



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 01:13 PM UTC

PDB ID : 1UYP / pdb_00001uyp
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.

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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

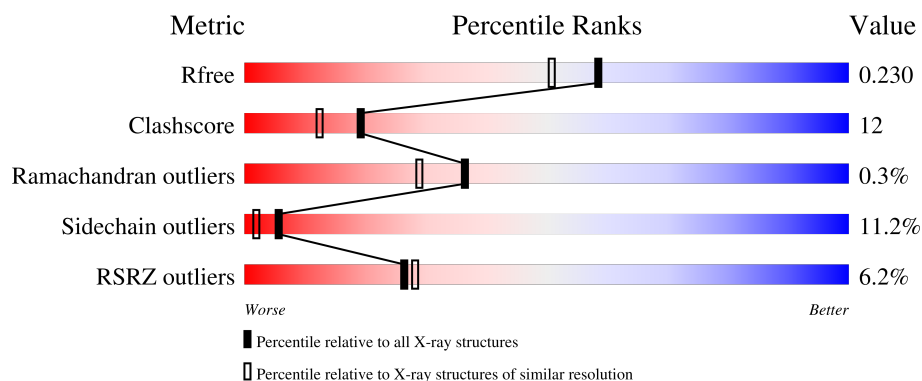
1 Overall quality at a glance

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	432	3% 78% 17% 5%
1	B	432	6% 73% 21% 5%
1	C	432	7% 75% 19% 5%
1	D	432	6% 74% 21% 5%
1	E	432	7% 73% 22% 5%

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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	B	1435	-	-	X	-
2	SO4	C	1435	-	-	X	-
2	SO4	F	1433	-	-	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:

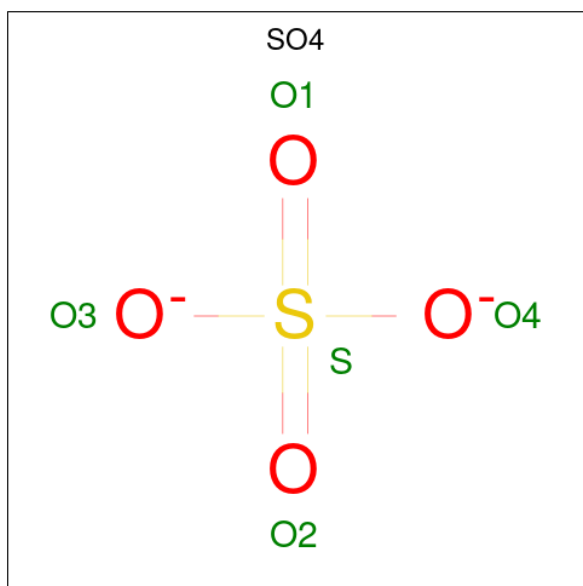
Chain	Residue	Modelled	Actual	Comment	Reference
A	1	LEU	MET	conflict	UNP O33833
B	1	LEU	MET	conflict	UNP O33833
C	1	LEU	MET	conflict	UNP O33833
D	1	LEU	MET	conflict	UNP O33833
E	1	LEU	MET	conflict	UNP O33833
F	1	LEU	MET	conflict	UNP O33833
A	108	VAL	ALA	conflict	UNP O33833
B	108	VAL	ALA	conflict	UNP 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 (CCD ID: SO4) (formula: O₄S).



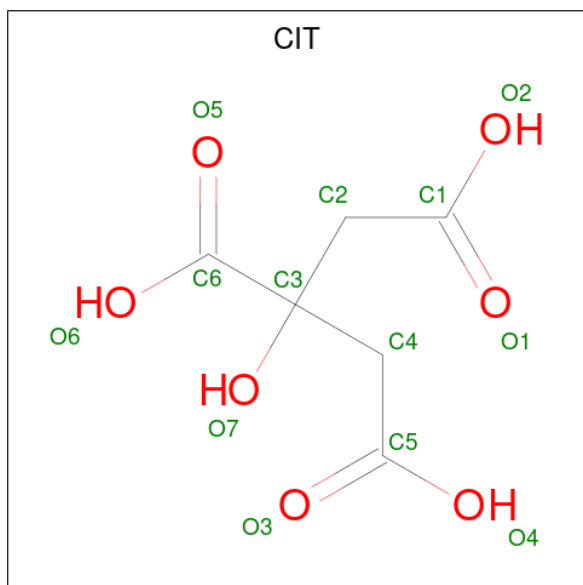
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	O	S	0	0
			5	4	1		
2	A	1	Total	O	S	0	0
			5	4	1		
2	A	1	Total	O	S	0	0
			5	4	1		
2	B	1	Total	O	S	0	0
			5	4	1		
2	B	1	Total	O	S	0	0
			5	4	1		
2	B	1	Total	O	S	0	0
			5	4	1		
2	B	1	Total	O	S	0	0
			5	4	1		
2	C	1	Total	O	S	0	0
			5	4	1		
2	C	1	Total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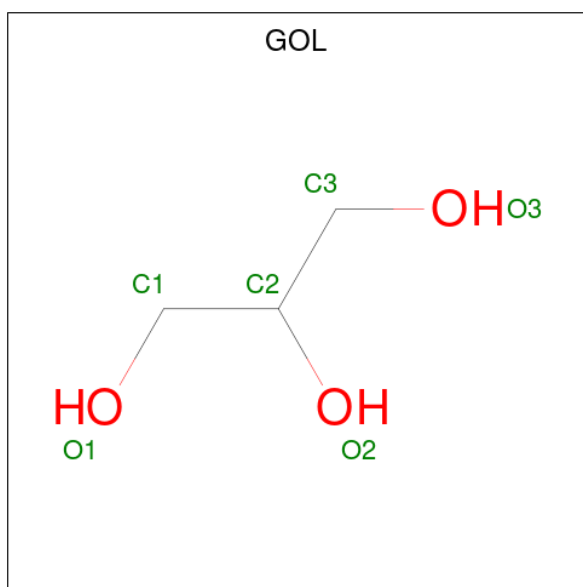
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	F	1	Total	O	S	0	0
			5	4	1		
2	F	1	Total	O	S	0	0
			5	4	1		
2	F	1	Total	O	S	0	0
			5	4	1		

- Molecule 3 is CITRIC ACID (CCD ID: 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 (CCD ID: 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 (CCD ID: 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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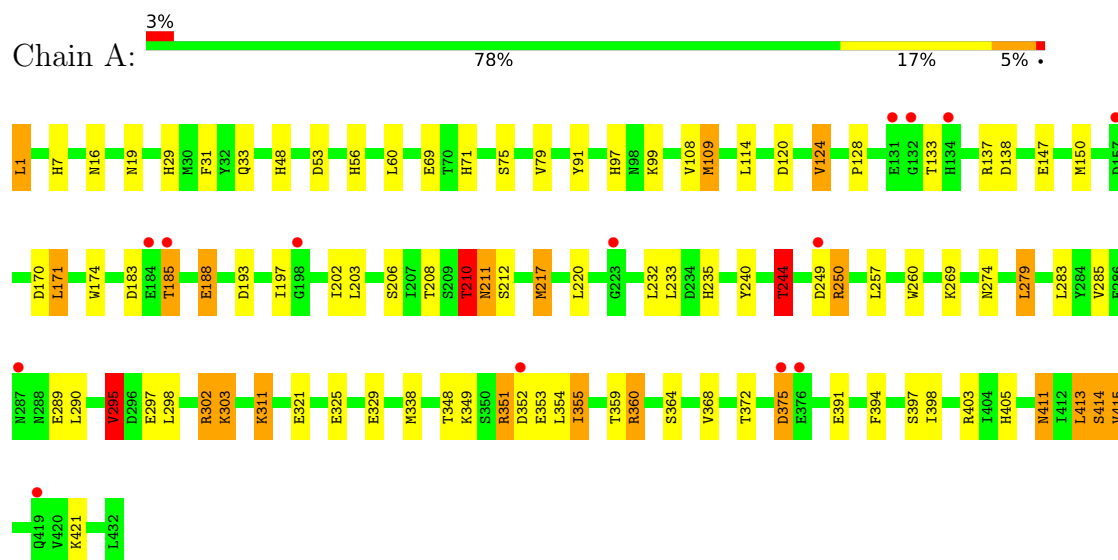
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	C	298	Total 298	O 298	0	0
6	D	286	Total 286	O 286	0	0
6	E	294	Total 294	O 294	0	0
6	F	277	Total 277	O 277	0	0

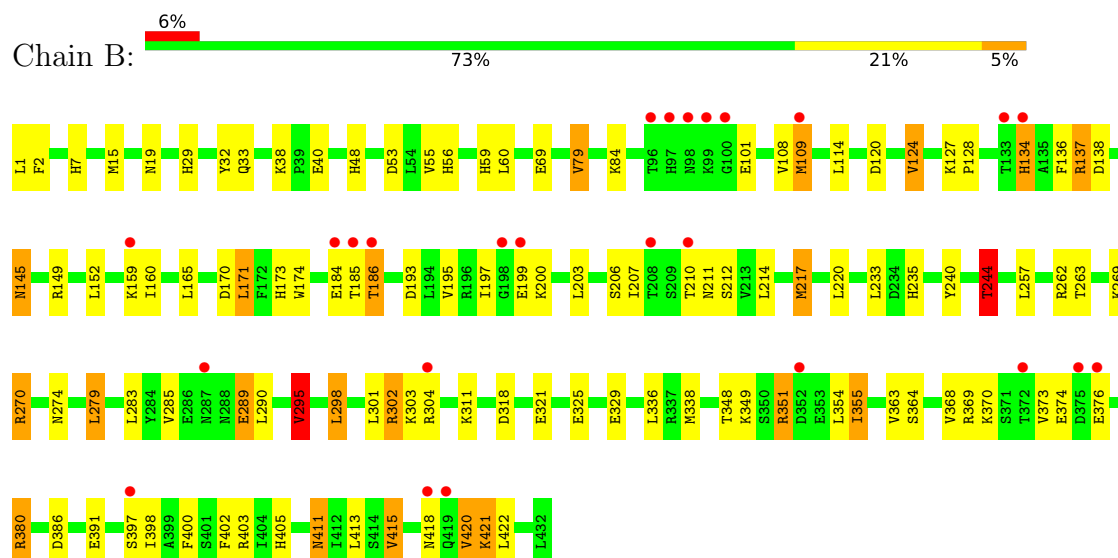
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

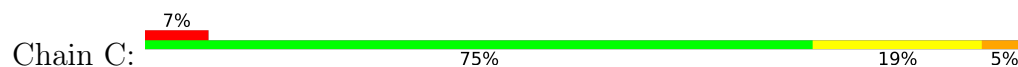
• Molecule 1: BETA-FRUCTOSIDASE

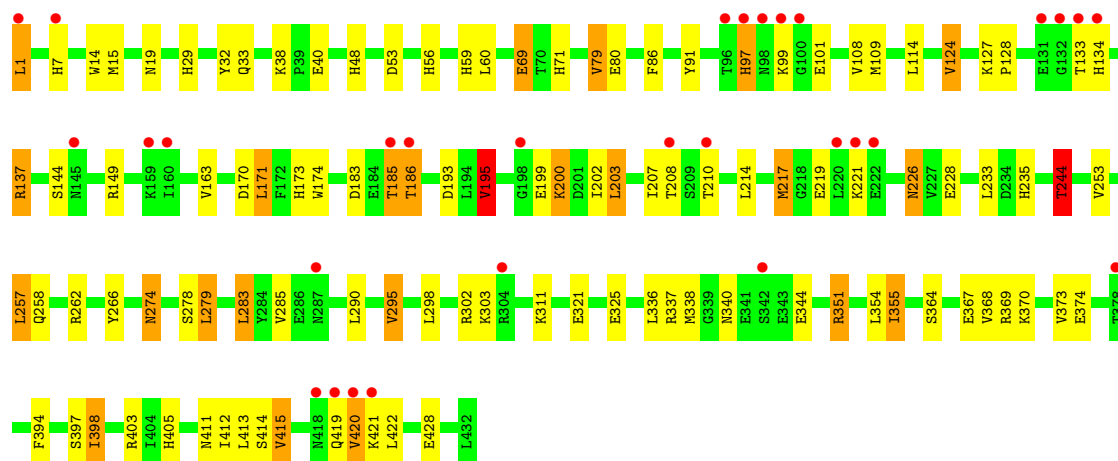


• Molecule 1: BETA-FRUCTOSIDASE

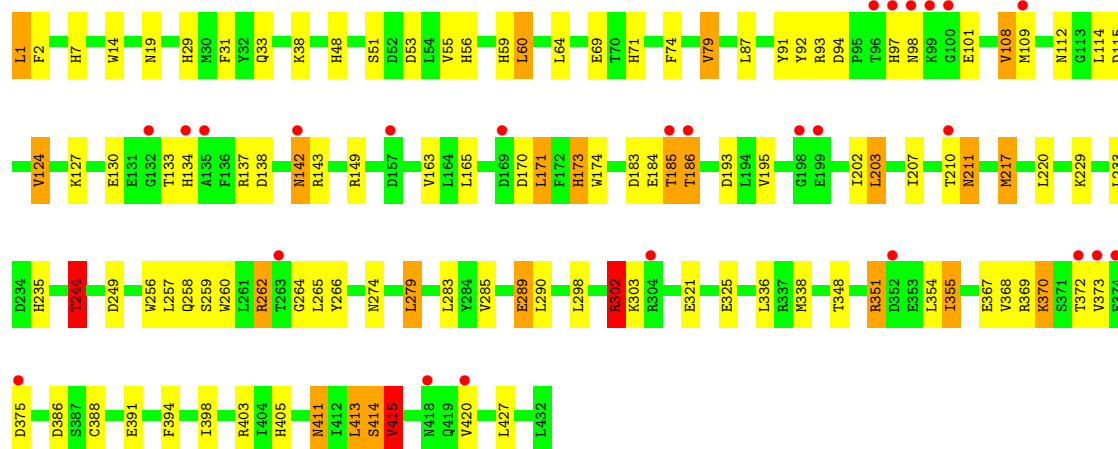
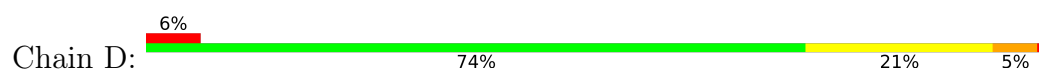


• Molecule 1: BETA-FRUCTOSIDASE

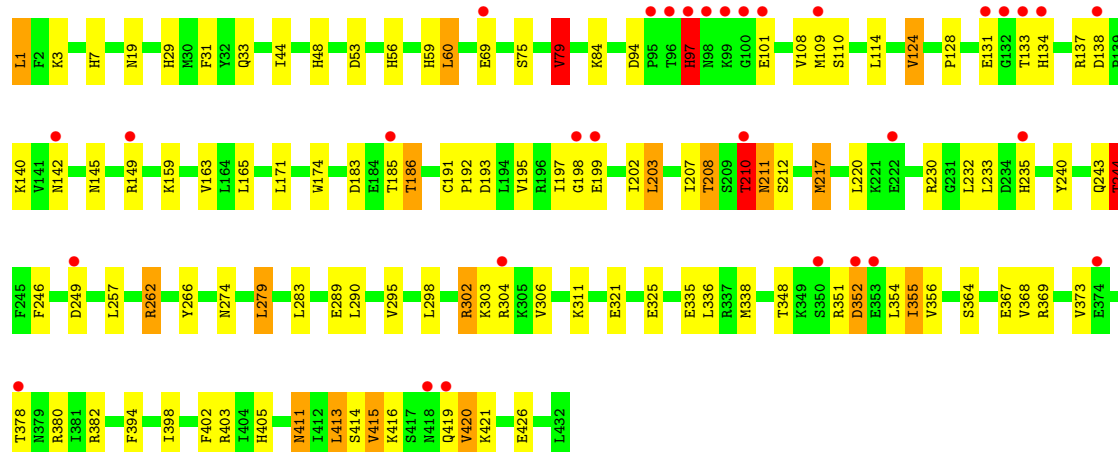
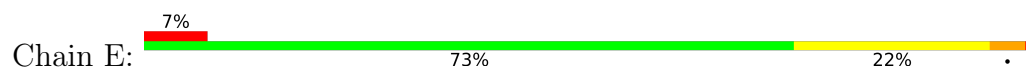




• Molecule 1: BETA-FRUCTOSIDASE

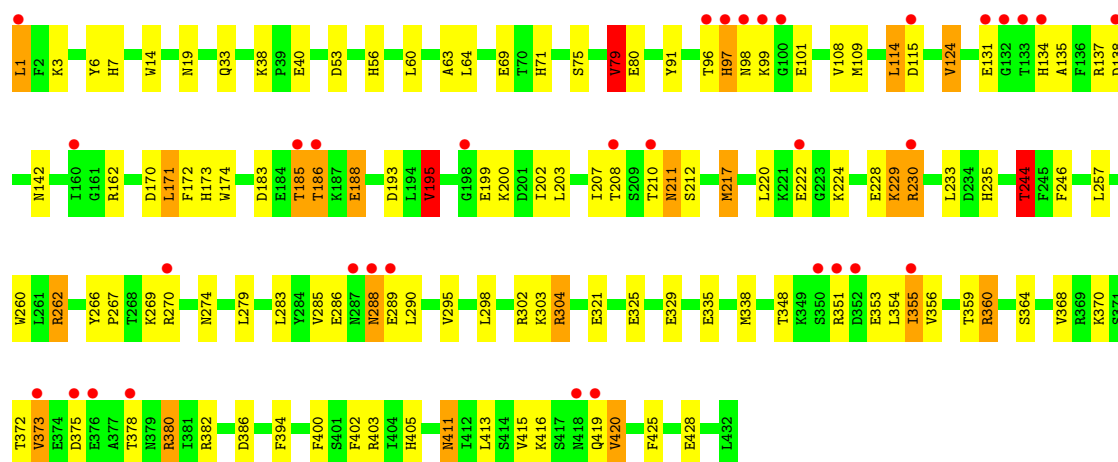


• Molecule 1: BETA-FRUCTOSIDASE



• Molecule 1: BETA-FRUCTOSIDASE

Chain F:  8% 71% 23% 5%



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 – 1.90 128.44 – 1.90	Depositor EDS
% Data completeness (in resolution range)	99.1 (129.10-1.90) 99.1 (128.44-1.90)	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 (5.02%)	wwPDB-VP
Wilson B-factor (Å ²)	21.2	Xtriage
Anisotropy	0.317	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.38 , 49.3	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	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, 0.333 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: NA, SO4, CIT, GOL

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	0.96	5/3611 (0.1%)	1.05	8/4886 (0.2%)
1	B	0.92	3/3611 (0.1%)	1.01	7/4886 (0.1%)
1	C	0.92	2/3611 (0.1%)	1.02	10/4886 (0.2%)
1	D	0.93	4/3611 (0.1%)	1.04	9/4886 (0.2%)
1	E	0.92	2/3611 (0.1%)	1.01	10/4886 (0.2%)
1	F	0.92	2/3611 (0.1%)	1.03	12/4886 (0.2%)
All	All	0.93	18/21666 (0.1%)	1.03	56/29316 (0.2%)

All (18) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	338	MET	SD-CE	-11.41	1.51	1.79
1	C	217	MET	SD-CE	-10.62	1.53	1.79
1	A	109	MET	SD-CE	9.60	2.03	1.79
1	F	217	MET	SD-CE	-8.52	1.58	1.79
1	D	217	MET	SD-CE	-8.28	1.58	1.79
1	B	338	MET	SD-CE	-8.02	1.59	1.79
1	A	217	MET	SD-CE	-7.73	1.60	1.79
1	E	217	MET	SD-CE	-7.08	1.61	1.79
1	E	338	MET	SD-CE	-6.13	1.64	1.79
1	F	338	MET	SD-CE	-6.02	1.64	1.79
1	A	244	THR	CB-CG2	-5.83	1.33	1.52
1	A	338	MET	SD-CE	-5.48	1.65	1.79
1	A	150	MET	SD-CE	-5.43	1.66	1.79
1	D	74	PHE	C-O	-5.27	1.18	1.23
1	D	262	ARG	CD-NE	-5.25	1.38	1.46
1	B	109	MET	SD-CE	5.14	1.92	1.79
1	C	338	MET	SD-CE	-5.12	1.66	1.79
1	B	217	MET	SD-CE	-5.03	1.67	1.79

All (56) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	262	ARG	NE-CZ-NH2	-9.14	110.97	119.20
1	D	137	ARG	N-CA-C	8.53	121.06	108.60
1	D	415	VAL	CB-CA-C	-8.20	97.87	110.50
1	F	38	LYS	N-CA-CB	-8.15	99.44	110.77
1	B	145	ASN	CB-CA-C	-8.06	100.03	111.80
1	A	210	THR	N-CA-CB	-7.65	100.33	110.88
1	C	244	THR	N-CA-CB	-7.60	98.69	110.85
1	C	415	VAL	CB-CA-C	-7.01	99.70	110.50
1	F	38	LYS	CA-CB-CG	6.71	127.53	114.10
1	D	262	ARG	CG-CD-NE	-6.70	97.26	112.00
1	F	262	ARG	NE-CZ-NH2	-6.67	113.20	119.20
1	C	137	ARG	N-CA-C	6.66	118.98	108.79
1	A	415	VAL	CB-CA-C	-6.66	100.25	110.50
1	F	244	THR	N-CA-CB	-6.61	100.27	110.85
1	D	244	THR	N-CA-CB	-6.57	100.34	110.85
1	E	415	VAL	CB-CA-C	-6.36	99.71	110.71
1	B	420	VAL	CB-CA-C	-6.33	102.34	111.34
1	B	244	THR	N-CA-CB	-6.24	100.86	110.85
1	E	420	VAL	CB-CA-C	-6.17	101.88	111.26
1	E	210	THR	OG1-CB-CG2	-6.15	97.01	109.30
1	C	79	VAL	N-CA-CB	-6.13	101.02	112.36
1	A	137	ARG	N-CA-C	6.13	118.17	108.79
1	D	302	ARG	NE-CZ-NH1	6.05	127.55	121.50
1	B	137	ARG	N-CA-C	6.03	118.01	108.79
1	E	244	THR	N-CA-CB	-6.03	101.21	110.85
1	B	295	VAL	N-CA-CB	-5.98	100.08	110.13
1	C	420	VAL	CB-CA-C	-5.96	102.21	111.26
1	E	137	ARG	N-CA-C	5.93	118.08	109.07
1	C	195	VAL	N-CA-CB	-5.82	102.67	112.44
1	E	262	ARG	NE-CZ-NH2	-5.82	113.97	119.20
1	F	420	VAL	N-CA-CB	5.79	118.19	110.26
1	E	302	ARG	CB-CG-CD	5.72	124.46	111.30
1	A	295	VAL	CB-CA-C	5.69	120.59	111.32
1	C	344	GLU	CB-CA-C	-5.64	97.92	109.94
1	F	137	ARG	N-CA-C	5.54	117.26	108.79
1	A	250	ARG	NE-CZ-NH1	-5.52	115.98	121.50
1	F	114	LEU	CA-C-N	-5.47	114.09	122.62
1	F	114	LEU	C-N-CA	-5.47	114.09	122.62
1	D	302	ARG	CB-CG-CD	5.47	123.87	111.30
1	E	171	LEU	N-CA-CB	-5.45	108.65	114.10
1	A	303	LYS	CB-CA-C	5.43	117.82	109.03
1	A	250	ARG	NE-CZ-NH2	5.41	124.07	119.20
1	B	79	VAL	N-CA-CB	-5.39	100.95	112.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	79	VAL	N-CA-CB	-5.38	102.41	112.36
1	D	302	ARG	NE-CZ-NH2	-5.34	114.39	119.20
1	F	79	VAL	N-CA-CB	-5.33	102.50	112.36
1	D	94	ASP	CB-CA-C	-5.32	100.14	109.61
1	F	195	VAL	N-CA-CB	-5.27	103.58	112.44
1	E	94	ASP	CB-CA-C	-5.24	100.28	109.61
1	F	420	VAL	CB-CA-C	-5.18	103.99	111.34
1	C	38	LYS	CA-CB-CG	5.15	124.39	114.10
1	C	295	VAL	CB-CA-C	5.14	119.70	111.32
1	A	16	ASN	N-CA-CB	5.07	116.30	111.59
1	F	230	ARG	N-CA-CB	-5.05	101.85	111.00
1	B	415	VAL	CB-CA-C	-5.01	102.78	110.50
1	C	420	VAL	N-CA-CB	5.01	117.94	110.13

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3520	0	3413	64	0
1	B	3520	0	3413	73	0
1	C	3520	0	3413	84	0
1	D	3520	0	3413	79	0
1	E	3520	0	3413	100	0
1	F	3520	0	3413	98	0
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	1	0
4	D	6	0	8	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
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	31	0
6	F	277	0	0	30	0
All	All	22996	0	20531	489	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 (489) 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:7:HIS:CG	6:F:2010:HOH:O	2.12	1.03
1:E:235:HIS:ND1	1:E:398:ILE:HD11	1.73	1.02
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
1:F:7:HIS:CD2	6:F:2010:HOH:O	2.22	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:C:33:GLN:OE1	4:C:1436:GOL:O2	1.96	0.83
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:115:ASP:HB2	6:F:2101:HOH:O	1.80	0.80
1:F:142:ASN:HB3	6:F:2122:HOH:O	1.81	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:F:202:ILE:HD11	1:F:217:MET:HE3	1.67	0.76
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:C:373:VAL:HG11	1:C:394:PHE:CE2	2.22	0.74
1:D:373:VAL:HG11	1:D:394:PHE:CE2	2.23	0.74
1:F:7:HIS:ND1	6:F:2010:HOH:O	1.96	0.74
1:E:53:ASP:OD2	1:E:56:HIS:HD2	1.71	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:C:69:GLU:CD	1:C:69:GLU:H	1.95	0.72
1:E:348:THR:HG21	6:E:2238:HOH:O	1.89	0.72
1:A:302:ARG:HD3	1:A:325:GLU:OE1	1.88	0.72
1:C:134:HIS:CE1	6:C:2119:HOH:O	2.41	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:F:200:LYS:HZ1	1:F:288:ASN:HD21	1.39	0.70
1:E:249:ASP:HB2	6:E:2178:HOH:O	1.90	0.69
1:C:217:MET:HE1	1:C:285:VAL:CG2	2.23	0.69
1:A:138:ASP:OD2	6:A:2114:HOH:O	2.10	0.69
1:B:418:ASN:HA	6:B:2303:HOH:O	1.92	0.69
1:E:138:ASP:HB3	6:E:2067:HOH:O	1.92	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:A:235:HIS:ND1	1:A:398:ILE:HD11	2.08	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:D:235:HIS:CE1	1:D:398:ILE:HD11	2.27	0.68
1:A:349:LYS:NZ	1:A:375:ASP:OD2	2.19	0.68
1:C:208:THR:HB	6:C:2154:HOH:O	1.92	0.67
1:C:235:HIS:ND1	1:C:398:ILE:HD11	2.08	0.67
1:D:134:HIS:HB2	6:D:2060:HOH:O	1.94	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:B:200:LYS:HD3	1:B:217:MET:HE2	1.76	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:C:1:LEU:HD13	6:C:2278:HOH:O	1.93	0.66
1:F:1:LEU:N	6:F:2002:HOH:O	2.27	0.66
1:A:413:LEU:HD12	1:A:414:SER:N	2.10	0.66
1:B:19:ASN:HD21	1:B:33:GLN:HE21	1.42	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:C:186:THR:CG2	1:C:207:ILE:HG23	2.27	0.65
1:E:31:PHE:CZ	1:E:48:HIS:CD2	2.84	0.65
1:F:359:THR:OG1	1:F:360:ARG:HD3	1.96	0.65
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:F:6:TYR:CE1	1:F:7:HIS:HE1	2.15	0.64
1:C:217:MET:HE1	1:C:285:VAL:HG22	1.80	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:84:LYS:NZ	6:E:2073:HOH:O	2.31	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:7:HIS:CE1	1:C:279:LEU:HD13	2.34	0.63
1:C:53:ASP:OD2	1:C:56:HIS:HD2	1.82	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:F:69:GLU:CD	1:F:69:GLU:H	2.08	0.62
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:A:403:ARG:HH21	1:A:405:HIS:HE1	1.49	0.60
1:C:7:HIS:ND1	1:C:279:LEU:HD13	2.16	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:B:270:ARG:H	1:B:270:ARG:HD2	1.67	0.60
1:A:217:MET:HE1	1:A:285:VAL:HG22	1.84	0.60
1:A:359:THR:OG1	1:A:360:ARG:HD3	2.02	0.59
1:D:112:ASN:ND2	1:D:115:ASP:OD2	2.23	0.59
1:E:131:GLU:OE1	1:E:131:GLU:HA	2.02	0.59
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:D:264:GLY:C	6:D:2177:HOH:O	2.45	0.59
1:E:364:SER:OG	1:E:405:HIS:HD2	1.86	0.59
1:E:367:GLU:OE1	1:E:369:ARG:NH2	2.36	0.58
1:C:364:SER:OG	1:C:405:HIS:HD2	1.86	0.58
1:D:149:ARG:HG3	1:D:165:LEU:HD11	1.84	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:C:202:ILE:HD11	1:C:217:MET:HE3	1.85	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:D:217:MET:HE1	1:D:285:VAL:HG22	1.86	0.57
1:E:149:ARG:HG2	1:E:165:LEU:HD11	1.86	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:D:55:VAL:C	6:D:2049:HOH:O	2.48	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:D:217:MET:HE1	1:D:285:VAL:CG2	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:134:HIS:CD2	6:E:2130:HOH:O	2.59	0.56
1:E:352:ASP:HB3	6:E:2244:HOH:O	2.06	0.56
1:B:269:LYS:HB2	6:B:2195:HOH:O	2.05	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:F:134:HIS:CG	1:F:135:ALA:H	2.24	0.56
1:C:336:LEU:HD11	1:C:413:LEU:HD11	1.88	0.55
1:E:243:GLN:HG3	6:E:2152:HOH:O	2.05	0.55
1:F:142:ASN:CB	6:F:2122:HOH:O	2.48	0.55
1:C:403:ARG:HH21	1:C:405:HIS:HE1	1.53	0.55
1:E:244:THR:CG2	6:E:2172:HOH:O	2.54	0.55
1:D:186:THR:HG23	1:D:207:ILE:HG23	1.88	0.55
1:E:348:THR:HG23	6:E:2247:HOH:O	2.06	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:B:149:ARG:HG3	1:B:165:LEU:HD11	1.89	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: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:A:1:LEU:HD12	1:A:1:LEU:H3	1.72	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:253:VAL:HG21	1:C:283:LEU:HD22	1.89	0.54
1:D:59:HIS:HD2	6:D:2029:HOH:O	1.91	0.54
1:D:170:ASP:O	1:D:171:LEU:HB2	2.08	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:A:411:ASN:HD22	1:A:411:ASN:H	1.56	0.54
1:E:208:THR:HG23	6:E:2145:HOH:O	2.08	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:F:217:MET:HE1	1:F:285:VAL:CG2	2.38	0.53
1:B:120:ASP:HB2	6:B:2111:HOH:O	2.08	0.53
1:E:59:HIS:HD2	6:E:2028:HOH:O	1.90	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:A:250:ARG:NH1	1:A:295:VAL:HG22	2.22	0.53
1:E:124:VAL:HG13	1:E:174:TRP:CD1	2.43	0.53
1:D:109:MET:HE1	6:D:2097:HOH:O	2.08	0.53
1:F:101:GLU:OE2	1:F:134:HIS:NE2	2.40	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
1:C:170:ASP:OD2	1:C:173:HIS:HD2	1.92	0.52
1:C:340:ASN:HA	1:C:412:ILE:HD12	1.91	0.52
1:F:109:MET:HE2	6:F:2045:HOH:O	2.07	0.52
1:C:217:MET:HE1	1:C:285:VAL:HG21	1.90	0.52
1:A:364:SER:OG	1:A:405:HIS:HD2	1.93	0.52
1:B:210:THR:HG21	6:B:2172:HOH:O	2.09	0.52
1:B:235:HIS:ND1	1:B:398:ILE:CD1	2.70	0.52
1:B:364:SER:OG	1:B:405:HIS:HD2	1.92	0.52
1:A:217:MET:HE1	1:A:285:VAL:CG2	2.38	0.52
1:B:124:VAL:HG13	1:B:174:TRP:CD1	2.44	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:A:352:ASP:OD1	1:C:228:GLU:OE2	2.27	0.52
1:A:250:ARG:HD3	2:A:1434:SO4:O3	2.09	0.52
1:A:302:ARG:CD	1:A:325:GLU:OE1	2.55	0.52
1:B:235:HIS:CE1	1:B:398:ILE:HD11	2.44	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:D:289:GLU:HG2	6:D:2256:HOH:O	2.10	0.52
1:F:134:HIS:CD2	1:F:135:ALA:N	2.75	0.52
1:F:217:MET:HE1	1:F:285:VAL:HG22	1.92	0.52
1:E:193:ASP:CG	6:E:2152:HOH:O	2.52	0.51
1:A:69:GLU:CD	1:A:69:GLU:H	2.18	0.51
1:B:15:MET:HG3	1:B:32:TYR:CD1	2.45	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:F:138:ASP:HB3	6:F:2079:HOH:O	2.10	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:B:403:ARG:HH21	1:B:405:HIS:HE1	1.58	0.51
1:C:19:ASN:HD21	1:C:33:GLN:NE2	2.09	0.51
1:F:355:ILE:CD1	1:F:368:VAL:HG13	2.40	0.51
1:C:124:VAL:HG13	1:C:174:TRP:CD1	2.46	0.51
1:C:355:ILE:HB	1:C:370:LYS:HG2	1.92	0.51
1:F:411:ASN:HD22	1:F:411:ASN:H	1.58	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:B:369:ARG:NE	6:B:2281:HOH:O	2.40	0.50
1:E:335:GLU:HG3	1:E:348:THR:HG22	1.94	0.50
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:B:1:LEU:HD11	1:B:2:PHE:CE1	2.47	0.50
1:B:200:LYS:CD	1:B:217:MET:HE2	2.41	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: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:E:336:LEU:CD1	1:E:413:LEU:HD11	2.42	0.50
1:F:124:VAL:HG13	1:F:174:TRP:CD1	2.46	0.50
1:A:188:GLU:CD	6:A:2139:HOH:O	2.55	0.49
1:A:372:THR:OG1	1:C:226:ASN:OD1	2.29	0.49
1:D:7:HIS:CE1	1:D:279:LEU:HD13	2.47	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:199:GLU:O	1:C:219:GLU:OE2	2.30	0.49
1:C:200:LYS:HG2	1:C:217:MET:HE2	1.93	0.49
1:C:373:VAL:HG11	1:C:394:PHE:HE2	1.70	0.49
1:A:71:HIS:HD2	1:A:91:TYR:CE2	2.30	0.49
1:B:422:LEU:HD23	1:B:422:LEU:C	2.37	0.49
1:F:200:LYS:HG3	1:F:217:MET:HE2	1.95	0.49
1:E:207:ILE:HG22	1:E:210:THR:HG22	1.95	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:C:373:VAL:HG12	1:C:374:GLU:N	2.28	0.49
1:E:183:ASP:OD1	1:E:185:THR:HB	2.13	0.49
1:C:134:HIS:NE2	6:C:2119:HOH:O	2.34	0.49
1:D:235:HIS:CE1	1:D:398:ILE:CD1	2.96	0.49
1:A:97:HIS:CE1	6:A:2085:HOH:O	2.66	0.48
1:A:355:ILE:HD12	1:A:368:VAL:HG13	1.95	0.48
1:C:1:LEU:N	6:C:2003:HOH:O	2.45	0.48
1:D:133:THR:CG2	6:D:2122:HOH:O	2.60	0.48
1:A:249:ASP:CB	1:D:249:ASP:OD1	2.61	0.48
1:B:1:LEU:HD13	6:B:2295:HOH:O	2.12	0.48
1:B:336:LEU:CD1	1:B:413:LEU:HD11	2.43	0.48
1:D:355:ILE:CD1	1:D:368:VAL:HG13	2.43	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: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:B:304:ARG:HG2	6:B:2226:HOH:O	2.13	0.47
1:F:124:VAL:HG22	1:F:172:PHE:HA	1.96	0.47
1:F:230:ARG:HD2	6:F:2160:HOH:O	2.13	0.47
1:A:120:ASP:CG	3:A:1436:CIT:H22	2.39	0.47
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:B:7:HIS:CE1	1:B:391:GLU:OE1	2.61	0.47
1:D:138:ASP:HB3	6:D:2063:HOH:O	2.14	0.47
1:D:170:ASP:OD2	1:D:173:HIS:CD2	2.68	0.47
1:D:186:THR:CG2	1:D:207:ILE:HG23	2.44	0.47
1:E:411:ASN:H	1:E:411:ASN:HD22	1.62	0.47
1:F:356:VAL:HG11	1:F:402:PHE:CE2	2.49	0.47
1:F:364:SER:OG	1:F:405:HIS:HD2	1.98	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:210:THR:HG1	1:E:212:SER:HG	1.46	0.47
1:B:411:ASN:H	1:B:411:ASN:HD22	1.62	0.47
1:C:128:PRO:HB2	1:C:133:THR:OG1	2.15	0.47
1:C:14:TRP:CD1	1:C:14:TRP:C	2.93	0.47
1:E:31:PHE:CD2	1:E:48:HIS:HD2	2.33	0.47
1:E:29:HIS:HE1	6:E:2022:HOH:O	1.98	0.46
1:E:33:GLN:OE1	1:E:44:ILE:HG21	2.14	0.46
1:E:75:SER:HB2	1:E:138:ASP:OD1	2.15	0.46
1:F:79:VAL:HG22	1:F:246:PHE:CE1	2.49	0.46
1:C:128:PRO:CB	1:C:133:THR:OG1	2.64	0.46
1:D:69:GLU:CG	6:D:2031:HOH:O	2.62	0.46
1:D:202:ILE:HD11	1:D:217:MET:HE3	1.97	0.46
1:F:71:HIS:HD2	1:F:91:TYR:CE2	2.33	0.46
1:F:373:VAL:CG1	1:F:394:PHE:CE2	2.98	0.46
1:D:29:HIS:HE1	6:D:2022:HOH:O	1.98	0.46
1:D:411:ASN:H	1:D:411:ASN:HD22	1.62	0.46
1:E:336:LEU:HD11	1:E:413:LEU:HD11	1.97	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:C:170:ASP:O	1:C:171:LEU:HB2	2.16	0.46
1:D:207:ILE:HG22	1:D:210:THR:HG22	1.97	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:C:183:ASP:OD1	1:C:185:THR:HB	2.16	0.46
1:C:214:LEU:N	1:C:214:LEU:HD12	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:A:29:HIS:HE1	6:A:2019:HOH:O	1.99	0.46
1:E:232:LEU:CD1	1:E:235:HIS:HD2	2.29	0.46
1:B:69:GLU:CG	6:B:2034:HOH:O	2.63	0.46
1:C:144:SER:CB	1:C:149:ARG:HD2	2.46	0.46
1:C:336:LEU:CD1	1:C:413:LEU:HD11	2.45	0.46
1:C:422:LEU:C	1:C:422:LEU:HD23	2.41	0.46
1:D:142:ASN:HD22	1:D:143:ARG:N	2.14	0.46
1:F:359:THR:OG1	1:F:360:ARG:NH1	2.49	0.46
1:F:403:ARG:HH21	1:F:405:HIS:HE1	1.63	0.46
1:F:19:ASN:HD21	1:F:33:GLN:HG2	1.81	0.45
1:B:400:PHE:HB3	1:B:402:PHE:CE2	2.51	0.45
1:D:413:LEU:HD12	1:D:414:SER:N	2.31	0.45
1:F:211:ASN:HD21	1:F:260:TRP:HB2	1.80	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:128:PRO:CB	1:A:133:THR:OG1	2.65	0.45
1:D:87:LEU:HB2	1:D:108:VAL:HG12	1.97	0.45
1:B:69:GLU:HG3	6:B:2034:HOH:O	2.15	0.45
1:E:193:ASP:CB	6:E:2152:HOH:O	2.62	0.45
1:A:206:SER:HB3	1:A:240:TYR:CE1	2.51	0.45
1:C:15:MET:HG3	1:C:32:TYR:CD1	2.51	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:E:149:ARG:CG	1:E:165:LEU:HD11	2.45	0.45
1:F:235:HIS:HD2	6:F:2248:HOH:O	1.99	0.45
1:B:421:LYS:NZ	6:B:2305:HOH:O	2.43	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:F:228:GLU:C	1:F:229:LYS:HG2	2.42	0.45
1:F:98:ASN:CG	6:F:2091:HOH:O	2.59	0.45
1:E:142:ASN:ND2	6:E:2116:HOH:O	2.41	0.45
1:E:202:ILE:CG1	1:E:217:MET:HG3	2.47	0.45
1:E:355:ILE:HD12	1:E:368:VAL:HG13	2.00	0.45
1:A:185:THR:HG21	6:A:2063:HOH:O	2.16	0.44
1:E:235:HIS:ND1	1:E:398:ILE:CD1	2.62	0.44
1:E:262:ARG:HD3	1:E:266:TYR:OH	2.17	0.44
1:A:232:LEU:HD12	1:A:235:HIS:CD2	2.53	0.44
1:B:7:HIS:CE1	1:B:279:LEU:HD13	2.52	0.44
1:B:244:THR:CG2	6:B:2187:HOH:O	2.64	0.44
1:D:1:LEU:CD1	1:D:2:PHE:CD1	3.00	0.44
1:E:369:ARG:NE	6:E:2256:HOH:O	2.36	0.44
1:F:1:LEU:HD11	2:F:1433:SO4:O1	2.17	0.44
1:F:14:TRP:CD1	1:F:14:TRP:C	2.94	0.44
1:E:128:PRO:HB2	1:E:133:THR:OG1	2.18	0.44
1:A:250:ARG:NH1	1:A:297:GLU:OE1	2.50	0.44
1:A:394:PHE:HB3	1:A:398:ILE:CG2	2.48	0.44
1:C:59:HIS:HD2	6:C:2023:HOH:O	2.00	0.44
1:A:351:ARG:NE	6:A:2237:HOH:O	2.49	0.44
1:B:170:ASP:O	1:B:171:LEU:HB2	2.17	0.44
1:F:142:ASN:CG	6:F:2122:HOH:O	2.60	0.44
1:F:244:THR:CG2	6:F:2173:HOH:O	2.65	0.44
1:A:232:LEU:HD12	1:A:235:HIS:HD2	1.83	0.44
1:B:160:ILE:HD12	1:B:184:GLU:CG	2.47	0.44
1:C:29:HIS:CD2	1:C:48:HIS:NE2	2.73	0.44
1:E:232:LEU:HD13	1:E:235:HIS:HD2	1.83	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:266:TYR:HA	1:F:267:PRO:HD3	1.92	0.44
1:D:211:ASN:HD21	1:D:260:TRP:HB2	1.83	0.44
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:F:69:GLU:CD	1:F:69:GLU:N	2.76	0.43
1:F:69:GLU:CG	6:F:2038:HOH:O	2.65	0.43
1:E:69:GLU:CD	1:E:69:GLU:H	2.26	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:A:128:PRO:HB2	1:A:133:THR:OG1	2.19	0.43
1:C:7:HIS:CE1	1:C:279:LEU:CD1	2.99	0.43
1:C:337:ARG:O	1:C:413:LEU:HD12	2.18	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:D:256:TRP:CE2	1:D:258:GLN:HB3	2.54	0.43
1:E:356:VAL:HG11	1:E:402:PHE:CE2	2.53	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:C:149:ARG:NH1	6:C:2131:HOH:O	2.51	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: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:HD3	1:F:360:ARG:N	2.34	0.42
1:C:217:MET:CE	1:C:285:VAL:HG21	2.49	0.42
1:F:40:GLU:OE2	1:F:269:LYS:HD3	2.19	0.42
1:F:286:GLU:CD	6:F:2192:HOH:O	2.62	0.42
1:A:329:GLU:OE1	1:E:304:ARG:CZ	2.68	0.42
1:A:353:GLU:OE2	1:C:226:ASN:ND2	2.53	0.42
1:B:348:THR:HG21	6:B:2254:HOH:O	2.18	0.42
1:F:210:THR:HG23	1:F:212:SER:HG	1.85	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
1:E:109:MET:SD	1:E:110:SER:N	2.92	0.42
1:E:416:LYS:NZ	6:E:2281:HOH:O	2.43	0.42
1:B:59:HIS:HE1	6:B:2011:HOH:O	2.02	0.42
1:C:195:VAL:HG21	1:C:244:THR:HG21	2.00	0.42
1:D:109:MET:CE	6:D:2097:HOH:O	2.66	0.42
1:D:403:ARG:HH21	1:D:405:HIS:CE1	2.37	0.42
1:E:3:LYS:NZ	6:E:2005:HOH:O	2.52	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:262:ARG:NH2	6:C:2183:HOH:O	2.53	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: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:388:CYS:HB2	1:D:405:HIS:CE1	2.55	0.41
1:C:262:ARG:HD3	1:C:266:TYR:OH	2.20	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:B:40:GLU:HG3	6:B:2041:HOH:O	2.19	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:79:VAL:HG22	1:E:246:PHE:CE1	2.55	0.41
1:E:163:VAL:HG21	1:E:203:LEU:HD11	2.02	0.41
1:F:131:GLU:OE1	1:F:131:GLU:HA	2.21	0.41
1:A:413:LEU:HD12	1:A:413:LEU:C	2.46	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:F:7:HIS:NE2	1:F:386:ASP:HB2	2.35	0.41
1:E:31:PHE:CZ	1:E:48:HIS:HD2	2.34	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:71:HIS:HA	1:D:92:TYR:O	2.21	0.41
1:D:259:SER:HB3	1:D:262:ARG:HB2	2.01	0.41
1:E:145:ASN:HA	1:F:80:GLU:O	2.21	0.41
1:A:69:GLU:CG	6:A:2030:HOH:O	2.68	0.41
1:A:311:LYS:HE3	1:A:311:LYS:HB3	1.88	0.41
1:B:235:HIS:ND1	1:B:398:ILE:CG1	2.83	0.41
1:C:257:LEU:HG	1:C:278:SER:HA	2.03	0.41
1:F:98:ASN:OD1	6:F:2091:HOH:O	2.21	0.41
1:F:170:ASP:OD2	1:F:173:HIS:CD2	2.73	0.41
1:B:1:LEU:H3	1:B:1:LEU:HG	1.82	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:C:56:HIS:HE1	1:C:428:GLU:OE1	2.04	0.41
1:C:311:LYS:NZ	6:C:2224:HOH:O	2.54	0.41
1:F:302:ARG:HD2	1:F:425:PHE:CG	2.56	0.41
1:B:207:ILE:HD12	1:B:214:LEU:HD13	2.02	0.40
1:D:14:TRP:CD1	1:D:14:TRP:C	2.98	0.40
1:D:79:VAL:HG11	1:D:171:LEU:HD21	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:E:202:ILE:HG13	1:E:217:MET:HG3	2.02	0.40
1:F:400:PHE:HB3	1:F:402:PHE:CE2	2.56	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: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
1:D:367:GLU:OE1	1:D:369:ARG:NH2	2.53	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

There are no symmetry-related clashes.

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	430/432 (100%)	414 (96%)	16 (4%)	0	100	100
1	B	430/432 (100%)	412 (96%)	17 (4%)	1 (0%)	43	36
1	C	430/432 (100%)	411 (96%)	18 (4%)	1 (0%)	43	36
1	D	430/432 (100%)	415 (96%)	13 (3%)	2 (0%)	24	16
1	E	430/432 (100%)	412 (96%)	16 (4%)	2 (0%)	24	16
1	F	430/432 (100%)	414 (96%)	13 (3%)	3 (1%)	18	10
All	All	2580/2592 (100%)	2478 (96%)	93 (4%)	9 (0%)	36	29

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 [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	387/387 (100%)	346 (89%)	41 (11%)	6	2
1	B	387/387 (100%)	339 (88%)	48 (12%)	4	1
1	C	387/387 (100%)	350 (90%)	37 (10%)	8	3
1	D	387/387 (100%)	343 (89%)	44 (11%)	5	2
1	E	387/387 (100%)	347 (90%)	40 (10%)	7	2
1	F	387/387 (100%)	337 (87%)	50 (13%)	4	1
All	All	2322/2322 (100%)	2062 (89%)	260 (11%)	6	2

All (260) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1	LEU
1	A	60	LEU
1	A	79	VAL
1	A	99	LYS
1	A	108	VAL
1	A	114	LEU
1	A	124	VAL
1	A	147	GLU
1	A	171	LEU
1	A	185	THR

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Mol	Chain	Res	Type
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	283	LEU
1	A	289	GLU
1	A	290	LEU
1	A	295	VAL
1	A	298	LEU
1	A	302	ARG
1	A	303	LYS
1	A	311	LYS
1	A	321	GLU
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
1	B	134	HIS
1	B	159	LYS
1	B	171	LEU
1	B	185	THR
1	B	186	THR

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Mol	Chain	Res	Type
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	263	THR
1	B	270	ARG
1	B	274	ASN
1	B	279	LEU
1	B	283	LEU
1	B	289	GLU
1	B	290	LEU
1	B	295	VAL
1	B	298	LEU
1	B	302	ARG
1	B	303	LYS
1	B	311	LYS
1	B	318	ASP
1	B	321	GLU
1	B	349	LYS
1	B	351	ARG
1	B	354	LEU
1	B	355	ILE
1	B	363	VAL
1	B	370	LYS
1	B	373	VAL
1	B	374	GLU
1	B	376	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	69	GLU
1	C	79	VAL
1	C	97	HIS

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Mol	Chain	Res	Type
1	C	108	VAL
1	C	114	LEU
1	C	124	VAL
1	C	127	LYS
1	C	171	LEU
1	C	185	THR
1	C	186	THR
1	C	195	VAL
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	295	VAL
1	C	298	LEU
1	C	321	GLU
1	C	351	ARG
1	C	354	LEU
1	C	355	ILE
1	C	397	SER
1	C	398	ILE
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	127	LYS

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Mol	Chain	Res	Type
1	D	142	ASN
1	D	171	LEU
1	D	173	HIS
1	D	184	GLU
1	D	185	THR
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	302	ARG
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	411	ASN
1	D	413	LEU
1	D	414	SER
1	D	415	VAL
1	D	420	VAL
1	E	1	LEU
1	E	60	LEU
1	E	79	VAL
1	E	97	HIS
1	E	101	GLU
1	E	108	VAL
1	E	114	LEU
1	E	124	VAL

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Mol	Chain	Res	Type
1	E	159	LYS
1	E	186	THR
1	E	195	VAL
1	E	203	LEU
1	E	208	THR
1	E	210	THR
1	E	211	ASN
1	E	220	LEU
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	311	LYS
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	96	THR
1	F	97	HIS
1	F	99	LYS
1	F	108	VAL
1	F	114	LEU
1	F	124	VAL
1	F	171	LEU

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Mol	Chain	Res	Type
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
1	F	222	GLU
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	283	LEU
1	F	288	ASN
1	F	289	GLU
1	F	290	LEU
1	F	295	VAL
1	F	298	LEU
1	F	303	LYS
1	F	321	GLU
1	F	354	LEU
1	F	355	ILE
1	F	360	ARG
1	F	370	LYS
1	F	373	VAL
1	F	375	ASP
1	F	378	THR
1	F	380	ARG
1	F	382	ARG
1	F	411	ASN
1	F	413	LEU
1	F	415	VAL
1	F	416	LYS
1	F	419	GLN
1	F	420	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (67) 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	97	HIS
1	A	134	HIS
1	A	173	HIS
1	A	211	ASN
1	A	274	ASN
1	A	288	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
1	B	59	HIS
1	B	173	HIS
1	B	274	ASN
1	B	288	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	173	HIS
1	C	211	ASN
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	274	ASN
1	D	288	ASN
1	D	405	HIS

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Mol	Chain	Res	Type
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
1	F	7	HIS
1	F	19	ASN
1	F	56	HIS
1	F	59	HIS
1	F	71	HIS
1	F	173	HIS
1	F	211	ASN
1	F	235	HIS
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 oligosaccharides 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	1434	-	4,4,4	0.31	0	6,6,6	0.20	0
2	SO4	C	1433	-	4,4,4	0.51	0	6,6,6	0.60	0
2	SO4	B	1433	-	4,4,4	0.35	0	6,6,6	0.56	0
4	GOL	C	1436	-	5,5,5	0.69	0	5,5,5	1.18	1 (20%)
3	CIT	A	1436	5	12,12,12	1.14	1 (8%)	17,17,17	2.39	7 (41%)
2	SO4	C	1434	-	4,4,4	0.22	0	6,6,6	0.25	0
2	SO4	B	1434	-	4,4,4	0.24	0	6,6,6	0.20	0
2	SO4	B	1437	-	4,4,4	0.33	0	6,6,6	0.66	0
4	GOL	E	1434	-	5,5,5	0.71	0	5,5,5	0.66	0
4	GOL	B	1436	-	5,5,5	0.41	0	5,5,5	0.38	0
4	GOL	A	1437	-	5,5,5	0.48	0	5,5,5	0.77	0
2	SO4	A	1435	-	4,4,4	0.41	0	6,6,6	0.52	0
2	SO4	E	1433	-	4,4,4	0.18	0	6,6,6	0.39	0
2	SO4	C	1435	-	4,4,4	0.37	0	6,6,6	0.43	0
2	SO4	F	1435	-	4,4,4	0.41	0	6,6,6	0.20	0
2	SO4	B	1435	-	4,4,4	0.38	0	6,6,6	0.25	0
2	SO4	F	1434	-	4,4,4	0.31	0	6,6,6	0.38	0
2	SO4	F	1433	-	4,4,4	0.28	0	6,6,6	0.67	0
2	SO4	A	1433	-	4,4,4	0.61	0	6,6,6	0.45	0
4	GOL	D	1433	-	5,5,5	0.44	0	5,5,5	0.47	0
4	GOL	F	1436	-	5,5,5	0.41	0	5,5,5	0.59	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
4	GOL	E	1434	-	-	4/4/4/4	-
4	GOL	B	1436	-	-	3/4/4/4	-
4	GOL	C	1436	-	-	2/4/4/4	-
3	CIT	A	1436	5	-	2/16/16/16	-
4	GOL	A	1437	-	-	4/4/4/4	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	GOL	D	1433	-	-	3/4/4/4	-
4	GOL	F	1436	-	-	2/4/4/4	-

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	1436	CIT	C2-C3	-2.13	1.51	1.54

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	1436	CIT	C4-C3-C2	4.62	121.16	109.31
3	A	1436	CIT	C2-C3-C6	-4.54	100.00	110.03
3	A	1436	CIT	O6-C6-C3	4.24	121.27	113.14
3	A	1436	CIT	O4-C5-C4	2.99	123.83	114.35
3	A	1436	CIT	O7-C3-C6	2.55	112.58	108.96
3	A	1436	CIT	O4-C5-O3	-2.07	118.00	123.33
4	C	1436	GOL	C3-C2-C1	2.06	119.36	111.80
3	A	1436	CIT	O6-C6-O5	-2.04	117.33	123.86

There are no chirality outliers.

All (20) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	1437	GOL	C1-C2-C3-O3
4	A	1437	GOL	O2-C2-C3-O3
4	C	1436	GOL	C1-C2-C3-O3
4	E	1434	GOL	C1-C2-C3-O3
4	E	1434	GOL	O2-C2-C3-O3
4	F	1436	GOL	C1-C2-C3-O3
4	A	1437	GOL	O1-C1-C2-C3
4	B	1436	GOL	C1-C2-C3-O3
4	D	1433	GOL	C1-C2-C3-O3
4	E	1434	GOL	O1-C1-C2-C3
4	F	1436	GOL	O2-C2-C3-O3
4	B	1436	GOL	O2-C2-C3-O3
4	C	1436	GOL	O2-C2-C3-O3
4	D	1433	GOL	O2-C2-C3-O3
4	E	1434	GOL	O1-C1-C2-O2
4	A	1437	GOL	O1-C1-C2-O2
4	D	1433	GOL	O1-C1-C2-O2

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Mol	Chain	Res	Type	Atoms
3	A	1436	CIT	C6-C3-C4-C5
4	B	1436	GOL	O1-C1-C2-O2
3	A	1436	CIT	C2-C3-C4-C5

There are no ring outliers.

6 monomers are involved in 12 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	1434	SO4	1	0
4	C	1436	GOL	1	0
3	A	1436	CIT	1	0
2	C	1435	SO4	2	0
2	B	1435	SO4	3	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%)	0.21	14 (3%)	50	54	13, 24, 41, 50	4 (0%)
1	B	432/432 (100%)	0.28	25 (5%)	29	30	14, 24, 41, 51	6 (1%)
1	C	432/432 (100%)	0.34	30 (6%)	23	24	13, 24, 41, 51	8 (1%)
1	D	432/432 (100%)	0.30	26 (6%)	27	29	14, 24, 41, 52	8 (1%)
1	E	432/432 (100%)	0.29	31 (7%)	21	23	13, 24, 42, 51	9 (2%)
1	F	432/432 (100%)	0.39	34 (7%)	18	20	13, 25, 41, 51	10 (2%)
All	All	2592/2592 (100%)	0.30	160 (6%)	26	28	13, 24, 41, 52	45 (1%)

All (160) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	E	100	GLY	8.3
1	D	100	GLY	8.0
1	B	96	THR	7.9
1	B	100	GLY	7.5
1	C	96	THR	7.4
1	F	100	GLY	7.4
1	F	99	LYS	7.2
1	F	96	THR	6.9
1	E	97	HIS	6.6
1	E	99	LYS	6.5
1	F	97	HIS	6.4
1	D	96	THR	6.4
1	D	99	LYS	6.3
1	C	100	GLY	6.2
1	C	98	ASN	5.8
1	D	97	HIS	5.7
1	E	96	THR	5.5
1	D	98	ASN	5.3
1	C	99	LYS	5.3

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Mol	Chain	Res	Type	RSRZ
1	C	97	HIS	5.1
1	F	198	GLY	4.7
1	B	99	LYS	4.6
1	C	134	HIS	4.0
1	A	352	ASP	4.0
1	E	98	ASN	4.0
1	B	97	HIS	3.9
1	C	185	THR	3.9
1	C	419	GLN	3.9
1	F	98	ASN	3.8
1	A	134	HIS	3.8
1	F	134	HIS	3.8
1	C	418	ASN	3.7
1	B	134	HIS	3.7
1	B	98	ASN	3.7
1	B	419	GLN	3.6
1	D	132	GLY	3.5
1	C	133	THR	3.5
1	C	145	ASN	3.5
1	F	287	ASN	3.5
1	D	352	ASP	3.4
1	A	419	GLN	3.3
1	F	419	GLN	3.3
1	B	208	THR	3.2
1	D	185	THR	3.1
1	C	7	HIS	3.0
1	E	134	HIS	3.0
1	D	198	GLY	3.0
1	B	109	MET	3.0
1	F	222	GLU	3.0
1	D	373	VAL	2.9
1	B	375	ASP	2.9
1	E	352	ASP	2.9
1	D	134	HIS	2.9
1	B	185	THR	2.8
1	B	418	ASN	2.8
1	C	132	GLY	2.8
1	D	169	ASP	2.8
1	E	133	THR	2.7
1	F	288	ASN	2.7
1	F	418	ASN	2.7
1	E	249	ASP	2.7

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Mol	Chain	Res	Type	RSRZ
1	F	350	SER	2.6
1	A	287	ASN	2.6
1	C	1	LEU	2.6
1	C	221	LYS	2.6
1	A	223	GLY	2.6
1	A	376	GLU	2.6
1	C	208	THR	2.6
1	D	186	THR	2.6
1	F	378	THR	2.6
1	E	185	THR	2.5
1	A	375	ASP	2.5
1	E	138	ASP	2.5
1	B	304	ARG	2.5
1	D	109	MET	2.5
1	B	133	THR	2.5
1	F	352	ASP	2.5
1	C	131	GLU	2.4
1	F	375	ASP	2.4
1	E	142	ASN	2.4
1	A	198	GLY	2.4
1	B	352	ASP	2.4
1	C	378	THR	2.4
1	E	131	GLU	2.4
1	F	376	GLU	2.4
1	D	418	ASN	2.4
1	E	198	GLY	2.4
1	D	157	ASP	2.3
1	B	376	GLU	2.3
1	D	210	THR	2.3
1	F	289	GLU	2.3
1	E	235	HIS	2.3
1	F	1	LEU	2.3
1	F	208	THR	2.3
1	A	132	GLY	2.3
1	C	421	LYS	2.3
1	E	132	GLY	2.3
1	F	138	ASP	2.3
1	A	184	GLU	2.3
1	E	199	GLU	2.3
1	B	287	ASN	2.3
1	C	210	THR	2.3
1	C	159	LYS	2.3

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Mol	Chain	Res	Type	RSRZ
1	B	397	SER	2.3
1	D	375	ASP	2.3
1	E	101	GLU	2.3
1	B	372	THR	2.3
1	F	210	THR	2.3
1	C	304	ARG	2.2
1	F	115	ASP	2.2
1	E	419	GLN	2.2
1	A	185	THR	2.2
1	B	210	THR	2.2
1	F	133	THR	2.2
1	C	198	GLY	2.2
1	A	249	ASP	2.2
1	D	142	ASN	2.2
1	C	186	THR	2.2
1	E	210	THR	2.2
1	C	220	LEU	2.2
1	C	342	SER	2.2
1	E	109	MET	2.2
1	F	131	GLU	2.2
1	D	135	ALA	2.2
1	E	222	GLU	2.1
1	E	374	GLU	2.1
1	C	160	ILE	2.1
1	B	186	THR	2.1
1	D	263	THR	2.1
1	D	420	VAL	2.1
1	A	131	GLU	2.1
1	D	374	GLU	2.1
1	F	185	THR	2.1
1	B	198	GLY	2.1
1	F	230	ARG	2.1
1	F	373	VAL	2.1
1	B	159	LYS	2.1
1	B	184	GLU	2.1
1	C	222	GLU	2.1
1	E	353	GLU	2.1
1	A	157	ASP	2.1
1	E	304	ARG	2.1
1	F	270	ARG	2.1
1	B	199	GLU	2.1
1	D	199	GLU	2.1

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Mol	Chain	Res	Type	RSRZ
1	E	95	PRO	2.1
1	D	304	ARG	2.1
1	E	149	ARG	2.1
1	E	69	GLU	2.0
1	E	350	SER	2.0
1	D	372	THR	2.0
1	E	378	THR	2.0
1	F	186	THR	2.0
1	F	132	GLY	2.0
1	F	351	ARG	2.0
1	F	160	ILE	2.0
1	F	355	ILE	2.0
1	C	287	ASN	2.0
1	E	418	ASN	2.0
1	C	420	VAL	2.0

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	SO4	B	1435	5/5	0.69	0.15	54,55,56,58	0
2	SO4	A	1435	5/5	0.71	0.16	57,63,66,67	0
2	SO4	B	1434	5/5	0.73	0.12	75,75,76,76	0
2	SO4	A	1433	5/5	0.77	0.25	32,39,47,49	0
2	SO4	A	1434	5/5	0.81	0.14	60,63,63,64	0
2	SO4	C	1435	5/5	0.82	0.12	51,52,53,53	0
2	SO4	F	1433	5/5	0.82	0.12	52,53,57,57	0
2	SO4	C	1434	5/5	0.84	0.12	63,64,65,66	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	CIT	A	1436	13/13	0.86	0.12	49,50,51,54	0
4	GOL	C	1436	6/6	0.86	0.15	18,30,34,41	0
4	GOL	A	1437	6/6	0.90	0.12	22,35,36,39	0
4	GOL	D	1433	6/6	0.92	0.11	26,37,37,42	0
2	SO4	E	1433	5/5	0.93	0.11	36,37,40,42	0
4	GOL	F	1436	6/6	0.93	0.14	23,34,39,40	0
4	GOL	E	1434	6/6	0.94	0.10	19,29,33,34	0
4	GOL	B	1436	6/6	0.94	0.09	30,36,37,37	0
2	SO4	F	1435	5/5	0.95	0.11	30,34,37,37	0
2	SO4	C	1433	5/5	0.96	0.08	29,31,32,35	0
2	SO4	F	1434	5/5	0.97	0.12	31,32,33,34	0
5	NA	A	1438	1/1	0.97	0.09	46,46,46,46	0
2	SO4	B	1437	5/5	0.98	0.06	29,34,34,36	0
2	SO4	B	1433	5/5	0.99	0.05	24,25,25,27	0

6.5 Other polymers [i](#)

There are no such residues in this entry.