL
1	A	114	LEU
1	A	124	VAL
1	A	127	LYS
1	A	171	LEU
1	A	188	GLU
1	A	203	LEU
1	A	208	THR
1	A	210	THR
1	A	211	ASN
1	A	220	LEU
1	A	233	LEU
1	A	244	THR
1	A	257	LEU
1	A	269	LYS
1	A	274	ASN
1	A	279	LEU
1	A	288	ASN
1	A	289	GLU
1	A	290	LEU
1	A	295	VAL
1	A	298	LEU
1	A	303	LYS
1	A	311	LYS
1	A	351	ARG
1	A	354	LEU
1	A	355	ILE
1	A	360	ARG
1	A	375	ASP
1	A	397	SER
1	A	411	ASN
1	A	413	LEU
1	A	414	SER
1	A	415	VAL
1	B	38	LYS
1	B	60	LEU
1	B	79	VAL
1	B	108	VAL
1	B	114	LEU
1	B	124	VAL

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Mol	Chain	Res	Type
1	B	134	HIS
1	B	159	LYS
1	B	186	THR
1	B	195	VAL
1	B	199	GLU
1	B	203	LEU
1	B	211	ASN
1	B	220	LEU
1	B	233	LEU
1	B	244	THR
1	B	257	LEU
1	B	270	ARG
1	B	274	ASN
1	B	279	LEU
1	B	283	LEU
1	B	288	ASN
1	B	289	GLU
1	B	290	LEU
1	B	295	VAL
1	B	298	LEU
1	B	303	LYS
1	B	311	LYS
1	B	318	ASP
1	B	349	LYS
1	B	351	ARG
1	B	354	LEU
1	B	355	ILE
1	B	363	VAL
1	B	374	GLU
1	B	380	ARG
1	B	397	SER
1	B	411	ASN
1	B	415	VAL
1	B	420	VAL
1	B	421	LYS
1	C	1	LEU
1	C	60	LEU
1	C	79	VAL
1	C	97	HIS
1	C	114	LEU
1	C	124	VAL
1	C	127	LYS

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Mol	Chain	Res	Type
1	C	131	GLU
1	C	171	LEU
1	C	186	THR
1	C	196	ARG
1	C	200	LYS
1	C	203	LEU
1	C	226	ASN
1	C	233	LEU
1	C	244	THR
1	C	257	LEU
1	C	274	ASN
1	C	279	LEU
1	C	283	LEU
1	C	290	LEU
1	C	293	LYS
1	C	295	VAL
1	C	298	LEU
1	C	308	GLU
1	C	321	GLU
1	C	351	ARG
1	C	354	LEU
1	C	355	ILE
1	C	397	SER
1	C	411	ASN
1	C	414	SER
1	C	415	VAL
1	C	419	GLN
1	C	420	VAL
1	C	421	LYS
1	D	1	LEU
1	D	38	LYS
1	D	60	LEU
1	D	79	VAL
1	D	98	ASN
1	D	101	GLU
1	D	108	VAL
1	D	114	LEU
1	D	124	VAL
1	D	131	GLU
1	D	142	ASN
1	D	171	LEU
1	D	185	THR

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Mol	Chain	Res	Type
1	D	186	THR
1	D	195	VAL
1	D	203	LEU
1	D	211	ASN
1	D	220	LEU
1	D	229	LYS
1	D	233	LEU
1	D	244	THR
1	D	257	LEU
1	D	274	ASN
1	D	279	LEU
1	D	283	LEU
1	D	289	GLU
1	D	290	LEU
1	D	298	LEU
1	D	303	LYS
1	D	321	GLU
1	D	351	ARG
1	D	354	LEU
1	D	355	ILE
1	D	370	LYS
1	D	372	THR
1	D	375	ASP
1	D	380	ARG
1	D	411	ASN
1	D	413	LEU
1	D	414	SER
1	D	415	VAL
1	D	420	VAL
1	E	60	LEU
1	E	79	VAL
1	E	97	HIS
1	E	101	GLU
1	E	114	LEU
1	E	124	VAL
1	E	159	LYS
1	E	186	THR
1	E	203	LEU
1	E	208	THR
1	E	210	THR
1	E	211	ASN
1	E	220	LEU

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Mol	Chain	Res	Type
1	E	230	ARG
1	E	233	LEU
1	E	244	THR
1	E	257	LEU
1	E	274	ASN
1	E	279	LEU
1	E	283	LEU
1	E	289	GLU
1	E	290	LEU
1	E	295	VAL
1	E	298	LEU
1	E	303	LYS
1	E	304	ARG
1	E	321	GLU
1	E	352	ASP
1	E	354	LEU
1	E	355	ILE
1	E	411	ASN
1	E	413	LEU
1	E	414	SER
1	E	415	VAL
1	E	419	GLN
1	E	420	VAL
1	E	421	LYS
1	F	1	LEU
1	F	60	LEU
1	F	79	VAL
1	F	97	HIS
1	F	99	LYS
1	F	108	VAL
1	F	114	LEU
1	F	124	VAL
1	F	171	LEU
1	F	185	THR
1	F	186	THR
1	F	188	GLU
1	F	195	VAL
1	F	199	GLU
1	F	203	LEU
1	F	208	THR
1	F	211	ASN
1	F	220	LEU

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Mol	Chain	Res	Type
1	F	224	LYS
1	F	229	LYS
1	F	233	LEU
1	F	244	THR
1	F	257	LEU
1	F	274	ASN
1	F	279	LEU
1	F	288	ASN
1	F	289	GLU
1	F	290	LEU
1	F	295	VAL
1	F	298	LEU
1	F	354	LEU
1	F	355	ILE
1	F	360	ARG
1	F	370	LYS
1	F	375	ASP
1	F	380	ARG
1	F	382	ARG
1	F	411	ASN
1	F	413	LEU
1	F	415	VAL
1	F	420	VAL

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (70) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	19	ASN
1	A	29	HIS
1	A	56	HIS
1	A	71	HIS
1	A	134	HIS
1	A	173	HIS
1	A	211	ASN
1	A	243	GLN
1	A	274	ASN
1	A	405	HIS
1	A	411	ASN
1	B	7	HIS
1	B	19	ASN
1	B	29	HIS
1	B	56	HIS

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Mol	Chain	Res	Type
1	B	59	HIS
1	B	173	HIS
1	B	243	GLN
1	B	274	ASN
1	B	405	HIS
1	B	411	ASN
1	C	19	ASN
1	C	29	HIS
1	C	56	HIS
1	C	59	HIS
1	C	134	HIS
1	C	142	ASN
1	C	173	HIS
1	C	211	ASN
1	C	243	GLN
1	C	274	ASN
1	C	405	HIS
1	C	411	ASN
1	D	7	HIS
1	D	19	ASN
1	D	29	HIS
1	D	56	HIS
1	D	59	HIS
1	D	71	HIS
1	D	98	ASN
1	D	142	ASN
1	D	235	HIS
1	D	243	GLN
1	D	274	ASN
1	D	405	HIS
1	D	411	ASN
1	E	19	ASN
1	E	29	HIS
1	E	48	HIS
1	E	56	HIS
1	E	59	HIS
1	E	173	HIS
1	E	235	HIS
1	E	243	GLN
1	E	274	ASN
1	E	405	HIS
1	E	411	ASN

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Mol	Chain	Res	Type
1	F	7	HIS
1	F	19	ASN
1	F	56	HIS
1	F	59	HIS
1	F	71	HIS
1	F	142	ASN
1	F	173	HIS
1	F	235	HIS
1	F	243	GLN
1	F	274	ASN
1	F	288	ASN
1	F	405	HIS
1	F	411	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

Of 22 ligands modelled in this entry, 1 is monoatomic - leaving 21 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	$\# Z > 2$
2	SO4	A	1433	-	4,4,4	1.00	0	6,6,6	0.48	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	SO4	A	1434	-	4,4,4	0.29	0	6,6,6	0.31	0
2	SO4	A	1435	-	4,4,4	0.29	0	6,6,6	0.39	0
3	CIT	A	1436	5	3,12,12	1.61	1 (33%)	3,17,17	3.05	1 (33%)
4	GOL	A	1437	-	5,5,5	0.46	0	5,5,5	0.72	0
2	SO4	B	1433	-	4,4,4	0.71	0	6,6,6	0.45	0
2	SO4	B	1434	-	4,4,4	0.13	0	6,6,6	0.23	0
2	SO4	B	1435	-	4,4,4	0.28	0	6,6,6	0.26	0
4	GOL	B	1436	-	5,5,5	0.41	0	5,5,5	0.38	0
2	SO4	B	1437	-	4,4,4	0.54	0	6,6,6	0.77	0
2	SO4	C	1433	-	4,4,4	0.43	0	6,6,6	0.54	0
2	SO4	C	1434	-	4,4,4	0.20	0	6,6,6	0.40	0
2	SO4	C	1435	-	4,4,4	0.23	0	6,6,6	0.58	0
4	GOL	C	1436	1	5,5,5	0.70	0	5,5,5	1.14	1 (20%)
4	GOL	D	1433	-	5,5,5	0.42	0	5,5,5	0.44	0
2	SO4	E	1433	-	4,4,4	0.33	0	6,6,6	0.23	0
4	GOL	E	1434	-	5,5,5	0.67	0	5,5,5	0.68	0
2	SO4	F	1433	-	4,4,4	0.16	0	6,6,6	0.56	0
2	SO4	F	1434	-	4,4,4	0.45	0	6,6,6	0.49	0
2	SO4	F	1435	-	4,4,4	0.35	0	6,6,6	0.25	0
4	GOL	F	1436	-	5,5,5	0.38	0	5,5,5	0.56	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. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	SO4	A	1433	-	-	0/0/0/0	0/0/0/0
2	SO4	A	1434	-	-	0/0/0/0	0/0/0/0
2	SO4	A	1435	-	-	0/0/0/0	0/0/0/0
3	CIT	A	1436	5	-	0/6/16/16	0/0/0/0
4	GOL	A	1437	-	-	0/4/4/4	0/0/0/0
2	SO4	B	1433	-	-	0/0/0/0	0/0/0/0
2	SO4	B	1434	-	-	0/0/0/0	0/0/0/0
2	SO4	B	1435	-	-	0/0/0/0	0/0/0/0
4	GOL	B	1436	-	-	0/4/4/4	0/0/0/0
2	SO4	B	1437	-	-	0/0/0/0	0/0/0/0
2	SO4	C	1433	-	-	0/0/0/0	0/0/0/0
2	SO4	C	1434	-	-	0/0/0/0	0/0/0/0
2	SO4	C	1435	-	-	0/0/0/0	0/0/0/0
4	GOL	C	1436	1	-	0/4/4/4	0/0/0/0
4	GOL	D	1433	-	-	0/4/4/4	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	SO4	E	1433	-	-	0/0/0/0	0/0/0/0
4	GOL	E	1434	-	-	0/4/4/4	0/0/0/0
2	SO4	F	1433	-	-	0/0/0/0	0/0/0/0
2	SO4	F	1434	-	-	0/0/0/0	0/0/0/0
2	SO4	F	1435	-	-	0/0/0/0	0/0/0/0
4	GOL	F	1436	-	-	0/4/4/4	0/0/0/0

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	1436	CIT	C2-C3	-2.23	1.51	1.54

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	C	1436	GOL	C3-C2-C1	2.10	119.36	111.12
3	A	1436	CIT	C4-C3-C2	4.75	121.16	109.81

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

5 monomers are involved in 11 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	1434	SO4	1	0
3	A	1436	CIT	1	0
2	B	1435	SO4	3	0
2	C	1435	SO4	2	0
2	F	1433	SO4	4	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	432/432 (100%)	0.18	19 (4%)	38	41	13, 24, 41, 50	4 (0%)
1	B	432/432 (100%)	0.24	25 (5%)	26	29	14, 24, 43, 51	6 (1%)
1	C	432/432 (100%)	0.32	33 (7%)	17	18	13, 24, 43, 51	8 (1%)
1	D	432/432 (100%)	0.28	29 (6%)	21	23	14, 24, 43, 52	8 (1%)
1	E	432/432 (100%)	0.32	32 (7%)	17	19	13, 24, 43, 54	9 (2%)
1	F	432/432 (100%)	0.37	29 (6%)	21	23	13, 25, 43, 51	10 (2%)
All	All	2592/2592 (100%)	0.28	167 (6%)	23	25	13, 24, 43, 54	45 (1%)

All (167) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	E	97	HIS	13.2
1	C	97	HIS	11.8
1	B	97	HIS	11.6
1	E	98	ASN	11.5
1	D	98	ASN	9.8
1	D	97	HIS	8.0
1	E	99	LYS	7.9
1	B	96	THR	5.8
1	C	96	THR	5.8
1	F	97	HIS	5.7
1	F	134	HIS	5.5
1	D	99	LYS	5.3
1	B	98	ASN	5.1
1	E	95	PRO	5.0
1	F	198	GLY	4.9
1	E	134	HIS	4.9
1	E	159	LYS	4.7
1	D	351	ARG	4.7
1	F	222	GLU	4.6

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Mol	Chain	Res	Type	RSRZ
1	A	223	GLY	4.5
1	C	419	GLN	4.5
1	C	99	LYS	4.5
1	F	419	GLN	4.4
1	D	134	HIS	4.4
1	C	131	GLU	4.4
1	A	222	GLU	4.3
1	C	134	HIS	4.3
1	D	198	GLY	4.3
1	B	99	LYS	4.2
1	D	287	ASN	4.2
1	E	351	ARG	4.2
1	B	134	HIS	4.1
1	A	159	LYS	4.1
1	F	159	LYS	4.1
1	C	351	ARG	4.1
1	F	131	GLU	4.1
1	E	222	GLU	4.1
1	A	287	ASN	4.0
1	F	157	ASP	3.9
1	C	418	ASN	3.9
1	A	145	ASN	3.8
1	D	132	GLY	3.8
1	C	222	GLU	3.8
1	A	134	HIS	3.8
1	E	96	THR	3.7
1	A	419	GLN	3.7
1	F	98	ASN	3.6
1	F	287	ASN	3.6
1	B	419	GLN	3.5
1	C	159	LYS	3.4
1	B	350	SER	3.4
1	D	352	ASP	3.4
1	E	374	GLU	3.4
1	F	184	GLU	3.4
1	D	374	GLU	3.3
1	D	145	ASN	3.3
1	B	375	ASP	3.3
1	E	352	ASP	3.3
1	D	157	ASP	3.2
1	E	184	GLU	3.2
1	A	184	GLU	3.2

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Mol	Chain	Res	Type	RSRZ
1	F	99	LYS	3.2
1	B	208	THR	3.1
1	C	98	ASN	3.1
1	C	350	SER	3.1
1	B	159	LYS	3.1
1	D	184	GLU	3.1
1	F	376	GLU	3.1
1	E	133	THR	3.0
1	B	418	ASN	3.0
1	F	351	ARG	2.9
1	A	198	GLY	2.9
1	F	418	ASN	2.9
1	A	224	LYS	2.9
1	B	133	THR	2.9
1	C	421	LYS	2.9
1	C	184	GLU	2.9
1	D	289	GLU	2.9
1	D	221	LYS	2.9
1	F	350	SER	2.8
1	D	304	ARG	2.8
1	F	377	ALA	2.8
1	E	157	ASP	2.8
1	D	159	LYS	2.8
1	C	145	ASN	2.8
1	A	221	LYS	2.8
1	A	169	ASP	2.7
1	F	352	ASP	2.7
1	C	377	ALA	2.7
1	D	96	THR	2.7
1	E	350	SER	2.7
1	F	187	LYS	2.7
1	F	158	GLU	2.7
1	C	304	ARG	2.7
1	C	287	ASN	2.6
1	F	160	ILE	2.6
1	E	419	GLN	2.6
1	B	158	GLU	2.6
1	B	131	GLU	2.6
1	C	158	GLU	2.6
1	D	158	GLU	2.6
1	C	100	GLY	2.5
1	C	198	GLY	2.5

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Mol	Chain	Res	Type	RSRZ
1	A	187	LYS	2.5
1	E	221	LYS	2.5
1	F	156	LYS	2.5
1	E	156	LYS	2.5
1	A	146	GLY	2.5
1	C	352	ASP	2.5
1	C	129	PRO	2.5
1	D	95	PRO	2.5
1	B	287	ASN	2.4
1	F	169	ASP	2.4
1	B	376	GLU	2.4
1	A	303	LYS	2.4
1	F	289	GLU	2.4
1	C	133	THR	2.4
1	D	288	ASN	2.4
1	E	185	THR	2.4
1	B	187	LYS	2.3
1	E	101	GLU	2.3
1	B	351	ARG	2.3
1	B	199	GLU	2.3
1	E	100	GLY	2.3
1	E	129	PRO	2.3
1	C	223	GLY	2.3
1	E	254	ILE	2.3
1	A	157	ASP	2.3
1	B	157	ASP	2.3
1	D	135	ALA	2.3
1	F	378	THR	2.3
1	C	255	GLY	2.3
1	F	100	GLY	2.3
1	C	221	LYS	2.3
1	A	158	GLU	2.3
1	C	95	PRO	2.3
1	E	158	GLU	2.3
1	E	288	ASN	2.2
1	E	130	GLU	2.2
1	D	350	SER	2.2
1	E	372	THR	2.2
1	D	69	GLU	2.2
1	E	131	GLU	2.2
1	D	169	ASP	2.2
1	D	375	ASP	2.2

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Mol	Chain	Res	Type	RSRZ
1	B	184	GLU	2.2
1	F	208	THR	2.2
1	A	288	ASN	2.1
1	B	156	LYS	2.1
1	B	374	GLU	2.1
1	B	352	ASP	2.1
1	F	155	GLY	2.1
1	C	241	ALA	2.1
1	E	242	ALA	2.1
1	D	418	ASN	2.1
1	E	127	LYS	2.1
1	B	100	GLY	2.1
1	F	221	LYS	2.0
1	A	132	GLY	2.0
1	C	7	HIS	2.0
1	C	378	THR	2.0
1	C	160	ILE	2.0
1	E	132	GLY	2.0
1	C	186	THR	2.0
1	D	185	THR	2.0
1	D	303	LYS	2.0
1	E	289	GLU	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 carbohydrates 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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. 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	LLDF	B-factors(\AA^2)	Q<0.9
2	SO4	A	1435	5/5	0.66	0.28	8.31	57,63,66,67	0
4	GOL	C	1436	6/6	0.90	0.18	3.98	18,30,34,41	0
2	SO4	A	1433	5/5	0.80	0.26	3.75	32,39,47,49	0
4	GOL	A	1437	6/6	0.90	0.15	3.38	22,35,36,39	0
2	SO4	B	1435	5/5	0.88	0.33	1.84	54,55,56,58	0
4	GOL	D	1433	6/6	0.93	0.14	1.67	26,37,37,42	0
4	GOL	F	1436	6/6	0.94	0.16	1.59	23,34,39,40	0
2	SO4	F	1434	5/5	0.97	0.12	0.93	31,32,33,34	0
3	CIT	A	1436	13/13	0.80	0.16	0.56	49,50,51,54	0
2	SO4	C	1435	5/5	0.91	0.19	0.29	51,52,53,53	0
2	SO4	A	1434	5/5	0.94	0.13	0.23	60,63,63,64	0
4	GOL	B	1436	6/6	0.95	0.11	0.11	30,36,37,37	0
4	GOL	E	1434	6/6	0.95	0.11	0.10	19,29,33,34	0
2	SO4	B	1437	5/5	0.99	0.06	-1.40	29,34,34,36	0
2	SO4	B	1433	5/5	0.99	0.06	-1.55	24,25,25,27	0
5	NA	A	1438	1/1	0.97	0.08	-1.75	46,46,46,46	0
2	SO4	C	1433	5/5	0.98	0.04	-3.55	29,31,32,35	0
2	SO4	C	1434	5/5	0.93	0.22	-	63,64,65,66	0
2	SO4	F	1435	5/5	0.98	0.08	-	30,34,37,37	0
2	SO4	E	1433	5/5	0.97	0.09	-	36,37,40,42	0
2	SO4	F	1433	5/5	0.91	0.16	-	52,53,57,57	0
2	SO4	B	1434	5/5	0.86	0.32	-	75,75,76,76	0

6.5 Other polymers ⓘ

There are no such residues in this entry.