



# Full wwPDB X-ray Structure Validation Report ⓘ

Dec 12, 2023 – 05:56 pm GMT

PDB ID : 4AV7  
Title : Structure determination of the double mutant S233Y F250G from the sec-alkyl sulfatase PisA1  
Authors : Knaus, T.; Schober, M.; Faber, K.; Macharaux, P.; Wagner, U.  
Deposited on : 2012-05-24  
Resolution : 3.00 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](mailto:validation@mail.wwpdb.org)

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity : 4.02b-467  
Mogul : 1.8.4, CSD as541be (2020)  
Xtriage (Phenix) : 1.13  
EDS : 2.36  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
Refmac : 5.8.0158  
CCP4 : 7.0.044 (Gargrove)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.36

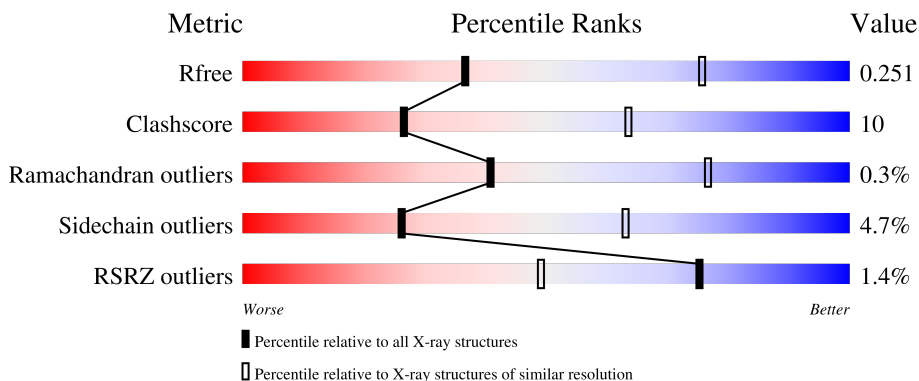
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 3.00 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



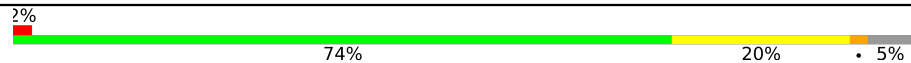
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	130704	2092 (3.00-3.00)
Clashscore	141614	2416 (3.00-3.00)
Ramachandran outliers	138981	2333 (3.00-3.00)
Sidechain outliers	138945	2336 (3.00-3.00)
RSRZ outliers	127900	1990 (3.00-3.00)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 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	668	
1	B	668	
1	C	668	
1	D	668	
1	E	668	

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Mol	Chain	Length	Quality of chain
1	F	668	 <p>A horizontal bar chart representing the quality of chain. The bar is divided into four segments: a small red segment at the beginning labeled '2%', a large green segment labeled '74%', a yellow segment labeled '20%', and a small grey segment at the end labeled '5%'.</p>

## 2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 30000 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 SEC-ALKYLSULFATASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	634	4936	3125	863	929	19	0	0	0
1	B	637	4966	3143	872	932	19	0	0	0
1	C	634	4936	3125	863	929	19	0	0	0
1	D	634	4936	3125	863	929	19	0	0	0
1	E	634	4936	3125	863	929	19	0	0	0
1	F	634	4930	3120	863	928	19	0	0	0

There are 66 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	661	LEU	-	expression tag	UNP F8KAY7
A	662	GLU	-	expression tag	UNP F8KAY7
A	663	HIS	-	expression tag	UNP F8KAY7
A	664	HIS	-	expression tag	UNP F8KAY7
A	665	HIS	-	expression tag	UNP F8KAY7
A	666	HIS	-	expression tag	UNP F8KAY7
A	667	HIS	-	expression tag	UNP F8KAY7
A	668	HIS	-	expression tag	UNP F8KAY7
A	107	ARG	HIS	conflict	UNP F8KAY7
A	233	TYR	SER	engineered mutation	UNP F8KAY7
A	250	GLY	PHE	engineered mutation	UNP F8KAY7
B	661	LEU	-	expression tag	UNP F8KAY7
B	662	GLU	-	expression tag	UNP F8KAY7
B	663	HIS	-	expression tag	UNP F8KAY7
B	664	HIS	-	expression tag	UNP F8KAY7
B	665	HIS	-	expression tag	UNP F8KAY7
B	666	HIS	-	expression tag	UNP F8KAY7

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Chain	Residue	Modelled	Actual	Comment	Reference
B	667	HIS	-	expression tag	UNP F8KAY7
B	668	HIS	-	expression tag	UNP F8KAY7
B	107	ARG	HIS	conflict	UNP F8KAY7
B	233	TYR	SER	engineered mutation	UNP F8KAY7
B	250	GLY	PHE	engineered mutation	UNP F8KAY7
C	661	LEU	-	expression tag	UNP F8KAY7
C	662	GLU	-	expression tag	UNP F8KAY7
C	663	HIS	-	expression tag	UNP F8KAY7
C	664	HIS	-	expression tag	UNP F8KAY7
C	665	HIS	-	expression tag	UNP F8KAY7
C	666	HIS	-	expression tag	UNP F8KAY7
C	667	HIS	-	expression tag	UNP F8KAY7
C	668	HIS	-	expression tag	UNP F8KAY7
C	107	ARG	HIS	conflict	UNP F8KAY7
C	233	TYR	SER	engineered mutation	UNP F8KAY7
C	250	GLY	PHE	engineered mutation	UNP F8KAY7
D	661	LEU	-	expression tag	UNP F8KAY7
D	662	GLU	-	expression tag	UNP F8KAY7
D	663	HIS	-	expression tag	UNP F8KAY7
D	664	HIS	-	expression tag	UNP F8KAY7
D	665	HIS	-	expression tag	UNP F8KAY7
D	666	HIS	-	expression tag	UNP F8KAY7
D	667	HIS	-	expression tag	UNP F8KAY7
D	668	HIS	-	expression tag	UNP F8KAY7
D	107	ARG	HIS	conflict	UNP F8KAY7
D	233	TYR	SER	engineered mutation	UNP F8KAY7
D	250	GLY	PHE	engineered mutation	UNP F8KAY7
E	661	LEU	-	expression tag	UNP F8KAY7
E	662	GLU	-	expression tag	UNP F8KAY7
E	663	HIS	-	expression tag	UNP F8KAY7
E	664	HIS	-	expression tag	UNP F8KAY7
E	665	HIS	-	expression tag	UNP F8KAY7
E	666	HIS	-	expression tag	UNP F8KAY7
E	667	HIS	-	expression tag	UNP F8KAY7
E	668	HIS	-	expression tag	UNP F8KAY7
E	107	ARG	HIS	conflict	UNP F8KAY7
E	233	TYR	SER	engineered mutation	UNP F8KAY7
E	250	GLY	PHE	engineered mutation	UNP F8KAY7
F	661	LEU	-	expression tag	UNP F8KAY7
F	662	GLU	-	expression tag	UNP F8KAY7
F	663	HIS	-	expression tag	UNP F8KAY7
F	664	HIS	-	expression tag	UNP F8KAY7

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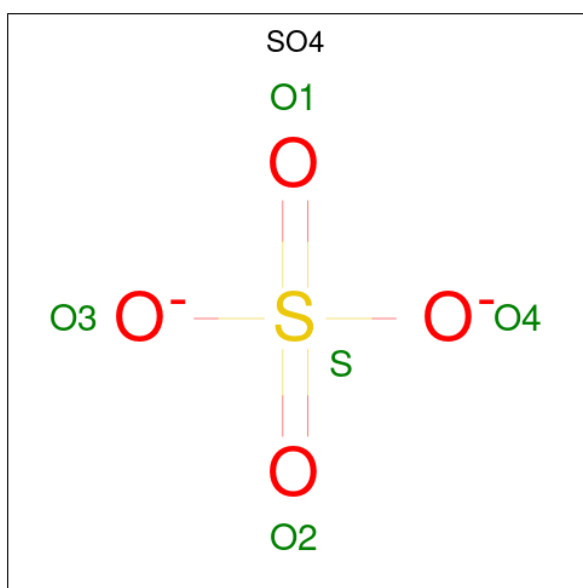
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Chain	Residue	Modelled	Actual	Comment	Reference
F	665	HIS	-	expression tag	UNP F8KAY7
F	666	HIS	-	expression tag	UNP F8KAY7
F	667	HIS	-	expression tag	UNP F8KAY7
F	668	HIS	-	expression tag	UNP F8KAY7
F	107	ARG	HIS	conflict	UNP F8KAY7
F	233	TYR	SER	engineered mutation	UNP F8KAY7
F	250	GLY	PHE	engineered mutation	UNP F8KAY7

- Molecule 2 is ZINC ION (three-letter code: ZN) (formula: Zn).

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

- Molecule 3 is SULFATE ION (three-letter code: SO4) (formula: O<sub>4</sub>S).



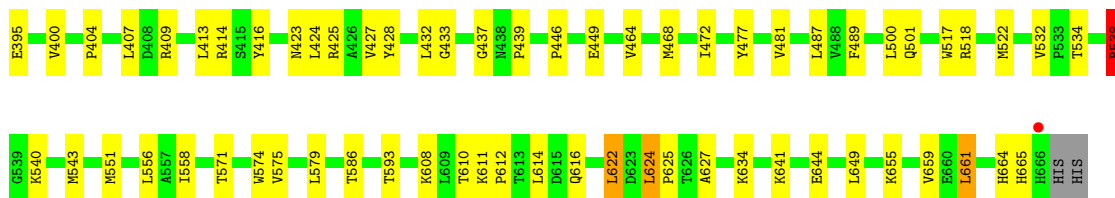
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	O	S	0	0
			5	4	1		
3	B	1	Total	O	S	0	0
			5	4	1		
3	C	1	Total	O	S	0	0
			5	4	1		
3	D	1	Total	O	S	0	0
			5	4	1		
3	E	1	Total	O	S	0	0
			5	4	1		
3	F	1	Total	O	S	0	0
			5	4	1		

- Molecule 4 is water.

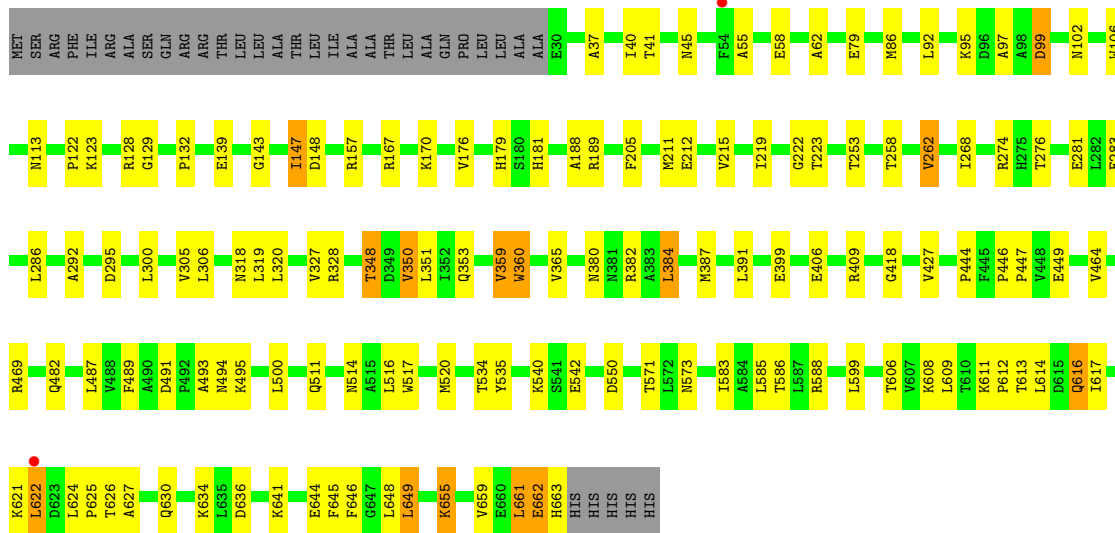
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	87	Total	O	0	0
			87	87		
4	B	71	Total	O	0	0
			71	71		
4	C	44	Total	O	0	0
			44	44		
4	D	39	Total	O	0	0
			39	39		
4	E	51	Total	O	0	0
			51	51		
4	F	26	Total	O	0	0
			26	26		



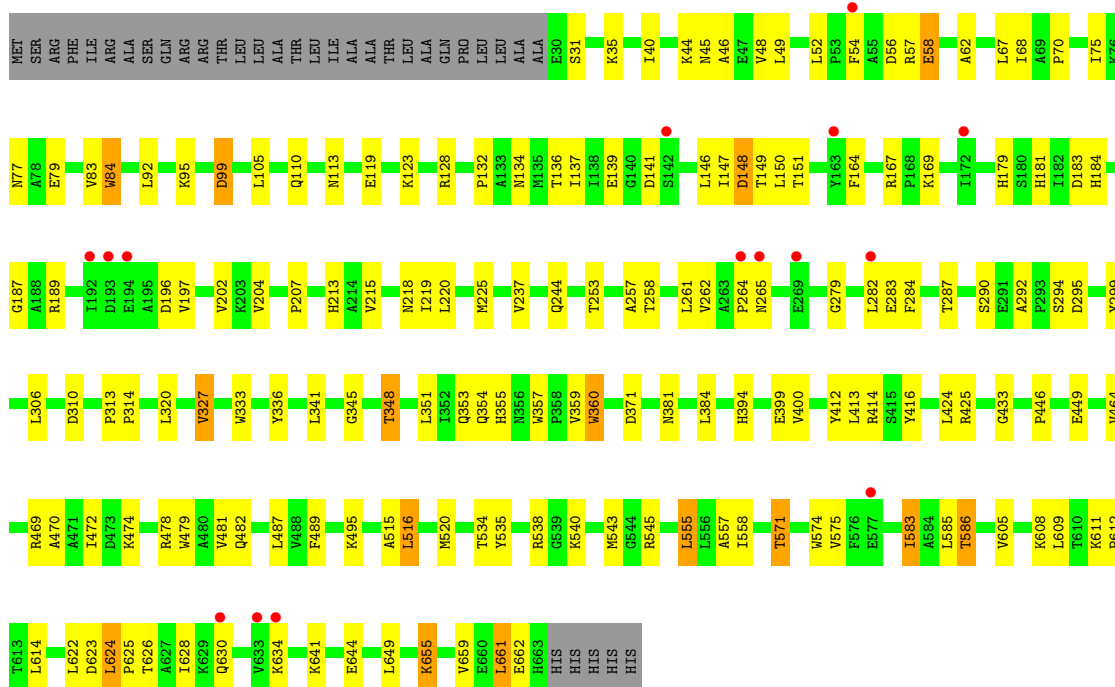




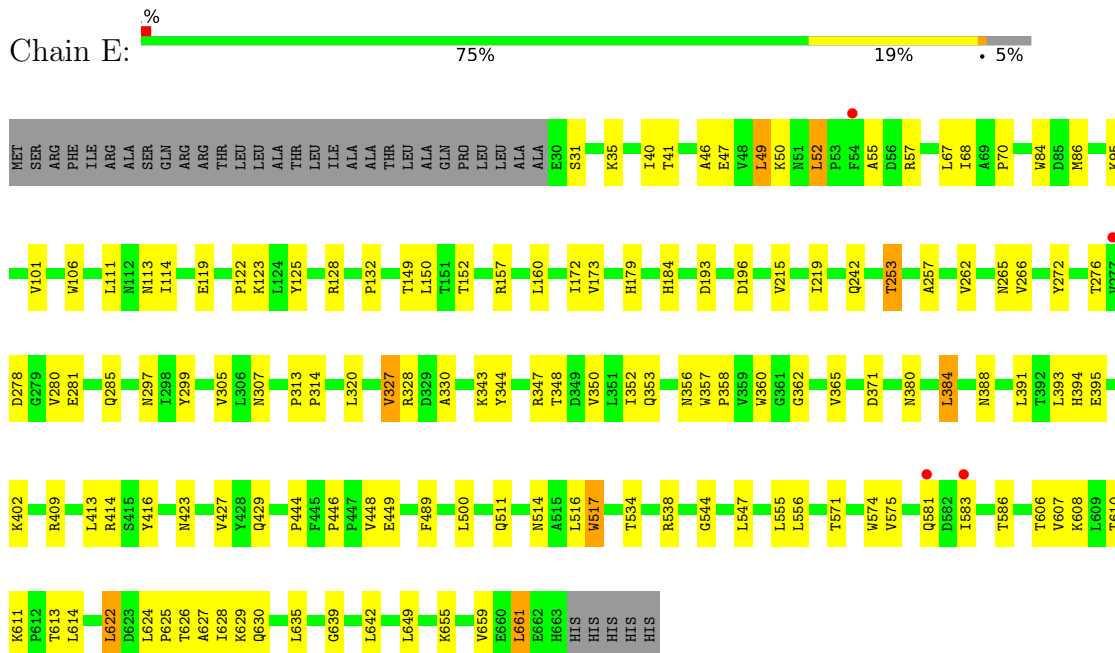
• Molecule 1: SEC-ALKYLSULFATASE



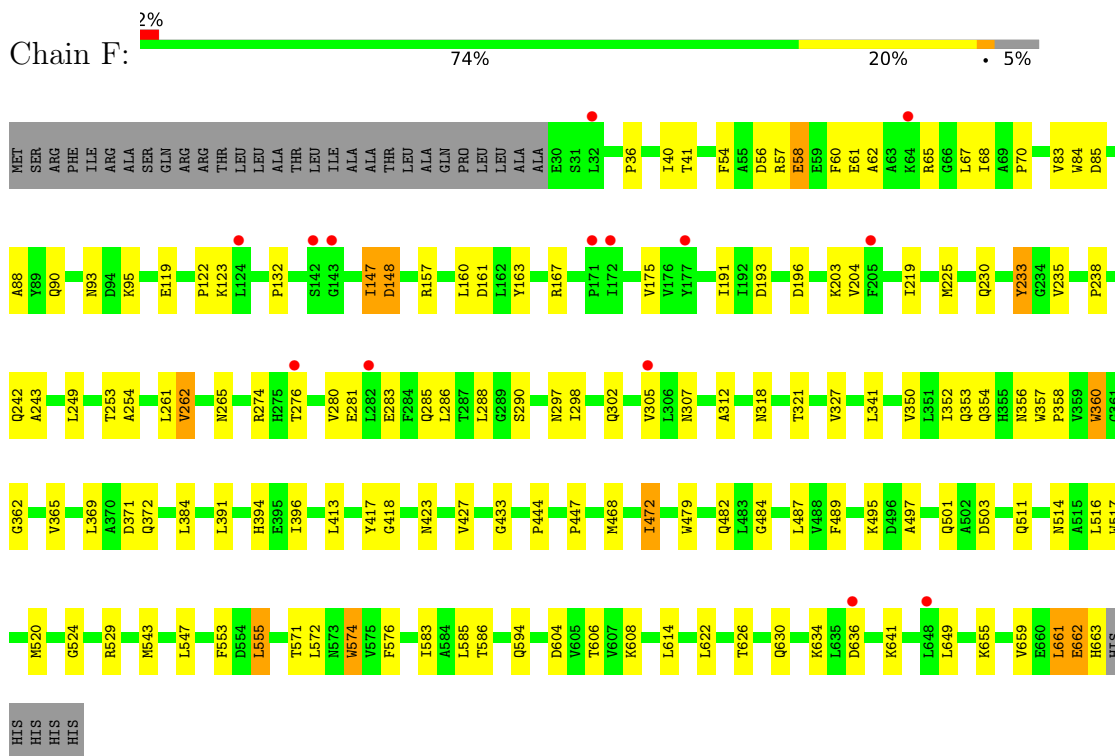
• Molecule 1: SEC-ALKYLSULFATASE



- Molecule 1: SEC-ALKYLSULFATASE



- Molecule 1: SEC-ALKYLSULFATASE



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	75.20Å 201.96Å 248.50Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	45.65 – 3.00 44.59 – 3.00	Depositor EDS
% Data completeness (in resolution range)	99.8 (45.65-3.00) 99.8 (44.59-3.00)	Depositor EDS
$R_{merge}$	0.07	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.18 (at 3.01Å)	Xtrriage
Refinement program	REFMAC 5.6.0117	Depositor
R, $R_{free}$	0.186 , 0.256 0.185 , 0.251	Depositor DCC
$R_{free}$ test set	3840 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	78.9	Xtrriage
Anisotropy	0.053	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.33 , 60.5	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.46$ , $\langle L^2 \rangle = 0.29$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	30000	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	86.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.87% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical values of  $\langle |L| \rangle$ ,  $\langle L^2 \rangle$  for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

## 5 Model quality i

### 5.1 Standard geometry i

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
1	A	0.60	2/5041 (0.0%)	0.68	0/6838
1	B	0.66	6/5074 (0.1%)	0.69	3/6883 (0.0%)
1	C	0.57	1/5041 (0.0%)	0.67	0/6838
1	D	0.65	7/5041 (0.1%)	0.74	5/6838 (0.1%)
1	E	0.60	5/5041 (0.1%)	0.67	2/6838 (0.0%)
1	F	0.59	5/5034 (0.1%)	0.64	0/6828
All	All	0.61	26/30272 (0.1%)	0.68	10/41063 (0.0%)

All (26) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	545	ARG	CZ-NH2	12.77	1.49	1.33
1	D	57	ARG	CZ-NH2	10.08	1.46	1.33
1	B	202	VAL	CB-CG1	10.07	1.74	1.52
1	E	629	LYS	CD-CE	9.26	1.74	1.51
1	F	233	TYR	CB-CG	-6.51	1.41	1.51
1	B	538	ARG	CZ-NH1	6.32	1.41	1.33
1	F	641	LYS	CE-NZ	6.13	1.64	1.49
1	C	360	TRP	CD2-CE2	5.96	1.48	1.41
1	E	517	TRP	CD2-CE2	5.95	1.48	1.41
1	F	574	TRP	CD2-CE2	5.87	1.48	1.41
1	A	360	TRP	CD2-CE2	5.63	1.48	1.41
1	D	360	TRP	CD2-CE2	5.60	1.48	1.41
1	A	574	TRP	CD2-CE2	5.45	1.47	1.41
1	D	84	TRP	CD2-CE2	5.39	1.47	1.41
1	B	574	TRP	CD2-CE2	5.37	1.47	1.41
1	E	84	TRP	CD2-CE2	5.35	1.47	1.41
1	B	517	TRP	CD2-CE2	5.20	1.47	1.41
1	F	360	TRP	CD2-CE2	5.17	1.47	1.41
1	E	574	TRP	CD2-CE2	5.15	1.47	1.41
1	F	479	TRP	CD2-CE2	5.15	1.47	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	357	TRP	CD2-CE2	5.10	1.47	1.41
1	B	61	GLU	CD-OE1	5.10	1.31	1.25
1	E	360	TRP	CD2-CE2	5.10	1.47	1.41
1	D	479	TRP	CD2-CE2	5.09	1.47	1.41
1	B	357	TRP	CD2-CE2	5.06	1.47	1.41
1	D	333	TRP	CD2-CE2	5.04	1.47	1.41

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	545	ARG	NE-CZ-NH2	-19.81	110.39	120.30
1	D	545	ARG	NH1-CZ-NH2	11.31	131.84	119.40
1	E	57	ARG	NE-CZ-NH1	6.91	123.75	120.30
1	D	189	ARG	NE-CZ-NH2	-6.56	117.02	120.30
1	D	57	ARG	NE-CZ-NH2	6.46	123.53	120.30
1	B	57	ARG	NE-CZ-NH1	-6.14	117.23	120.30
1	B	52	LEU	CA-CB-CG	5.64	128.26	115.30
1	B	144	LEU	CA-CB-CG	5.59	128.16	115.30
1	D	545	ARG	NE-CZ-NH1	-5.27	117.67	120.30
1	E	52	LEU	CA-CB-CG	5.25	127.37	115.30

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	4936	0	4889	82	0
1	B	4966	0	4910	153	0
1	C	4936	0	4889	93	0
1	D	4936	0	4889	122	0
1	E	4936	0	4889	84	0
1	F	4930	0	4884	87	0
2	A	2	0	0	0	0
2	B	2	0	0	0	0
2	C	2	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	D	2	0	0	0	0
2	E	2	0	0	0	0
2	F	2	0	0	0	0
3	A	5	0	0	0	0
3	B	5	0	0	0	0
3	C	5	0	0	0	0
3	D	5	0	0	0	0
3	E	5	0	0	0	0
3	F	5	0	0	0	0
4	A	87	0	0	22	0
4	B	71	0	0	58	0
4	C	44	0	0	17	0
4	D	39	0	0	30	0
4	E	51	0	0	13	0
4	F	26	0	0	10	0
All	All	30000	0	29350	610	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 10.

All (610) 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:B:221:ALA:HA	4:B:2026:HOH:O	1.19	1.26
1:D:184:HIS:HA	4:D:2008:HOH:O	1.41	1.18
1:A:661:LEU:H	1:A:661:LEU:HD23	1.10	1.16
1:A:157:ARG:HB2	4:A:2022:HOH:O	1.45	1.15
1:D:264:PRO:HA	4:D:2017:HOH:O	1.44	1.15
1:A:215:VAL:HB	4:A:2032:HOH:O	1.47	1.15
1:B:138:ILE:HA	4:B:2008:HOH:O	1.47	1.13
1:C:661:LEU:H	1:C:661:LEU:HD23	1.10	1.12
1:C:37:ALA:HB3	4:C:2002:HOH:O	1.51	1.09
1:D:219:ILE:HG22	4:D:2014:HOH:O	1.51	1.09
1:B:661:LEU:N	1:B:661:LEU:HD23	1.67	1.09
1:D:555:LEU:HG	4:D:2014:HOH:O	1.49	1.09
1:B:661:LEU:HD23	1:B:661:LEU:H	0.91	1.04
1:B:661:LEU:H	1:B:661:LEU:CD2	1.68	1.04
1:B:144:LEU:HA	4:B:2012:HOH:O	1.56	1.03
1:A:181:HIS:HA	4:A:2028:HOH:O	1.60	1.01
1:E:661:LEU:HD23	1:E:661:LEU:H	1.22	1.01
1:B:664:HIS:HA	4:B:2071:HOH:O	1.59	1.01

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:265:ASN:HB2	4:E:2013:HOH:O	1.62	0.97
1:B:138:ILE:HB	1:B:145:VAL:HG13	1.47	0.97
1:A:53:PRO:HB2	4:A:2007:HOH:O	1.65	0.96
1:B:225:MET:HB2	4:B:2025:HOH:O	1.64	0.96
1:A:40:ILE:HB	4:B:2001:HOH:O	1.64	0.95
1:E:272:TYR:HA	4:E:2019:HOH:O	1.65	0.95
1:B:269:GLU:HG2	4:B:2033:HOH:O	1.64	0.95
1:D:661:LEU:HD23	1:D:661:LEU:H	1.33	0.93
1:B:175:VAL:HA	4:B:2014:HOH:O	1.68	0.93
1:E:534:THR:HA	1:E:655:LYS:HD2	1.52	0.91
1:C:662:GLU:HG3	1:C:663:HIS:HA	1.52	0.89
1:A:611:LYS:HE2	4:A:2082:HOH:O	1.73	0.88
1:C:99:ASP:HB2	4:C:2002:HOH:O	1.72	0.88
1:F:280:VAL:HA	1:F:302:GLN:HE22	1.39	0.88
1:F:62:ALA:O	1:F:360:TRP:HZ3	1.58	0.87
1:C:661:LEU:H	1:C:661:LEU:CD2	1.88	0.86
4:A:2056:HOH:O	1:D:558:ILE:HG12	1.76	0.85
1:A:606:THR:HB	1:A:636:ASP:HB2	1.59	0.85
1:D:495:LYS:HG2	4:D:2033:HOH:O	1.78	0.83
1:A:624:LEU:HB3	1:A:625:PRO:HD3	1.59	0.83
1:A:40:ILE:CB	4:B:2001:HOH:O	2.21	0.83
1:F:661:LEU:HD23	1:F:661:LEU:H	1.43	0.83
1:D:204:VAL:HB	4:D:2017:HOH:O	1.78	0.82
1:F:225:MET:HG3	4:F:2010:HOH:O	1.80	0.81
1:B:489:PHE:HA	1:B:661:LEU:HD22	1.63	0.81
1:B:188:ALA:HB3	4:B:2019:HOH:O	1.81	0.80
1:B:624:LEU:HG	4:B:2069:HOH:O	1.81	0.80
4:B:2048:HOH:O	1:C:520:MET:HE2	1.81	0.80
1:A:661:LEU:HD23	1:A:661:LEU:N	1.95	0.79
1:C:661:LEU:HD23	1:C:661:LEU:N	1.93	0.79
1:F:40:ILE:HD12	1:F:40:ILE:H	1.48	0.79
1:B:313:PRO:HD2	4:B:2036:HOH:O	1.82	0.78
1:B:202:VAL:O	1:B:265:ASN:ND2	2.16	0.78
1:C:189:ARG:NH1	1:C:542:GLU:OE1	2.17	0.78
1:A:40:ILE:CG2	4:B:2001:HOH:O	2.31	0.78
1:B:144:LEU:HD12	4:B:2012:HOH:O	1.85	0.77
1:A:534:THR:HA	1:A:655:LYS:HD2	1.65	0.77
1:E:265:ASN:CB	4:E:2013:HOH:O	2.27	0.76
1:E:305:VAL:HG12	1:E:350:VAL:HG13	1.67	0.75
1:B:624:LEU:HB3	1:B:625:PRO:HD3	1.67	0.75
1:D:624:LEU:HB3	1:D:625:PRO:HD3	1.67	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:391:LEU:HD23	1:E:395:GLU:HB3	1.68	0.74
1:C:181:HIS:HA	4:C:2012:HOH:O	1.86	0.74
1:B:464:VAL:HG23	1:B:487:LEU:HD22	1.69	0.74
1:B:54:PHE:HA	4:B:2002:HOH:O	1.87	0.73
1:B:320:LEU:HA	4:B:2037:HOH:O	1.87	0.73
1:F:62:ALA:O	1:F:360:TRP:CZ3	2.42	0.73
1:A:489:PHE:HA	1:A:661:LEU:HD22	1.71	0.73
1:C:188:ALA:HB3	4:C:2010:HOH:O	1.89	0.73
1:F:487:LEU:HD23	1:F:497:ALA:HB2	1.70	0.72
1:B:659:VAL:HG22	4:B:2030:HOH:O	1.88	0.72
1:C:276:THR:HG22	1:C:281:GLU:HG2	1.70	0.72
1:A:228:ARG:HD2	4:A:2036:HOH:O	1.89	0.72
1:A:661:LEU:H	1:A:661:LEU:CD2	1.88	0.72
1:B:344:TYR:O	1:B:348:THR:HG22	1.89	0.72
1:E:320:LEU:HA	4:E:2025:HOH:O	1.89	0.72
1:A:626:THR:HG22	1:A:630:GLN:HE21	1.55	0.72
4:A:2068:HOH:O	1:D:520:MET:HE2	1.88	0.72
1:A:381:ASN:HA	4:A:2056:HOH:O	1.90	0.72
1:D:611:LYS:HE3	4:D:2035:HOH:O	1.90	0.72
1:C:148:ASP:HB3	4:C:2009:HOH:O	1.90	0.71
1:C:608:LYS:HB2	1:C:634:LYS:HB2	1.72	0.71
1:D:225:MET:HE3	4:D:2013:HOH:O	1.88	0.71
1:B:59:GLU:HB2	1:B:107:ARG:HH22	1.56	0.71
1:E:661:LEU:HD23	1:E:661:LEU:N	2.03	0.70
1:C:274:ARG:HG3	1:C:283:GLU:HG3	1.72	0.70
1:A:166:HIS:HE1	4:A:2023:HOH:O	1.75	0.70
1:A:40:ILE:HG21	4:B:2001:HOH:O	1.90	0.70
1:E:635:LEU:HD22	1:E:639:GLY:HA2	1.73	0.70
1:B:144:LEU:HB2	4:B:2017:HOH:O	1.91	0.70
1:D:77:ASN:HD22	1:D:540:LYS:HE3	1.55	0.70
1:D:167:ARG:HA	4:D:2009:HOH:O	1.92	0.70
1:E:173:VAL:HG11	1:E:278:ASP:HB2	1.72	0.70
1:C:626:THR:HG22	1:C:630:GLN:HE21	1.57	0.69
1:D:661:LEU:HD23	1:D:661:LEU:N	2.05	0.69
1:E:67:LEU:HD21	1:E:70:PRO:HG3	1.73	0.69
1:C:655:LYS:HE3	1:C:655:LYS:HA	1.74	0.69
1:E:661:LEU:H	1:E:661:LEU:CD2	1.97	0.68
1:D:641:LYS:HA	1:D:644:GLU:HG2	1.76	0.68
1:A:101:VAL:HG11	1:A:106:TRP:CE3	2.29	0.68
1:C:534:THR:HA	1:C:655:LYS:HD3	1.76	0.68
1:B:207:PRO:HG3	1:B:296:MET:HG2	1.76	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:272:TYR:CE2	1:E:343:LYS:HD3	2.29	0.67
1:F:262:VAL:HG13	4:F:2008:HOH:O	1.95	0.67
1:C:489:PHE:HA	1:C:661:LEU:HD22	1.77	0.67
1:E:299:TYR:OH	1:E:347:ARG:O	2.09	0.67
1:E:611:LYS:HE3	4:E:2046:HOH:O	1.95	0.67
1:B:352:ILE:HG22	1:B:358:PRO:HB3	1.77	0.66
1:A:207:PRO:HG3	1:A:296:MET:HG2	1.76	0.66
1:B:351:LEU:HB3	1:B:359:VAL:HG13	1.75	0.66
1:D:141:ASP:HA	4:D:2006:HOH:O	1.95	0.66
1:A:40:ILE:HD13	1:A:475:GLY:HA3	1.77	0.65
1:B:128:ARG:HD3	4:B:2009:HOH:O	1.95	0.65
1:E:285:GLN:HA	4:E:2019:HOH:O	1.97	0.65
1:C:606:THR:HB	1:C:636:ASP:HB2	1.78	0.65
1:D:31:SER:HB3	1:D:35:LYS:HE3	1.78	0.65
1:E:157:ARG:HD3	4:E:2012:HOH:O	1.96	0.65
1:F:233:TYR:CG	4:F:2011:HOH:O	2.49	0.65
1:B:138:ILE:HG23	4:B:2008:HOH:O	1.97	0.64
1:C:406:GLU:OE2	1:C:409:ARG:NH1	2.30	0.64
1:B:193:ASP:N	4:B:2022:HOH:O	2.29	0.64
1:D:611:LYS:HB3	1:D:612:PRO:HD3	1.80	0.64
1:F:662:GLU:HG3	1:F:663:HIS:HA	1.80	0.64
1:C:624:LEU:HB3	1:C:625:PRO:HD3	1.80	0.64
1:D:626:THR:HG22	1:D:630:GLN:NE2	2.13	0.64
1:B:208:SER:N	4:B:2024:HOH:O	2.31	0.64
1:E:352:ILE:HG22	1:E:358:PRO:HG3	1.79	0.63
1:D:204:VAL:CB	4:D:2017:HOH:O	2.43	0.63
1:E:626:THR:HG22	1:E:630:GLN:HE21	1.62	0.63
1:A:351:LEU:HB3	1:A:359:VAL:HG13	1.79	0.63
1:A:292:ALA:HB3	1:A:295:ASP:HB2	1.81	0.63
1:B:207:PRO:C	4:B:2024:HOH:O	2.36	0.63
1:E:313:PRO:HD2	4:E:2024:HOH:O	1.99	0.63
1:B:262:VAL:CG1	4:B:2019:HOH:O	2.47	0.63
1:B:624:LEU:HA	4:B:2069:HOH:O	1.98	0.63
1:E:444:PRO:HG2	1:F:394:HIS:CE1	2.34	0.63
1:D:77:ASN:ND2	1:D:540:LYS:HE3	2.14	0.62
1:B:260:THR:HB	4:B:2021:HOH:O	1.99	0.62
1:D:110:GLN:O	1:D:113:ASN:HB2	1.99	0.62
1:D:292:ALA:HB3	1:D:295:ASP:HB2	1.82	0.62
1:F:67:LEU:HD21	1:F:70:PRO:HG3	1.82	0.62
1:C:292:ALA:HB3	1:C:295:ASP:HB2	1.82	0.62
1:B:518:ARG:O	1:B:522:MET:HG2	1.99	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:157:ARG:HD2	4:C:2015:HOH:O	2.00	0.61
1:D:179:HIS:CD2	1:D:181:HIS:HB2	2.35	0.61
1:B:299:TYR:OH	1:B:347:ARG:O	2.12	0.61
1:E:344:TYR:O	1:E:348:THR:HG22	2.00	0.61
1:F:321:THR:HG22	4:F:2013:HOH:O	2.00	0.61
1:B:144:LEU:CB	4:B:2017:HOH:O	2.46	0.61
1:D:611:LYS:HG2	4:D:2035:HOH:O	2.01	0.61
1:B:489:PHE:HA	1:B:661:LEU:CD2	2.31	0.60
1:B:204:VAL:HB	1:B:265:ASN:H	1.67	0.60
1:B:225:MET:HG3	4:B:2025:HOH:O	2.00	0.60
1:C:276:THR:CG2	1:C:281:GLU:HG2	2.31	0.60
1:A:122:PRO:O	1:A:123:LYS:HB2	1.99	0.60
1:B:101:VAL:HG11	1:B:106:TRP:CE3	2.36	0.60
1:F:489:PHE:HA	1:F:661:LEU:HD22	1.83	0.60
1:B:40:ILE:HD12	1:B:40:ILE:H	1.67	0.60
1:B:258:THR:HB	4:B:2015:HOH:O	2.00	0.60
1:B:280:VAL:HA	1:B:302:GLN:HE22	1.66	0.60
1:B:611:LYS:HE2	4:B:2060:HOH:O	2.02	0.60
1:C:626:THR:HG22	1:C:630:GLN:NE2	2.17	0.60
1:E:272:TYR:CG	4:E:2019:HOH:O	2.55	0.60
1:E:320:LEU:HD13	1:E:327:VAL:HG13	1.84	0.60
1:C:516:LEU:O	1:C:520:MET:HG3	2.01	0.60
1:B:68:ILE:HD11	1:B:119:GLU:HB2	1.85	0.59
1:B:258:THR:HG23	1:B:540:LYS:O	2.01	0.59
1:E:626:THR:HG22	1:E:630:GLN:NE2	2.17	0.59
1:A:259:ASN:ND2	1:A:538:ARG:HD2	2.18	0.59
1:C:147:ILE:HG13	1:C:147:ILE:O	2.02	0.59
1:A:261:LEU:HB2	1:A:543:MET:HG2	1.85	0.58
1:E:624:LEU:HD21	1:E:642:LEU:HD23	1.84	0.58
1:B:90:GLN:HA	1:B:93:ASN:HD22	1.68	0.58
1:D:469:ARG:O	1:D:472:ILE:HG13	2.04	0.58
1:F:219:ILE:HD13	1:F:547:LEU:HD11	1.84	0.58
1:B:341:LEU:HD13	1:B:369:LEU:HB2	1.86	0.58
1:C:351:LEU:HB3	1:C:359:VAL:HG13	1.86	0.58
1:E:394:HIS:CE1	1:F:444:PRO:HG2	2.38	0.58
1:E:610:THR:O	1:E:613:THR:HB	2.04	0.58
1:C:92:LEU:HD12	1:C:113:ASN:HD21	1.69	0.58
1:D:538:ARG:NH1	4:D:2013:HOH:O	2.37	0.58
1:E:119:GLU:HG2	4:E:2004:HOH:O	2.03	0.58
1:A:59:GLU:HB2	1:A:107:ARG:HH22	1.70	0.57
1:F:305:VAL:HG22	1:F:350:VAL:HG13	1.85	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:31:SER:HB3	1:B:35:LYS:HE3	1.85	0.57
1:D:197:VAL:HG21	4:D:2004:HOH:O	2.03	0.57
1:C:139:GLU:OE2	1:C:167:ARG:NE	2.36	0.57
1:C:211:MET:O	1:C:215:VAL:HG13	2.04	0.57
1:D:148:ASP:OD2	1:D:184:HIS:ND1	2.37	0.57
1:D:261:LEU:HB2	1:D:543:MET:HG2	1.86	0.57
1:D:516:LEU:O	1:D:520:MET:HG3	2.04	0.57
1:A:616:GLN:HB3	1:A:622:LEU:HB2	1.86	0.57
1:F:61:GLU:O	1:F:65:ARG:HB2	2.03	0.57
1:B:262:VAL:HG13	4:B:2019:HOH:O	2.04	0.57
1:B:593:THR:HB	4:B:2065:HOH:O	2.05	0.57
1:A:101:VAL:HG11	1:A:106:TRP:HE3	1.69	0.57
1:C:99:ASP:N	1:C:99:ASP:OD1	2.37	0.57
1:D:123:LYS:HG2	1:D:139:GLU:HB2	1.86	0.57
1:F:487:LEU:CD2	1:F:497:ALA:HB2	2.34	0.57
1:F:495:LYS:HG2	4:F:2023:HOH:O	2.03	0.57
1:B:394:HIS:CE1	1:C:444:PRO:HG2	2.40	0.57
1:C:300:LEU:HB3	4:C:2025:HOH:O	2.04	0.56
1:B:261:LEU:HB2	1:B:543:MET:HG2	1.86	0.56
1:B:202:VAL:HA	4:B:2018:HOH:O	2.05	0.56
1:B:203:LYS:HA	1:B:265:ASN:HD21	1.70	0.56
1:B:90:GLN:HA	1:B:93:ASN:ND2	2.19	0.56
1:A:489:PHE:HA	1:A:661:LEU:CD2	2.35	0.56
1:C:86:MET:HE1	1:C:113:ASN:HA	1.88	0.56
1:F:661:LEU:HD23	1:F:661:LEU:N	2.16	0.56
1:A:393:LEU:H	1:A:393:LEU:HD23	1.69	0.56
1:B:122:PRO:O	1:B:123:LYS:HB2	2.06	0.56
1:B:141:ASP:HA	4:B:2013:HOH:O	2.04	0.56
1:D:218:ASN:HA	4:D:2013:HOH:O	2.05	0.56
1:A:211:MET:O	1:A:215:VAL:HG22	2.06	0.55
1:B:92:LEU:HB2	1:B:113:ASN:ND2	2.21	0.55
1:A:170:LYS:HD2	4:A:2025:HOH:O	2.06	0.55
1:D:220:LEU:HD22	1:D:558:ILE:HD12	1.89	0.55
1:D:611:LYS:CE	4:D:2035:HOH:O	2.50	0.55
1:E:276:THR:HG22	1:E:281:GLU:HA	1.88	0.55
1:B:172:ILE:HD12	1:B:191:ILE:O	2.06	0.55
1:E:635:LEU:CD2	1:E:639:GLY:HA2	2.37	0.55
1:E:635:LEU:HD22	1:E:639:GLY:CA	2.36	0.55
1:A:40:ILE:HD11	4:A:2076:HOH:O	2.06	0.55
1:B:608:LYS:HB2	1:B:634:LYS:HB2	1.89	0.55
1:A:68:ILE:HD11	1:A:119:GLU:HB2	1.88	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:202:VAL:HG23	4:B:2023:HOH:O	2.06	0.55
1:B:534:THR:HA	1:B:655:LYS:HD2	1.89	0.54
1:F:148:ASP:HB2	1:F:354:GLN:HE21	1.72	0.54
1:F:341:LEU:HD13	1:F:369:LEU:HB2	1.87	0.54
1:D:52:LEU:HD12	4:D:2001:HOH:O	2.06	0.54
1:D:611:LYS:CG	4:D:2035:HOH:O	2.55	0.54
1:C:122:PRO:O	1:C:123:LYS:HB2	2.07	0.54
1:B:101:VAL:HG11	1:B:106:TRP:HE3	1.72	0.54
1:B:208:SER:HA	4:B:2024:HOH:O	2.08	0.54
1:D:626:THR:HG22	1:D:630:GLN:HE21	1.71	0.54
1:F:487:LEU:HD23	1:F:497:ALA:CB	2.35	0.54
1:A:506:GLU:HB3	4:A:2079:HOH:O	2.08	0.54
1:B:196:ASP:HB3	1:B:202:VAL:HG23	1.90	0.54
1:C:550:ASP:HB3	4:C:2040:HOH:O	2.07	0.54
1:E:380:ASN:O	1:E:384:LEU:HB2	2.08	0.54
1:C:143:GLY:HA2	1:C:170:LYS:HB3	1.90	0.54
1:C:622:LEU:HD22	1:C:627:ALA:HB2	1.89	0.54
1:A:301:PRO:HD2	4:A:2044:HOH:O	2.07	0.53
1:D:282:LEU:HD23	1:D:284:PHE:CZ	2.44	0.53
4:A:2068:HOH:O	1:D:520:MET:CE	2.51	0.53
1:D:608:LYS:HB2	1:D:634:LYS:HB2	1.90	0.53
1:D:583:ILE:HD11	1:D:585:LEU:HG	1.90	0.53
1:F:249:LEU:HG	1:F:417:TYR:CD1	2.42	0.53
1:C:655:LYS:HA	1:C:655:LYS:CE	2.39	0.53
1:D:40:ILE:H	1:D:40:ILE:HD12	1.74	0.53
1:E:31:SER:HB3	1:E:35:LYS:HE3	1.89	0.53
1:F:516:LEU:O	1:F:520:MET:HG3	2.09	0.53
1:D:310:ASP:OD1	1:D:355:HIS:HD2	1.90	0.53
1:E:122:PRO:O	1:E:123:LYS:HB2	2.09	0.53
1:E:272:TYR:CD2	4:E:2019:HOH:O	2.54	0.53
1:F:203:LYS:HA	1:F:265:ASN:HD21	1.73	0.53
1:C:305:VAL:HG22	1:C:350:VAL:HG13	1.90	0.53
1:F:132:PRO:HG3	1:F:253:THR:HA	1.91	0.53
1:C:489:PHE:HA	1:C:661:LEU:CD2	2.39	0.52
1:C:258:THR:HG23	1:C:540:LYS:O	2.10	0.52
1:D:148:ASP:HB3	4:D:2008:HOH:O	2.09	0.52
1:F:318:ASN:OD1	1:F:418:GLY:HA2	2.09	0.52
1:D:283:GLU:HB3	1:D:299:TYR:HB3	1.89	0.52
1:F:608:LYS:HB2	1:F:634:LYS:HB2	1.92	0.52
1:A:307:ASN:HA	1:A:352:ILE:O	2.10	0.52
4:A:2057:HOH:O	1:D:557:ALA:HB1	2.08	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:661:LEU:N	1:B:661:LEU:CD2	2.43	0.52
1:B:437:GLY:O	1:B:439:PRO:HD3	2.09	0.52
1:C:212:GLU:HB2	4:C:2018:HOH:O	2.09	0.52
1:D:571:THR:HG22	1:D:586:THR:HB	1.91	0.52
1:A:219:ILE:HD11	1:A:543:MET:HB3	1.92	0.52
1:A:320:LEU:HD11	1:D:433:GLY:HA3	1.92	0.51
1:B:138:ILE:O	4:B:2012:HOH:O	2.19	0.51
1:D:67:LEU:HD21	1:D:70:PRO:HG3	1.91	0.51
1:D:279:GLY:HA3	4:D:2007:HOH:O	2.09	0.51
1:D:575:VAL:CG1	1:D:608:LYS:HG2	2.40	0.51
1:E:40:ILE:HD12	1:E:40:ILE:H	1.74	0.51
1:B:472:ILE:HG23	1:B:477:TYR:HE1	1.76	0.51
1:E:330:ALA:HB3	1:E:380:ASN:HB2	1.92	0.51
1:C:646:PHE:HA	1:C:649:LEU:HD22	1.93	0.51
1:D:132:PRO:HG3	1:D:253:THR:HG22	1.92	0.51
1:F:489:PHE:HA	1:F:661:LEU:CD2	2.39	0.51
1:B:67:LEU:HD13	1:B:118:PHE:CE2	2.45	0.51
1:E:514:ASN:HB3	1:E:517:TRP:HB2	1.91	0.51
1:F:54:PHE:HA	4:F:2002:HOH:O	2.11	0.51
1:A:641:LYS:HA	1:A:644:GLU:HG2	1.91	0.51
1:E:423:ASN:O	1:E:427:VAL:HG23	2.11	0.51
1:F:352:ILE:HG22	1:F:358:PRO:HB3	1.91	0.51
1:F:371:ASP:HB3	1:F:413:LEU:HD11	1.93	0.51
1:B:371:ASP:HB3	1:B:413:LEU:HD11	1.93	0.51
1:D:137:ILE:HG23	1:D:146:LEU:HD12	1.93	0.51
1:F:161:ASP:HB2	4:F:2007:HOH:O	2.10	0.51
1:D:287:THR:HA	1:D:336:TYR:CE1	2.45	0.51
1:B:307:ASN:HA	1:B:352:ILE:O	2.11	0.50
1:D:313:PRO:HD2	4:D:2019:HOH:O	2.11	0.50
1:A:462:ASP:N	4:A:2075:HOH:O	2.44	0.50
1:F:56:ASP:C	1:F:58:GLU:H	2.15	0.50
1:F:312:ALA:HB1	1:F:372:GLN:HG3	1.93	0.50
1:B:208:SER:CA	4:B:2024:HOH:O	2.59	0.50
1:B:262:VAL:HG12	4:B:2019:HOH:O	2.10	0.50
1:D:661:LEU:H	1:D:661:LEU:CD2	2.04	0.50
1:E:160:LEU:HD21	1:E:172:ILE:HD11	1.93	0.50
1:A:286:LEU:HD22	1:A:288:LEU:HD21	1.92	0.50
1:D:207:PRO:HB2	1:D:294:SER:OG	2.12	0.50
1:F:661:LEU:HD11	4:F:2022:HOH:O	2.09	0.50
1:C:306:LEU:HB2	1:C:348:THR:HG21	1.94	0.50
1:E:101:VAL:HG11	1:E:106:TRP:CE3	2.46	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:143:GLY:HA2	1:B:171:PRO:HD2	1.93	0.50
1:B:147:ILE:HA	1:B:176:VAL:HB	1.93	0.50
1:B:270:LYS:HB2	1:B:273:GLU:HG3	1.94	0.50
1:B:135:MET:HG3	4:B:2011:HOH:O	2.10	0.49
1:C:573:ASN:HB3	1:C:599:LEU:HD22	1.94	0.49
1:C:645:PHE:O	1:C:648:LEU:HB2	2.12	0.49
1:D:137:ILE:HG23	1:D:146:LEU:CD1	2.42	0.49
1:A:160:LEU:HD21	1:A:172:ILE:HD11	1.93	0.49
1:E:305:VAL:CG1	1:E:350:VAL:HG13	2.41	0.49
1:A:544:GLY:HA2	1:A:547:LEU:HD22	1.95	0.49
1:C:40:ILE:HD12	1:C:40:ILE:H	1.77	0.49
1:C:387:MET:HE1	1:C:427:VAL:HG12	1.95	0.49
1:C:514:ASN:HB3	1:C:517:TRP:HB2	1.93	0.49
1:E:285:GLN:HB3	1:E:297:ASN:HB2	1.95	0.49
1:B:344:TYR:O	1:B:348:THR:CG2	2.59	0.49
1:B:209:GLY:O	1:B:213:HIS:HD2	1.96	0.49
1:D:75:ILE:HD12	1:D:84:TRP:HB3	1.94	0.49
1:D:218:ASN:O	1:D:219:ILE:HG13	2.13	0.49
1:B:207:PRO:HD2	1:B:210:PHE:HD1	1.78	0.49
1:C:132:PRO:HG3	1:C:253:THR:HG22	1.95	0.49
1:C:659:VAL:HG22	4:C:2022:HOH:O	2.13	0.49
1:D:105:LEU:HD11	1:D:515:ALA:HB2	1.95	0.49
1:D:262:VAL:HG22	4:D:2004:HOH:O	2.13	0.49
1:F:36:PRO:HA	1:F:242:GLN:NE2	2.27	0.49
1:F:90:GLN:HA	1:F:93:ASN:HD22	1.78	0.49
1:A:148:ASP:OD2	1:A:354:GLN:HG3	2.13	0.49
1:A:533:PRO:HD2	4:A:2081:HOH:O	2.12	0.49
1:D:215:VAL:HA	1:D:219:ILE:HD12	1.95	0.49
1:E:362:GLY:HA2	1:E:365:VAL:HG22	1.95	0.49
1:A:40:ILE:CD1	4:B:2001:HOH:O	2.60	0.48
1:A:381:ASN:ND2	4:A:2057:HOH:O	2.46	0.48
1:B:464:VAL:CG2	1:B:487:LEU:HD22	2.42	0.48
1:E:276:THR:HA	1:E:280:VAL:O	2.13	0.48
1:B:265:ASN:OD1	1:B:266:VAL:HG12	2.13	0.48
1:B:296:MET:HG3	4:B:2034:HOH:O	2.13	0.48
1:F:147:ILE:O	1:F:147:ILE:HG13	2.13	0.48
1:B:163:TYR:CE1	1:B:167:ARG:HG3	2.49	0.48
1:B:305:VAL:HG12	1:B:350:VAL:HG13	1.95	0.48
1:F:391:LEU:HB3	1:F:396:ILE:HG13	1.95	0.48
1:A:353:GLN:HG2	4:A:2046:HOH:O	2.13	0.48
1:B:428:TYR:CE1	1:B:432:LEU:HD12	2.49	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:276:THR:HG22	1:F:281:GLU:HG2	1.94	0.48
1:B:400:VAL:HB	1:B:424:LEU:CD1	2.43	0.48
1:C:464:VAL:HG23	1:C:487:LEU:HD22	1.95	0.48
1:A:611:LYS:HB3	1:A:612:PRO:HD3	1.96	0.48
1:B:622:LEU:HD22	1:B:627:ALA:HB2	1.95	0.48
1:D:196:ASP:HB3	1:D:202:VAL:HG23	1.95	0.48
1:D:258:THR:HG23	1:D:540:LYS:O	2.14	0.48
1:D:68:ILE:HD11	1:D:119:GLU:HB2	1.96	0.48
1:A:626:THR:HG22	1:A:630:GLN:NE2	2.26	0.48
1:C:320:LEU:HD12	4:C:2032:HOH:O	2.13	0.47
1:D:535:TYR:H	1:D:655:LYS:HD3	1.77	0.47
1:D:659:VAL:HG22	4:D:2015:HOH:O	2.14	0.47
1:F:553:PHE:CD1	1:F:585:LEU:HD11	2.49	0.47
1:D:341:LEU:O	1:D:345:GLY:HA3	2.14	0.47
1:F:286:LEU:HD22	1:F:288:LEU:HD21	1.97	0.47
1:B:177:TYR:CD2	1:B:210:PHE:CZ	3.02	0.47
1:D:197:VAL:HG13	1:D:265:ASN:ND2	2.30	0.47
1:E:371:ASP:HB3	1:E:413:LEU:HD11	1.97	0.47
1:E:111:LEU:HA	1:E:114:ILE:HD12	1.95	0.47
1:F:285:GLN:HB3	1:F:297:ASN:HB2	1.96	0.47
1:B:423:ASN:O	1:B:427:VAL:HG23	2.14	0.47
1:B:593:THR:CB	4:B:2065:HOH:O	2.62	0.47
1:D:54:PHE:HA	4:D:2001:HOH:O	2.14	0.47
1:D:56:ASP:O	1:D:58:GLU:N	2.37	0.47
1:E:414:ARG:HB2	1:E:416:TYR:CE2	2.49	0.47
1:A:152:THR:HG21	1:A:257:ALA:HB3	1.97	0.47
1:A:464:VAL:HG23	1:A:487:LEU:HD22	1.96	0.47
1:C:222:GLY:HA2	4:C:2020:HOH:O	2.15	0.47
1:C:41:THR:HG23	1:C:511:GLN:HG3	1.96	0.47
1:C:491:ASP:OD1	1:C:493:ALA:HB3	2.15	0.47
1:D:279:GLY:CA	4:D:2007:HOH:O	2.62	0.47
1:D:314:PRO:HA	1:D:412:TYR:HB2	1.97	0.47
1:F:193:ASP:HB3	1:F:196:ASP:OD2	2.15	0.47
4:B:2048:HOH:O	1:C:520:MET:CE	2.53	0.47
1:D:148:ASP:HB2	1:D:354:GLN:HE21	1.80	0.47
1:F:606:THR:HB	1:F:636:ASP:HB2	1.96	0.47
1:C:662:GLU:CG	1:C:663:HIS:HA	2.35	0.46
1:C:262:VAL:HA	4:C:2016:HOH:O	2.15	0.46
1:F:122:PRO:O	1:F:123:LYS:HB2	2.15	0.46
1:A:136:THR:HB	1:A:147:ILE:HB	1.97	0.46
1:D:207:PRO:C	4:D:2010:HOH:O	2.53	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:625:PRO:HA	1:E:628:ILE:HD12	1.97	0.46
1:B:124:LEU:HA	4:B:2008:HOH:O	2.15	0.46
1:C:469:ARG:HG3	1:C:500:LEU:HD21	1.96	0.46
1:E:47:GLU:OE2	1:E:50:LYS:HE2	2.16	0.46
1:F:423:ASN:O	1:F:427:VAL:HG23	2.15	0.46
1:D:320:LEU:HD13	1:D:327:VAL:HG13	1.96	0.46
1:B:101:VAL:CG1	1:B:106:TRP:CE3	2.98	0.46
1:F:41:THR:HG23	1:F:511:GLN:HG3	1.96	0.46
1:E:352:ILE:HG22	1:E:358:PRO:CG	2.45	0.46
1:F:157:ARG:HH21	1:F:191:ILE:HG22	1.78	0.46
1:B:414:ARG:HB2	1:B:416:TYR:CE2	2.50	0.46
1:C:62:ALA:O	1:C:360:TRP:HZ3	1.99	0.46
1:D:351:LEU:HB3	1:D:359:VAL:HG13	1.96	0.46
1:E:219:ILE:HD13	1:E:547:LEU:HD11	1.98	0.46
1:F:362:GLY:HA2	1:F:365:VAL:HG22	1.97	0.46
1:A:492:PRO:HG3	1:A:661:LEU:HD11	1.98	0.45
1:B:193:ASP:HB3	4:B:2022:HOH:O	2.16	0.45
1:C:318:ASN:OD1	1:C:418:GLY:HA2	2.16	0.45
1:F:356:ASN:HB3	1:F:357:TRP:CE3	2.51	0.45
1:B:216:SER:HA	1:B:220:LEU:HD12	1.96	0.45
1:C:276:THR:HG22	1:C:281:GLU:HA	1.97	0.45
1:D:218:ASN:C	1:D:219:ILE:HG13	2.36	0.45
1:B:610:THR:HB	1:B:612:PRO:HD2	1.98	0.45
1:D:371:ASP:HB3	1:D:413:LEU:HD11	1.97	0.45
1:E:393:LEU:HD23	1:E:393:LEU:H	1.81	0.45
1:F:281:GLU:H	1:F:302:GLN:NE2	2.14	0.45
1:B:556:LEU:HD22	1:B:649:LEU:HD13	1.99	0.45
4:B:2062:HOH:O	1:C:382:ARG:HD2	2.16	0.45
1:C:353:GLN:HG2	4:C:2029:HOH:O	2.15	0.45
1:F:57:ARG:HA	1:F:60:PHE:HB2	1.98	0.45
1:F:274:ARG:HG3	1:F:283:GLU:HG3	1.98	0.45
1:B:148:ASP:OD2	1:B:184:HIS:ND1	2.45	0.45
1:B:269:GLU:CG	4:B:2033:HOH:O	2.43	0.45
1:B:281:GLU:H	1:B:302:GLN:NE2	2.15	0.45
1:B:350:VAL:HG21	1:B:360:TRP:CE3	2.51	0.45
1:D:623:ASP:HB3	1:D:626:THR:OG1	2.16	0.45
1:F:68:ILE:HD11	1:F:119:GLU:HB2	1.99	0.45
1:F:175:VAL:HB	1:F:204:VAL:HG22	1.97	0.45
1:B:351:LEU:HB3	1:B:359:VAL:CG1	2.43	0.45
1:B:446:PRO:HG2	1:B:449:GLU:HB2	1.97	0.45
1:A:610:THR:HB	1:A:612:PRO:HD2	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:588:ARG:HD2	4:C:2043:HOH:O	2.16	0.45
1:D:62:ALA:O	1:D:360:TRP:HZ3	1.98	0.45
1:D:464:VAL:CG2	1:D:487:LEU:HD22	2.46	0.45
1:E:149:THR:O	1:E:150:LEU:HB2	2.15	0.45
1:F:276:THR:HA	1:F:280:VAL:O	2.16	0.45
1:A:36:PRO:HA	1:A:242:GLN:NE2	2.32	0.44
1:A:352:ILE:HG22	1:A:358:PRO:HB3	1.98	0.44
1:E:68:ILE:HD11	1:E:119:GLU:HB2	1.99	0.44
1:C:446:PRO:HG2	1:C:449:GLU:HB2	2.00	0.44
1:D:661:LEU:CD1	4:D:2032:HOH:O	2.65	0.44
1:E:556:LEU:HD22	1:E:649:LEU:HD22	1.99	0.44
1:F:626:THR:HG22	1:F:630:GLN:HE21	1.83	0.44
1:B:286:LEU:HD13	1:B:288:LEU:HD11	1.99	0.44
1:D:123:LYS:HA	1:D:139:GLU:OE1	2.16	0.44
1:E:86:MET:HE1	1:E:113:ASN:HA	1.99	0.44
1:C:380:ASN:O	1:C:384:LEU:HB2	2.18	0.44
1:D:400:VAL:HB	1:D:424:LEU:CD1	2.47	0.44
1:B:173:VAL:HG11	1:B:278:ASP:HB2	2.00	0.44
1:B:468:MET:HB3	1:B:500:LEU:HD23	1.99	0.44
1:F:163:TYR:CE1	1:F:167:ARG:HG3	2.52	0.44
1:B:59:GLU:HB2	1:B:107:ARG:NH2	2.29	0.44
1:B:274:ARG:HG2	1:B:283:GLU:HG3	2.00	0.44
1:B:321:THR:OG1	1:B:323:ARG:HG2	2.18	0.44
1:C:391:LEU:HD21	1:C:399:GLU:HG3	1.99	0.44
1:D:179:HIS:HD2	1:D:181:HIS:CG	2.35	0.44
1:D:237:VAL:HG12	1:D:244:GLN:HB2	1.99	0.44
1:B:101:VAL:CG1	1:B:106:TRP:HE3	2.30	0.44
1:B:290:SER:OG	1:B:291:GLU:N	2.51	0.44
1:E:49:LEU:O	1:E:52:LEU:HG	2.18	0.44
1:E:119:GLU:HG3	1:E:125:TYR:CE2	2.52	0.44
1:F:468:MET:O	1:F:472:ILE:HG12	2.17	0.44
1:C:62:ALA:O	1:C:360:TRP:CZ3	2.71	0.44
1:C:319:LEU:O	1:C:328:ARG:HD2	2.18	0.44
1:A:557:ALA:HB1	1:D:381:ASN:ND2	2.33	0.44
1:C:176:VAL:HG22	1:C:205:PHE:HB2	1.99	0.44
1:F:147:ILE:HD13	1:F:298:ILE:HD13	2.00	0.44
1:B:283:GLU:HB3	1:B:299:TYR:HB3	2.00	0.43
1:D:478:ARG:O	1:D:481:VAL:HG22	2.18	0.43
1:B:292:ALA:HB3	1:B:295:ASP:HB2	1.99	0.43
1:F:238:PRO:O	1:F:243:ALA:HB3	2.17	0.43
1:A:249:LEU:HG	1:A:417:TYR:CD1	2.54	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:255:THR:HA	1:A:535:TYR:OH	2.18	0.43
1:A:305:VAL:HG12	1:A:350:VAL:HG13	2.01	0.43
1:E:152:THR:HG21	1:E:257:ALA:HB3	2.00	0.43
1:F:472:ILE:HG12	1:F:472:ILE:H	1.57	0.43
1:B:77:ASN:HB2	4:B:2005:HOH:O	2.17	0.43
1:C:128:ARG:HA	4:C:2008:HOH:O	2.19	0.43
1:D:204:VAL:CG1	4:D:2017:HOH:O	2.65	0.43
1:E:622:LEU:HD22	1:E:627:ALA:HB2	2.00	0.43
1:F:286:LEU:HD22	1:F:288:LEU:CD2	2.49	0.43
1:B:215:VAL:HG21	1:B:551:MET:SD	2.59	0.43
1:C:45:ASN:OD1	1:C:102:ASN:HA	2.18	0.43
1:D:605:VAL:C	4:D:2039:HOH:O	2.56	0.43
1:A:392:THR:HG21	4:A:2060:HOH:O	2.18	0.43
1:D:136:THR:HB	1:D:147:ILE:HB	2.01	0.43
1:A:56:ASP:HA	1:A:107:ARG:HH21	1.84	0.43
1:B:160:LEU:HD22	1:B:191:ILE:HG22	2.00	0.43
1:D:62:ALA:O	1:D:360:TRP:CZ3	2.72	0.43
1:E:307:ASN:HA	1:E:352:ILE:O	2.19	0.43
1:F:85:ASP:OD2	1:F:88:ALA:HB2	2.18	0.43
1:B:664:HIS:HA	1:B:665:HIS:HA	1.88	0.43
1:D:46:ALA:HA	1:D:49:LEU:HD12	2.01	0.43
1:E:489:PHE:HA	1:E:661:LEU:HD22	2.00	0.43
1:F:219:ILE:HD11	1:F:543:MET:HB3	2.01	0.43
1:A:472:ILE:HG23	1:A:477:TYR:HE1	1.84	0.43
1:B:433:GLY:HA3	1:C:320:LEU:HD11	2.01	0.43
4:B:2042:HOH:O	1:C:447:PRO:HD2	2.19	0.43
1:D:306:LEU:HB2	1:D:348:THR:HG21	2.01	0.43
1:D:469:ARG:HA	1:D:472:ILE:CG1	2.48	0.43
1:D:470:ALA:O	1:D:474:LYS:HB2	2.19	0.43
1:E:446:PRO:HG2	1:E:449:GLU:HB2	2.01	0.43
1:F:157:ARG:NH2	1:F:160:LEU:HD22	2.34	0.43
1:F:307:ASN:HA	1:F:352:ILE:O	2.19	0.43
1:A:235:VAL:HG23	1:A:236:MET:HG2	2.01	0.42
1:B:67:LEU:HD13	1:B:118:PHE:CZ	2.54	0.42
1:B:579:LEU:HD11	1:B:611:LYS:HB2	2.01	0.42
1:F:574:TRP:HB3	1:F:576:PHE:HE1	1.84	0.42
1:A:464:VAL:CG2	1:A:487:LEU:HD22	2.50	0.42
1:A:624:LEU:CB	1:A:625:PRO:HD3	2.42	0.42
1:B:308:THR:HG21	1:B:351:LEU:HD11	2.01	0.42
1:B:393:LEU:HB3	1:B:428:TYR:CD2	2.55	0.42
1:B:394:HIS:ND1	1:B:425:ARG:HD3	2.35	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:477:TYR:N	4:B:2056:HOH:O	2.51	0.42
1:C:179:HIS:CD2	1:C:181:HIS:HB2	2.54	0.42
1:D:287:THR:HA	1:D:336:TYR:CD1	2.55	0.42
1:D:489:PHE:HA	1:D:661:LEU:HD22	2.00	0.42
1:E:356:ASN:HB3	1:E:357:TRP:CE3	2.54	0.42
1:A:179:HIS:CD2	1:A:181:HIS:HB2	2.54	0.42
1:B:400:VAL:HB	1:B:424:LEU:HD13	2.01	0.42
1:E:193:ASP:HB3	1:E:196:ASP:OD2	2.19	0.42
1:F:225:MET:HB2	4:F:2010:HOH:O	2.19	0.42
1:B:260:THR:CB	4:B:2021:HOH:O	2.64	0.42
1:E:215:VAL:O	1:E:219:ILE:HB	2.19	0.42
1:E:395:GLU:HG3	1:F:447:PRO:HD2	2.00	0.42
1:F:503:ASP:OD1	1:F:529:ARG:NH2	2.51	0.42
1:F:524:GLY:HA2	1:F:659:VAL:HG11	2.02	0.42
1:A:185:PHE:C	1:A:185:PHE:CD1	2.93	0.42
1:B:102:ASN:OD1	1:B:104:SER:HB3	2.20	0.42
1:B:148:ASP:HB2	1:B:354:GLN:HE21	1.85	0.42
1:B:664:HIS:CA	4:B:2071:HOH:O	2.40	0.42
1:C:215:VAL:O	1:C:219:ILE:HB	2.19	0.42
1:D:44:LYS:O	1:D:48:VAL:HG23	2.20	0.42
1:A:55:ALA:HB3	4:A:2007:HOH:O	2.20	0.42
1:C:616:GLN:HB3	1:C:622:LEU:HB2	2.00	0.42
1:D:213:HIS:CE1	4:D:2011:HOH:O	2.72	0.42
1:D:446:PRO:HG2	1:D:449:GLU:HB2	2.01	0.42
1:D:489:PHE:HA	1:D:661:LEU:CD2	2.50	0.42
1:B:69:ALA:HA	1:B:70:PRO:HD3	1.91	0.42
1:B:388:ASN:HB3	1:C:223:THR:HB	2.02	0.42
1:C:359:VAL:HG22	1:C:365:VAL:HG12	2.01	0.42
1:F:514:ASN:HB3	1:F:517:TRP:HB2	2.02	0.42
1:A:635:LEU:CD2	1:A:639:GLY:HA2	2.49	0.41
1:B:395:GLU:HG3	1:C:447:PRO:HD2	2.02	0.41
1:B:641:LYS:HA	1:B:644:GLU:HG2	2.02	0.41
1:D:414:ARG:HB2	1:D:416:TYR:CE2	2.55	0.41
1:A:661:LEU:N	1:A:661:LEU:CD2	2.66	0.41
1:A:662:GLU:H	1:A:662:GLU:HG2	1.63	0.41
1:D:151:THR:HA	1:D:183:ASP:HA	2.02	0.41
1:E:429:GLN:HE22	1:F:433:GLY:HA2	1.84	0.41
1:B:481:VAL:HA	1:B:501:GLN:OE1	2.20	0.41
1:C:613:THR:O	1:C:617:ILE:HG13	2.20	0.41
1:D:394:HIS:ND1	1:D:425:ARG:HD3	2.36	0.41
1:E:128:ARG:HD3	4:E:2006:HOH:O	2.19	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:179:HIS:CE1	1:E:184:HIS:CD2	3.08	0.41
1:E:328:ARG:HG2	4:E:2021:HOH:O	2.20	0.41
1:F:547:LEU:HD21	1:F:555:LEU:HD12	2.02	0.41
1:F:572:LEU:HB3	1:F:574:TRP:HE1	1.85	0.41
1:B:153:ALA:HB3	4:B:2015:HOH:O	2.21	0.41
1:B:186:GLY:HA2	1:B:260:THR:O	2.20	0.41
1:D:164:PHE:CE1	1:D:169:LYS:HA	2.56	0.41
1:F:84:TRP:CZ3	1:F:132:PRO:HD3	2.55	0.41
1:D:464:VAL:HG23	1:D:487:LEU:HD22	2.02	0.41
1:E:581:GLN:HE21	1:E:583:ILE:HD11	1.85	0.41
1:E:607:VAL:HG21	1:E:642:LEU:HD13	2.02	0.41
1:F:484:GLY:HA3	1:F:501:GLN:OE1	2.20	0.41
1:A:468:MET:HB3	1:A:500:LEU:HD23	2.03	0.41
1:C:129:GLY:N	4:C:2008:HOH:O	2.54	0.41
1:E:41:THR:HG23	1:E:511:GLN:HG3	2.03	0.41
1:A:207:PRO:O	1:A:208:SER:C	2.59	0.41
1:C:268:ILE:HG22	1:C:286:LEU:HD21	2.03	0.41
1:D:179:HIS:HD2	1:D:181:HIS:ND1	2.18	0.41
1:E:35:LYS:O	1:E:242:GLN:NE2	2.54	0.41
1:E:544:GLY:O	1:E:547:LEU:HB2	2.21	0.41
1:F:661:LEU:CD1	4:F:2022:HOH:O	2.69	0.41
1:B:135:MET:HG2	1:B:137:ILE:HG13	2.01	0.41
1:B:259:ASN:ND2	1:B:538:ARG:HD2	2.36	0.41
1:C:535:TYR:H	1:C:655:LYS:HD3	1.86	0.41
1:C:585:LEU:HD23	1:C:585:LEU:HA	1.90	0.41
1:D:92:LEU:HD12	1:D:113:ASN:HD21	1.86	0.41
1:D:128:ARG:HD2	1:D:134:ASN:ND2	2.36	0.41
1:D:149:THR:O	1:D:187:GLY:HA3	2.21	0.41
1:B:132:PRO:HG3	1:B:253:THR:HG22	2.01	0.41
1:B:225:MET:CB	4:B:2025:HOH:O	2.39	0.41
1:B:378:PHE:CE1	1:B:382:ARG:HD3	2.56	0.41
1:B:558:ILE:HG12	1:C:384:LEU:HB3	2.03	0.41
1:C:611:LYS:HB3	1:C:612:PRO:HD3	2.03	0.41
1:D:574:TRP:HE1	1:D:585:LEU:HD12	1.86	0.41
1:E:46:ALA:O	1:E:49:LEU:HB2	2.20	0.41
1:E:132:PRO:HG3	1:E:253:THR:HG22	2.01	0.41
1:E:575:VAL:CG1	1:E:608:LYS:HG2	2.50	0.41
1:E:606:THR:O	1:E:635:LEU:HA	2.21	0.41
1:F:83:VAL:HG13	1:F:254:ALA:HB1	2.03	0.41
1:F:281:GLU:H	1:F:302:GLN:CD	2.24	0.41
1:B:274:ARG:CG	1:B:283:GLU:HG3	2.51	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:128:ARG:HD2	1:A:134:ASN:ND2	2.35	0.40
1:A:167:ARG:HA	1:A:168:PRO:HD3	1.91	0.40
1:D:150:LEU:O	1:D:187:GLY:N	2.53	0.40
1:C:97:ALA:HA	1:C:106:TRP:CD2	2.56	0.40
1:D:83:VAL:CG1	1:D:257:ALA:HB2	2.51	0.40
1:D:624:LEU:HB3	1:D:625:PRO:CD	2.46	0.40
1:E:384:LEU:O	1:E:388:ASN:ND2	2.54	0.40
1:F:230:GLN:HA	1:F:235:VAL:HG22	2.03	0.40
1:F:585:LEU:HD23	1:F:594:GLN:HB3	2.02	0.40
1:B:665:HIS:CD2	4:B:2071:HOH:O	2.74	0.40
1:D:575:VAL:HG13	1:D:608:LYS:HG2	2.02	0.40
1:B:174:ALA:HB1	1:B:205:PHE:HE2	1.86	0.40
1:B:404:PRO:HG2	1:B:407:LEU:HD12	2.02	0.40
1:D:45:ASN:ND2	1:D:99:ASP:O	2.53	0.40
1:A:189:ARG:HB2	1:A:260:THR:CB	2.51	0.40
1:B:46:ALA:O	1:B:49:LEU:HB2	2.22	0.40
1:C:641:LYS:HA	1:C:644:GLU:HG2	2.03	0.40
1:D:625:PRO:HA	1:D:628:ILE:HD12	2.02	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	632/668 (95%)	600 (95%)	30 (5%)	2 (0%)	41	76
1	B	635/668 (95%)	590 (93%)	45 (7%)	0	100	100
1	C	632/668 (95%)	598 (95%)	32 (5%)	2 (0%)	41	76
1	D	632/668 (95%)	585 (93%)	45 (7%)	2 (0%)	41	76
1	E	632/668 (95%)	593 (94%)	38 (6%)	1 (0%)	47	82
1	F	632/668 (95%)	591 (94%)	38 (6%)	3 (0%)	29	68

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
All	All	3795/4008 (95%)	3557 (94%)	228 (6%)	10 (0%)	41 76

All (10) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	290	SER
1	E	55	ALA
1	A	56	ASP
1	C	494	ASN
1	F	148	ASP
1	F	290	SER
1	F	604	ASP
1	C	55	ALA
1	D	290	SER
1	D	148	ASP

### 5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	511/538 (95%)	484 (95%)	27 (5%)	22 58
1	B	514/538 (96%)	489 (95%)	25 (5%)	25 61
1	C	511/538 (95%)	486 (95%)	25 (5%)	25 61
1	D	511/538 (95%)	487 (95%)	24 (5%)	26 63
1	E	511/538 (95%)	489 (96%)	22 (4%)	29 66
1	F	510/538 (95%)	490 (96%)	20 (4%)	32 69
All	All	3068/3228 (95%)	2925 (95%)	143 (5%)	26 63

All (143) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	40	ILE
1	A	44	LYS

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	A	49	LEU
1	A	56	ASP
1	A	95	LYS
1	A	261	LEU
1	A	262	VAL
1	A	276	THR
1	A	327	VAL
1	A	350	VAL
1	A	359	VAL
1	A	384	LEU
1	A	516	LEU
1	A	532	VAL
1	A	538	ARG
1	A	550	ASP
1	A	555	LEU
1	A	571	THR
1	A	586	THR
1	A	604	ASP
1	A	609	LEU
1	A	614	LEU
1	A	616	GLN
1	A	622	LEU
1	A	651	SER
1	A	661	LEU
1	A	663	HIS
1	B	49	LEU
1	B	95	LYS
1	B	101	VAL
1	B	144	LEU
1	B	253	THR
1	B	262	VAL
1	B	266	VAL
1	B	321	THR
1	B	327	VAL
1	B	351	LEU
1	B	353	GLN
1	B	359	VAL
1	B	365	VAL
1	B	384	LEU
1	B	409	ARG
1	B	532	VAL
1	B	538	ARG

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	B	571	THR
1	B	575	VAL
1	B	586	THR
1	B	614	LEU
1	B	616	GLN
1	B	622	LEU
1	B	624	LEU
1	B	661	LEU
1	C	58	GLU
1	C	79	GLU
1	C	95	LYS
1	C	99	ASP
1	C	147	ILE
1	C	262	VAL
1	C	327	VAL
1	C	348	THR
1	C	350	VAL
1	C	359	VAL
1	C	384	LEU
1	C	482	GLN
1	C	495	LYS
1	C	571	THR
1	C	583	ILE
1	C	586	THR
1	C	609	LEU
1	C	614	LEU
1	C	616	GLN
1	C	621	LYS
1	C	622	LEU
1	C	649	LEU
1	C	655	LYS
1	C	661	LEU
1	C	662	GLU
1	D	58	GLU
1	D	79	GLU
1	D	95	LYS
1	D	99	ASP
1	D	327	VAL
1	D	348	THR
1	D	353	GLN
1	D	384	LEU
1	D	399	GLU

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	D	482	GLN
1	D	516	LEU
1	D	534	THR
1	D	555	LEU
1	D	571	THR
1	D	583	ILE
1	D	586	THR
1	D	609	LEU
1	D	614	LEU
1	D	622	LEU
1	D	624	LEU
1	D	649	LEU
1	D	655	LYS
1	D	661	LEU
1	D	662	GLU
1	E	49	LEU
1	E	95	LYS
1	E	253	THR
1	E	262	VAL
1	E	266	VAL
1	E	314	PRO
1	E	327	VAL
1	E	353	GLN
1	E	384	LEU
1	E	402	LYS
1	E	409	ARG
1	E	448	VAL
1	E	500	LEU
1	E	516	LEU
1	E	538	ARG
1	E	555	LEU
1	E	571	THR
1	E	586	THR
1	E	614	LEU
1	E	622	LEU
1	E	659	VAL
1	E	661	LEU
1	F	58	GLU
1	F	95	LYS
1	F	147	ILE
1	F	261	LEU
1	F	262	VAL

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Mol	Chain	Res	Type
1	F	327	VAL
1	F	353	GLN
1	F	384	LEU
1	F	472	ILE
1	F	482	GLN
1	F	555	LEU
1	F	571	THR
1	F	583	ILE
1	F	586	THR
1	F	614	LEU
1	F	622	LEU
1	F	649	LEU
1	F	655	LYS
1	F	661	LEU
1	F	662	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (35) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	93	ASN
1	A	165	GLN
1	A	166	HIS
1	A	242	GLN
1	A	259	ASN
1	A	581	GLN
1	A	630	GLN
1	B	93	ASN
1	B	213	HIS
1	B	242	GLN
1	B	256	ASN
1	B	259	ASN
1	B	275	HIS
1	B	302	GLN
1	C	93	ASN
1	C	242	GLN
1	C	259	ASN
1	C	307	ASN
1	C	354	GLN
1	C	630	GLN
1	D	256	ASN
1	D	630	GLN
1	E	90	GLN

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Mol	Chain	Res	Type
1	E	112	ASN
1	E	242	GLN
1	E	302	GLN
1	E	356	ASN
1	E	568	HIS
1	E	581	GLN
1	E	616	GLN
1	E	630	GLN
1	F	93	ASN
1	F	242	GLN
1	F	302	GLN
1	F	630	GLN

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

Of 18 ligands modelled in this entry, 12 are monoatomic - leaving 6 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z  > 2$	Counts	RMSZ	$\# Z  > 2$
3	SO4	F	801	-	4,4,4	0.42	0	6,6,6	0.49	0
3	SO4	D	801	-	4,4,4	0.34	0	6,6,6	0.28	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
3	SO4	C	801	-	4,4,4	0.48	0	6,6,6	0.67	0
3	SO4	B	801	-	4,4,4	0.36	0	6,6,6	0.47	0
3	SO4	E	801	-	4,4,4	0.39	0	6,6,6	0.34	0
3	SO4	A	801	-	4,4,4	0.35	0	6,6,6	0.47	0

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

## 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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	634/668 (94%)	-0.37	2 (0%) 94 84	39, 65, 123, 163	0
1	B	637/668 (95%)	-0.14	18 (2%) 53 25	39, 81, 154, 190	0
1	C	634/668 (94%)	-0.39	2 (0%) 94 84	46, 75, 113, 163	0
1	D	634/668 (94%)	-0.08	15 (2%) 59 30	40, 88, 143, 191	0
1	E	634/668 (94%)	-0.23	4 (0%) 89 72	51, 87, 133, 177	0
1	F	634/668 (94%)	-0.08	14 (2%) 62 33	49, 99, 143, 179	0
All	All	3807/4008 (94%)	-0.22	55 (1%) 75 49	39, 82, 140, 191	0

All (55) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	142	SER	5.5
1	D	193	ASP	4.4
1	B	666	HIS	3.8
1	D	54	PHE	3.8
1	F	142	SER	3.6
1	D	192	ILE	3.5
1	B	192	ILE	3.4
1	B	197	VAL	3.4
1	D	630	GLN	3.4
1	C	54	PHE	3.3
1	F	171	PRO	3.2
1	B	266	VAL	3.2
1	B	282	LEU	3.2
1	D	172	ILE	3.1
1	F	172	ILE	3.1
1	D	163	TYR	3.0
1	B	264	PRO	3.0
1	B	280	VAL	2.9
1	B	276	THR	2.9

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Mol	Chain	Res	Type	RSRZ
1	B	205	PHE	2.9
1	D	633	VAL	2.8
1	B	140	GLY	2.7
1	D	282	LEU	2.7
1	B	277	VAL	2.7
1	B	143	GLY	2.7
1	F	143	GLY	2.5
1	F	64	LYS	2.5
1	D	194	GLU	2.5
1	F	276	THR	2.5
1	A	633	VAL	2.5
1	D	577	GLU	2.4
1	B	278	ASP	2.4
1	F	32	LEU	2.4
1	D	264	PRO	2.4
1	D	265	ASN	2.4
1	E	54	PHE	2.3
1	B	141	ASP	2.3
1	E	277	VAL	2.3
1	C	622	LEU	2.3
1	F	636	ASP	2.2
1	B	267	LEU	2.2
1	F	305	VAL	2.2
1	A	618	ALA	2.2
1	F	648	LEU	2.2
1	F	177	TYR	2.2
1	D	634	LYS	2.1
1	D	269	GLU	2.1
1	E	581	GLN	2.1
1	E	583	ILE	2.1
1	B	173	VAL	2.1
1	F	282	LEU	2.1
1	D	142	SER	2.1
1	F	205	PHE	2.0
1	F	124	LEU	2.0
1	B	139	GLU	2.0

## 6.2 Non-standard residues in protein, DNA, RNA chains

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

### 6.3 Carbohydrates [i](#)

There are no monosaccharides 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, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
3	SO4	C	801	5/5	0.95	0.27	64,66,75,87	0
3	SO4	F	801	5/5	0.95	0.23	84,94,102,102	0
3	SO4	B	801	5/5	0.97	0.19	77,78,82,90	0
2	ZN	D	700	1/1	0.97	0.17	85,85,85,85	0
2	ZN	D	701	1/1	0.97	0.17	80,80,80,80	0
3	SO4	A	801	5/5	0.98	0.23	53,55,59,60	0
2	ZN	C	700	1/1	0.98	0.21	68,68,68,68	0
2	ZN	F	700	1/1	0.98	0.14	80,80,80,80	0
2	ZN	F	701	1/1	0.98	0.17	84,84,84,84	0
2	ZN	B	701	1/1	0.99	0.18	70,70,70,70	0
2	ZN	B	700	1/1	0.99	0.15	64,64,64,64	0
2	ZN	E	700	1/1	0.99	0.15	73,73,73,73	0
2	ZN	E	701	1/1	0.99	0.18	68,68,68,68	0
3	SO4	D	801	5/5	0.99	0.23	76,77,81,88	0
3	SO4	E	801	5/5	0.99	0.23	72,74,75,81	0
2	ZN	C	701	1/1	0.99	0.17	50,50,50,50	0
2	ZN	A	700	1/1	1.00	0.17	53,53,53,53	0
2	ZN	A	701	1/1	1.00	0.16	47,47,47,47	0

### 6.5 Other polymers [i](#)

There are no such residues in this entry.