



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 12, 2026 – 06:35 AM UTC

PDB ID : 4AV7 / pdb_00004av7
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

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

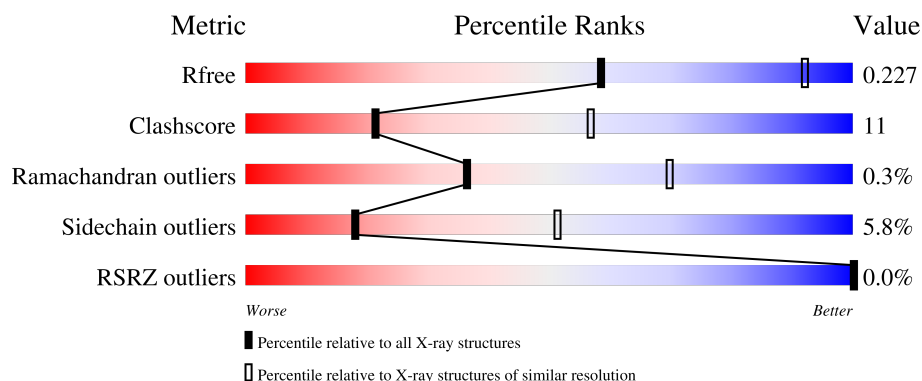
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

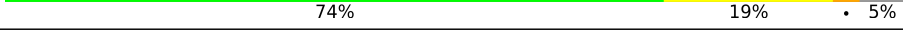
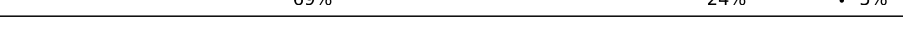
The reported resolution of this entry is 3.00 Å.

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}	180053	2672 (3.00-3.00)
Clashscore	190562	2977 (3.00-3.00)
Ramachandran outliers	187476	2877 (3.00-3.00)
Sidechain outliers	187428	2880 (3.00-3.00)
RSRZ outliers	180081	2671 (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 ≥ 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	 75% 18% • 5%
1	B	668	 65% 28% • 5%
1	C	668	 74% 19% • 5%
1	D	668	 69% 24% • 5%
1	E	668	 73% 20% • 5%

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Mol	Chain	Length	Quality of chain
1	F	668	71% 22% • 5%

2 Entry composition

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
1	A	634	Total	C	N	O	S	0	0	0
			4936	3125	863	929	19			
1	B	637	Total	C	N	O	S	0	0	0
			4966	3143	872	932	19			
1	C	634	Total	C	N	O	S	0	0	0
			4936	3125	863	929	19			
1	D	634	Total	C	N	O	S	0	0	0
			4936	3125	863	929	19			
1	E	634	Total	C	N	O	S	0	0	0
			4936	3125	863	929	19			
1	F	634	Total	C	N	O	S	0	0	0
			4930	3120	863	928	19			

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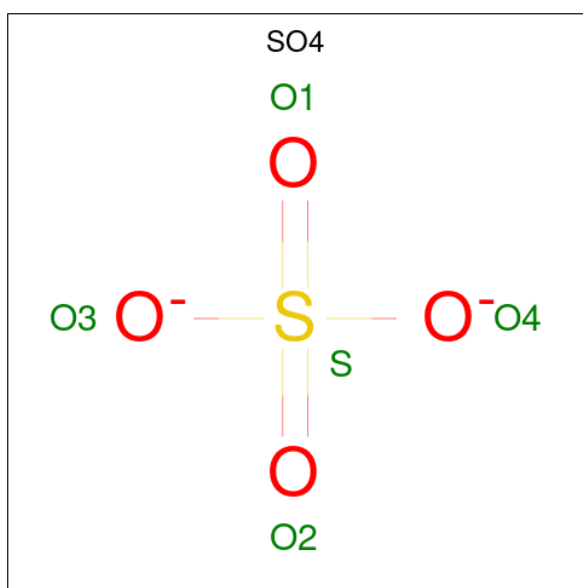
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Chain	Residue	Modelled	Actual	Comment	Reference
F	665	HIS	-	expression tag	UNP F8KAY7
F	666	HIS	-	expression tag	UNP F8KAY7
F	667	HIS	-	expression tag	UNP F8KAY7
F	668	HIS	-	expression tag	UNP F8KAY7
F	107	ARG	HIS	conflict	UNP F8KAY7
F	233	TYR	SER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

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



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

- Molecule 4 is water.

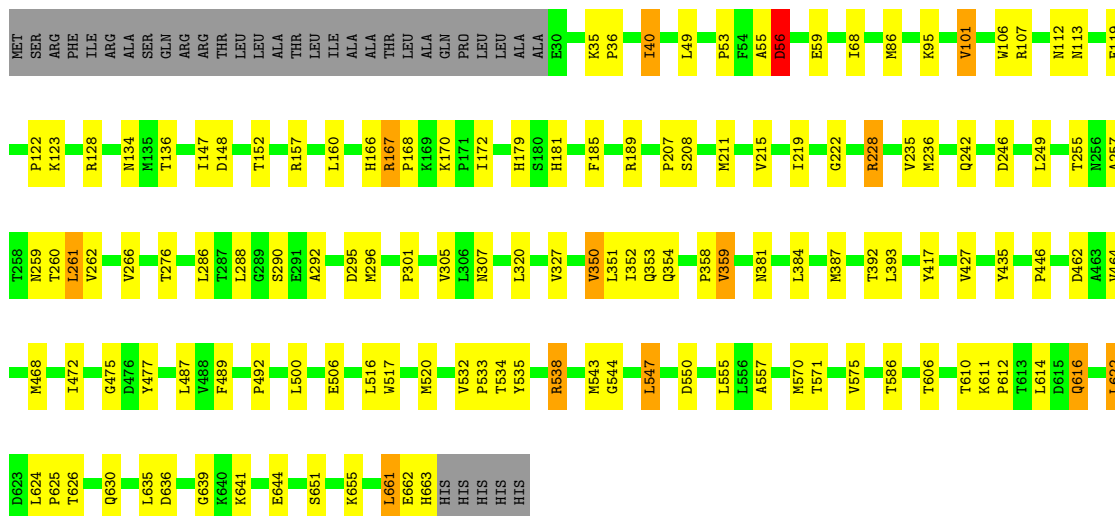
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	87	Total O 87 87	0	0
4	B	71	Total O 71 71	0	0
4	C	44	Total O 44 44	0	0
4	D	39	Total O 39 39	0	0
4	E	51	Total O 51 51	0	0
4	F	26	Total O 26 26	0	0

3 Residue-property plots

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.

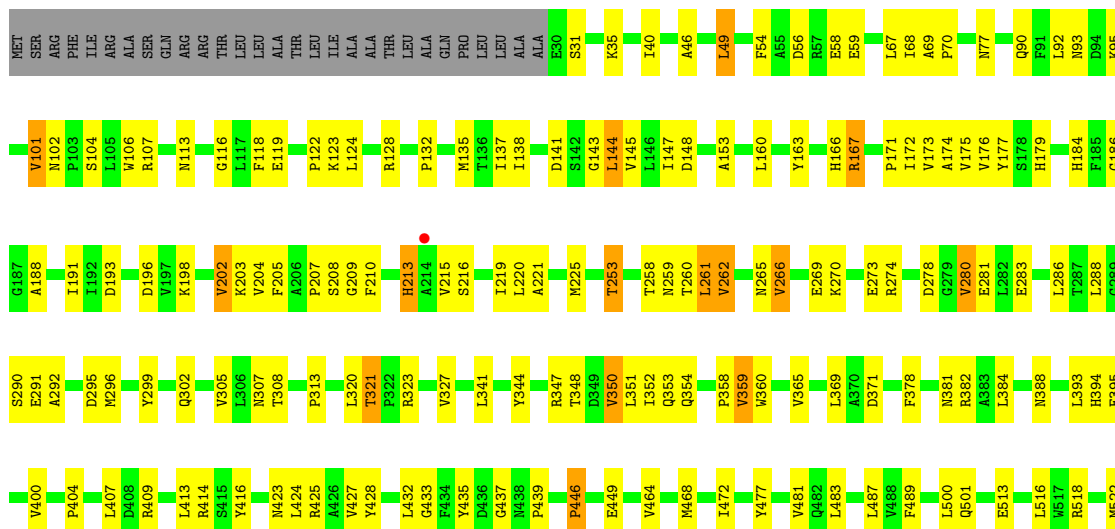
• Molecule 1: SEC-ALKYLSULFATASE

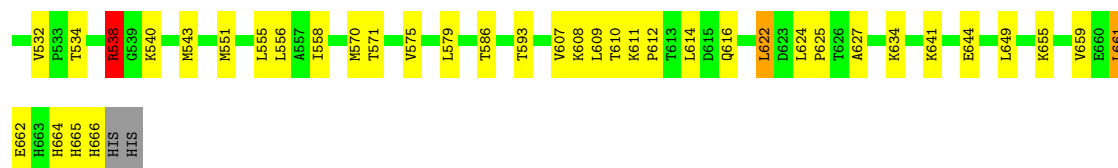
Chain A: 



• Molecule 1: SEC-ALKYLSULFATASE

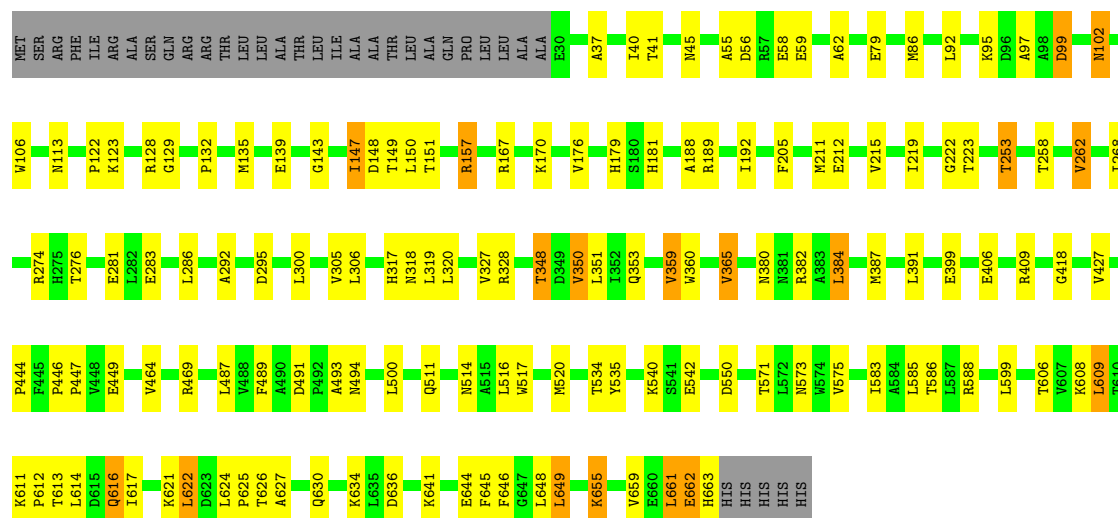
Chain B: 





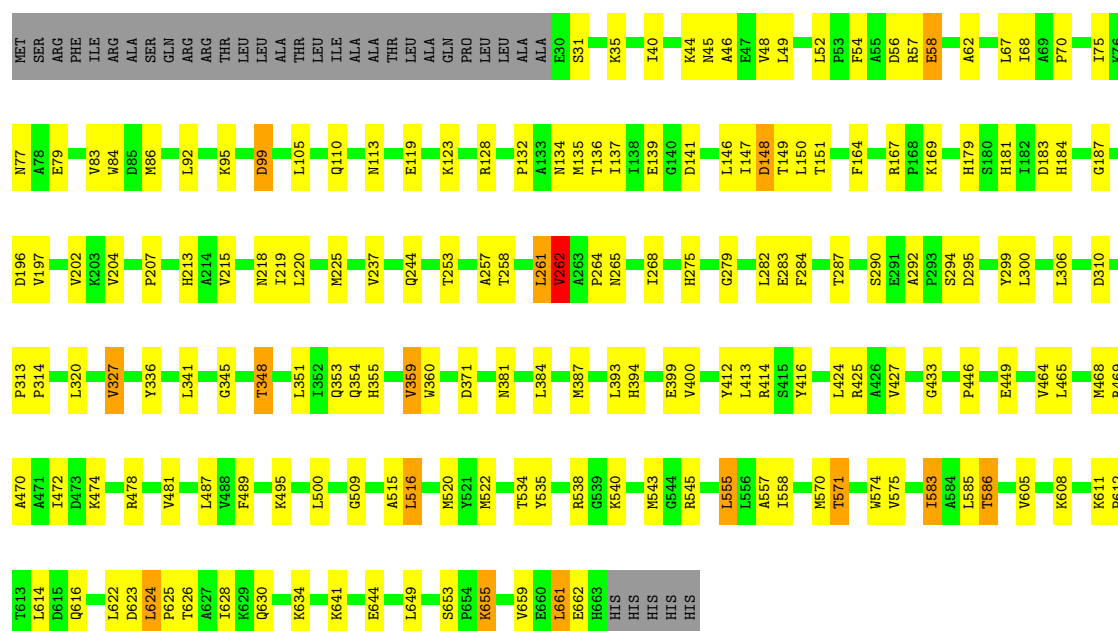
• Molecule 1: SEC-ALKYLSULFATASE

Chain C: 74% 19% 5%



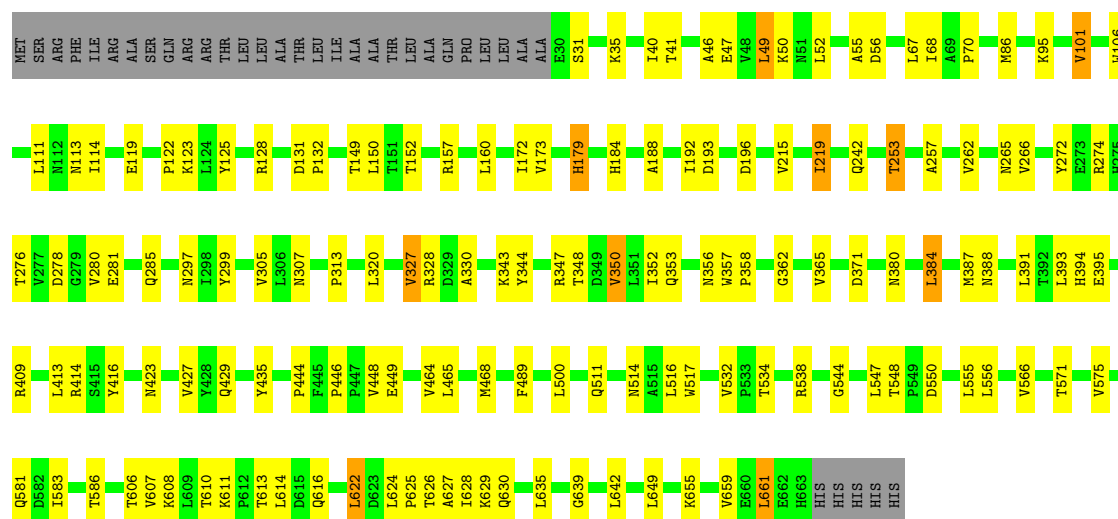
• Molecule 1: SEC-ALKYLSULFATASE

Chain D: 69% 24% 5%



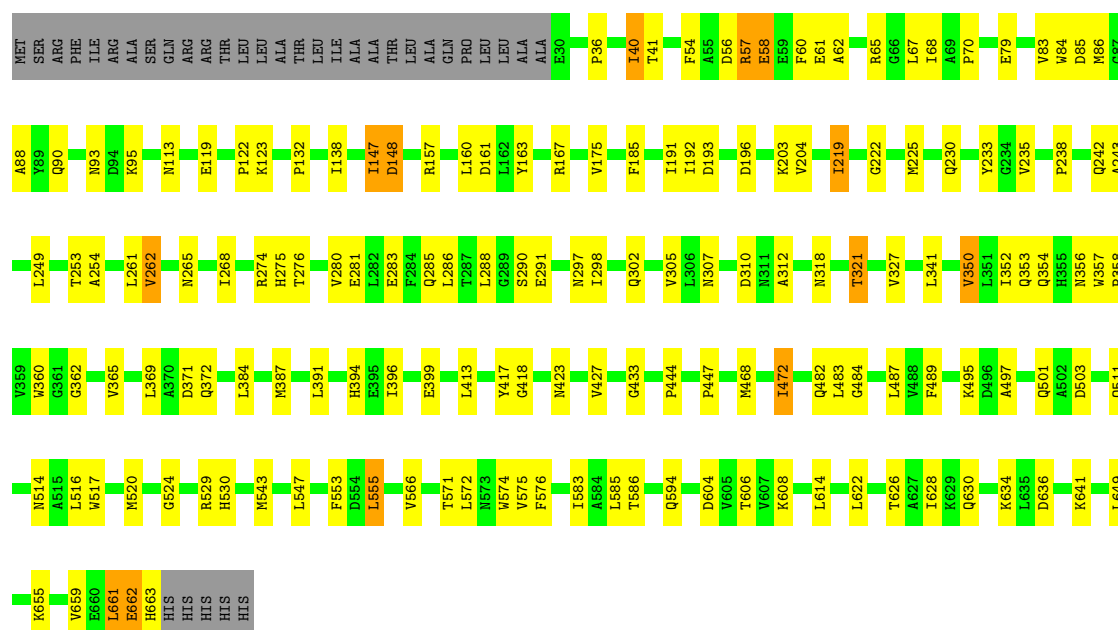
• Molecule 1: SEC-ALKYLSULFATASE

Chain E:  73% 20% • 5%



• Molecule 1: SEC-ALKYLSULFATASE

Chain F:  71% 22% • 5%



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	75.20Å 201.96Å 248.50Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	45.65 – 3.00 45.65 – 3.00	Depositor EDS
% Data completeness (in resolution range)	99.8 (45.65-3.00) 99.8 (45.65-3.00)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.18 (at 3.01Å)	Xtriage
Refinement program	REFMAC 5.6.0117	Depositor
R, R_{free}	0.186 , 0.256 (Not available) , 0.227	Depositor DCC
R_{free} test set	3840 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å ²)	78.9	Xtriage
Anisotropy	0.053	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 60.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.46$, $\langle L^2 \rangle = 0.29$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	30000	wwPDB-VP
Average B, all atoms (Å ²)	86.0	wwPDB-VP

Xtriage'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.*

¹Intensities estimated from amplitudes.

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

5 Model quality [i](#)

5.1 Standard geometry [i](#)

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

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	0.80	1/5041 (0.0%)	0.99	6/6838 (0.1%)
1	B	0.84	7/5074 (0.1%)	0.98	7/6883 (0.1%)
1	C	0.75	1/5041 (0.0%)	0.98	3/6838 (0.0%)
1	D	0.80	3/5041 (0.1%)	0.99	6/6838 (0.1%)
1	E	0.75	2/5041 (0.0%)	0.97	4/6838 (0.1%)
1	F	0.75	3/5034 (0.1%)	0.95	4/6828 (0.1%)
All	All	0.78	17/30272 (0.1%)	0.98	30/41063 (0.1%)

All (17) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	545	ARG	CZ-NH2	12.46	1.49	1.33
1	D	57	ARG	CZ-NH2	9.77	1.46	1.33
1	E	629	LYS	CD-CE	7.32	1.74	1.52
1	B	666	HIS	CG-CD2	7.17	1.43	1.35
1	A	446	PRO	CA-C	7.09	1.55	1.51
1	B	446	PRO	CA-C	6.83	1.55	1.51
1	B	202	VAL	CB-CG1	6.50	1.74	1.52
1	B	538	ARG	CZ-NH1	6.08	1.41	1.32
1	F	275	HIS	CG-CD2	5.61	1.42	1.35
1	B	666	HIS	CE1-NE2	5.49	1.38	1.32
1	B	213	HIS	CE1-NE2	5.43	1.38	1.32
1	E	56	ASP	CG-OD2	5.37	1.35	1.25
1	D	275	HIS	CG-CD2	5.32	1.41	1.35
1	B	166	HIS	CG-CD2	5.28	1.41	1.35
1	C	317	HIS	CG-CD2	5.23	1.41	1.35
1	F	530	HIS	CG-CD2	5.20	1.41	1.35
1	F	641	LYS	CE-NZ	5.01	1.64	1.49

All (30) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	545	ARG	NE-CZ-NH2	-9.78	110.39	119.20
1	D	545	ARG	NH1-CZ-NH2	9.65	131.84	119.30
1	B	381	ASN	N-CA-C	8.07	119.71	111.07
1	E	131	ASP	N-CA-C	-7.57	101.32	108.13
1	D	300	LEU	CA-C-N	7.17	126.70	119.24
1	D	300	LEU	C-N-CA	7.17	126.70	119.24
1	A	167	ARG	CA-C-N	6.31	126.68	119.93
1	A	167	ARG	C-N-CA	6.31	126.68	119.93
1	A	222	GLY	N-CA-C	5.80	119.23	112.50
1	E	179	HIS	N-CA-C	5.70	116.08	108.38
1	C	609	LEU	N-CA-C	5.70	115.76	108.24
1	B	116	GLY	N-CA-C	5.69	117.71	110.20
1	B	513	GLU	N-CA-C	-5.64	106.24	113.23
1	F	219	ILE	N-CA-C	5.59	116.03	111.62
1	C	102	ASN	CA-C-N	5.43	125.52	119.32
1	C	102	ASN	C-N-CA	5.43	125.52	119.32
1	A	228	ARG	N-CA-C	-5.38	105.98	112.54
1	E	188	ALA	N-CA-C	5.35	116.80	110.97
1	B	179	HIS	N-CA-C	5.27	116.29	108.60
1	B	167	ARG	CA-C-N	5.27	126.42	119.84
1	B	167	ARG	C-N-CA	5.27	126.42	119.84
1	B	662	GLU	N-CA-C	5.26	117.66	110.24
1	D	262	VAL	CB-CA-C	5.19	117.43	110.42
1	F	321	THR	CA-C-N	5.16	124.95	119.28
1	F	321	THR	C-N-CA	5.16	124.95	119.28
1	D	393	LEU	N-CA-C	5.14	117.55	111.33
1	E	387	MET	N-CA-C	-5.09	105.81	111.36
1	A	35	LYS	CA-C-N	-5.06	115.57	120.98
1	A	35	LYS	C-N-CA	-5.06	115.57	120.98
1	F	222	GLY	N-CA-C	5.02	118.75	112.73

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	4936	0	4889	88	0
1	B	4966	0	4910	160	0
1	C	4936	0	4889	96	0
1	D	4936	0	4889	130	0
1	E	4936	0	4889	89	0
1	F	4930	0	4884	93	0
2	A	2	0	0	0	0
2	B	2	0	0	0	0
2	C	2	0	0	0	0
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	14	0
4	F	26	0	0	10	0
All	All	30000	0	29350	641	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 11.

All (641) 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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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
4:B:2048:HOH:O	1:C:520:MET:HE2	1.74	0.86
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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
1:E:391:LEU:HD23	1:E:395:GLU:HB3	1.68	0.74
1:D:135:MET:HE3	1:D:150:LEU:HG	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
4:A:2068:HOH:O	1:D:520:MET:HE2	1.88	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
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:B:59:GLU:HB2	1:B:107:ARG:HH22	1.56	0.71
1:E:435:TYR:HE2	1:F:520:MET:HE1	1.56	0.70
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:D:225:MET:HE3	4:D:2013:HOH:O	1.90	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:C	4:B:2024:HOH:O	2.36	0.67
1:B:207:PRO:HG3	1:B:296:MET:HG2	1.76	0.67
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:E:313:PRO:HD2	4:E:2024:HOH:O	1.99	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:220:LEU:HD22	1:D:558:ILE:HD12	1.89	0.55
4:A:2068:HOH:O	1:D:520:MET:CE	2.51	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:F:56:ASP:C	1:F:58:GLU:H	2.15	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
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:C:387:MET:HE1	1:C:427:VAL:HG12	1.89	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:C:86:MET:HE1	1:C:113:ASN:HA	1.89	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:D:509:GLY:HA3	1:D:522:MET:HE2	1.90	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
1:D:608:LYS:HB2	1:D:634:LYS:HB2	1.90	0.53
1:B:435:TYR:HE2	1:C:520:MET:HE1	1.74	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:D:570:MET:HE1	1:D:644:GLU:HG3	1.91	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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:387:MET:HE1	1:D:427:VAL:HG12	1.91	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:207:PRO:C	4:D:2010:HOH:O	2.53	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: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:E:465:LEU:HA	1:E:468:MET:HE3	1.93	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
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:A:387:MET:HE1	1:A:427:VAL:HG12	1.95	0.49
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:514:ASN:HB3	1:C:517:TRP:HB2	1.93	0.49
1:D:218:ASN:C	1:D:219:ILE:HG13	2.36	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:296:MET:HE3	4:B:2034:HOH:O	2.14	0.48
1:B:428:TYR:CE1	1:B:432:LEU:HD12	2.49	0.48
1:E:435:TYR:CE2	1:F:520:MET:HE1	2.44	0.48
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:B:570:MET:HE1	1:B:644:GLU:HG3	1.95	0.48
1:C:464:VAL:HG23	1:C:487:LEU:HD22	1.95	0.48
1:F:86:MET:HE1	1:F:113:ASN:HA	1.96	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:605:VAL:C	4:D:2039:HOH:O	2.56	0.48
1:D:68:ILE:HD11	1:D:119:GLU:HB2	1.96	0.48
1:A:86:MET:HE1	1:A:113:ASN:HA	1.95	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
1:C:135:MET:HE3	1:C:150:LEU:HG	1.96	0.47
1:A:185:PHE:C	1:A:185:PHE:CD1	2.93	0.47
1:D:86:MET:HE1	1:D:113:ASN:HA	1.95	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:A:136:THR:HB	1:A:147:ILE:HB	1.97	0.46
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:F:122:PRO:O	1:F:123:LYS:HB2	2.15	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:A:207:PRO:O	1:A:208:SER:C	2.59	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:548:THR:OG1	1:E:550:ASP:OD1	2.32	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:F:281:GLU:H	1:F:302:GLN:CD	2.24	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:119:GLU:CD	4:E:2004:HOH:O	2.59	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
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:465:LEU:HA	1:D:468:MET:HE3	1.98	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:C:135:MET:HE2	1:C:149:THR:HA	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:185:PHE:CD1	1:F:185:PHE:C	2.95	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:54:PHE:C	1:B:56:ASP:H	2.26	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
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:D:653:SER:C	1:D:655:LYS:H	2.27	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:F:291:GLU:CD	1:F:310:ASP:HB2	2.43	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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:A:435:TYR:HE2	1:D:520:MET:HE1	1.84	0.42
1:C:56:ASP:C	1:C:58:GLU:H	2.28	0.42
1:F:524:GLY:HA2	1:F:659:VAL:HG11	2.02	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
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:387:MET:HE1	1:F:427:VAL:HG12	2.02	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:B:281:GLU:H	1:B:302:GLN:CD	2.28	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:86:MET:HE1	1:E:113:ASN:HA	2.02	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:A:517:TRP:HA	1:A:520:MET:HE3	2.01	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:259:ASN:CB	1:B:543:MET:HE2	2.51	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:B:274:ARG:CG	1:B:283:GLU:HG3	2.51	0.41
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:B:56:ASP:C	1:B:58:GLU:H	2.28	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:A:112:ASN:HD22	1:A:246:ASP:CG	2.30	0.40
1:A:570:MET:HE1	1:A:644:GLU:HG3	2.03	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 ⓘ

5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	283/668 (42%)	268 (95%)	13 (5%)	2 (1%)	18	53
1	B	301/668 (45%)	285 (95%)	16 (5%)	0	100	100
1	C	589/668 (88%)	558 (95%)	29 (5%)	2 (0%)	36	70
1	D	589/668 (88%)	543 (92%)	44 (8%)	2 (0%)	36	70
1	E	529/668 (79%)	495 (94%)	33 (6%)	1 (0%)	43	76
1	F	618/668 (92%)	579 (94%)	36 (6%)	3 (0%)	24	60
All	All	2909/4008 (73%)	2728 (94%)	171 (6%)	10 (0%)	36	70

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 ⓘ

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%)	483 (94%)	28 (6%)	19	53
1	B	514/538 (96%)	481 (94%)	33 (6%)	16	48
1	C	511/538 (95%)	482 (94%)	29 (6%)	18	52
1	D	511/538 (95%)	483 (94%)	28 (6%)	19	53
1	E	511/538 (95%)	482 (94%)	29 (6%)	18	52
1	F	510/538 (95%)	478 (94%)	32 (6%)	16	48
All	All	3068/3228 (95%)	2889 (94%)	179 (6%)	18	51

All (179) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	40	ILE
1	A	49	LEU
1	A	56	ASP
1	A	95	LYS
1	A	101	VAL
1	A	261	LEU
1	A	262	VAL

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Mol	Chain	Res	Type
1	A	266	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	547	LEU
1	A	550	ASP
1	A	555	LEU
1	A	571	THR
1	A	575	VAL
1	A	586	THR
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	198	LYS
1	B	219	ILE
1	B	253	THR
1	B	261	LEU
1	B	262	VAL
1	B	266	VAL
1	B	280	VAL
1	B	321	THR
1	B	327	VAL
1	B	350	VAL
1	B	353	GLN
1	B	359	VAL
1	B	365	VAL
1	B	384	LEU
1	B	409	ARG
1	B	483	LEU
1	B	516	LEU

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Mol	Chain	Res	Type
1	B	532	VAL
1	B	538	ARG
1	B	555	LEU
1	B	571	THR
1	B	575	VAL
1	B	586	THR
1	B	607	VAL
1	B	609	LEU
1	B	614	LEU
1	B	616	GLN
1	B	622	LEU
1	B	661	LEU
1	C	59	GLU
1	C	79	GLU
1	C	95	LYS
1	C	99	ASP
1	C	147	ILE
1	C	151	THR
1	C	157	ARG
1	C	192	ILE
1	C	253	THR
1	C	262	VAL
1	C	327	VAL
1	C	348	THR
1	C	350	VAL
1	C	359	VAL
1	C	365	VAL
1	C	384	LEU
1	C	571	THR
1	C	575	VAL
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

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Mol	Chain	Res	Type
1	D	79	GLU
1	D	95	LYS
1	D	99	ASP
1	D	261	LEU
1	D	262	VAL
1	D	268	ILE
1	D	327	VAL
1	D	348	THR
1	D	353	GLN
1	D	359	VAL
1	D	384	LEU
1	D	399	GLU
1	D	500	LEU
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	614	LEU
1	D	616	GLN
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	101	VAL
1	E	192	ILE
1	E	219	ILE
1	E	253	THR
1	E	262	VAL
1	E	266	VAL
1	E	274	ARG
1	E	327	VAL
1	E	350	VAL
1	E	353	GLN
1	E	384	LEU
1	E	409	ARG
1	E	448	VAL

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Mol	Chain	Res	Type
1	E	464	VAL
1	E	500	LEU
1	E	516	LEU
1	E	532	VAL
1	E	538	ARG
1	E	555	LEU
1	E	566	VAL
1	E	571	THR
1	E	586	THR
1	E	614	LEU
1	E	616	GLN
1	E	622	LEU
1	E	659	VAL
1	E	661	LEU
1	F	40	ILE
1	F	57	ARG
1	F	58	GLU
1	F	79	GLU
1	F	95	LYS
1	F	138	ILE
1	F	147	ILE
1	F	192	ILE
1	F	261	LEU
1	F	262	VAL
1	F	268	ILE
1	F	327	VAL
1	F	350	VAL
1	F	353	GLN
1	F	384	LEU
1	F	399	GLU
1	F	472	ILE
1	F	482	GLN
1	F	483	LEU
1	F	555	LEU
1	F	566	VAL
1	F	571	THR
1	F	575	VAL
1	F	583	ILE
1	F	586	THR
1	F	614	LEU
1	F	622	LEU
1	F	628	ILE

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Mol	Chain	Res	Type
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 (62) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	90	GLN
1	A	134	ASN
1	A	166	HIS
1	A	242	GLN
1	A	259	ASN
1	A	441	ASN
1	A	600	ASN
1	A	630	GLN
1	B	93	ASN
1	B	113	ASN
1	B	126	GLN
1	B	134	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	B	307	ASN
1	B	354	GLN
1	B	441	ASN
1	C	93	ASN
1	C	134	ASN
1	C	165	GLN
1	C	242	GLN
1	C	256	ASN
1	C	259	ASN
1	C	307	ASN
1	C	354	GLN
1	C	441	ASN
1	C	600	ASN
1	C	630	GLN
1	D	113	ASN
1	D	126	GLN

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Mol	Chain	Res	Type
1	D	165	GLN
1	D	259	ASN
1	D	353	GLN
1	D	356	ASN
1	D	381	ASN
1	D	441	ASN
1	D	630	GLN
1	E	90	GLN
1	E	110	GLN
1	E	302	GLN
1	E	307	ASN
1	E	441	ASN
1	E	568	HIS
1	E	581	GLN
1	E	600	ASN
1	E	616	GLN
1	E	630	GLN
1	F	93	ASN
1	F	165	GLN
1	F	242	GLN
1	F	259	ASN
1	F	302	GLN
1	F	307	ASN
1	F	311	ASN
1	F	354	GLN
1	F	441	ASN
1	F	600	ASN
1	F	630	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry [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	C	801	-	4,4,4	0.55	0	6,6,6	0.65	0
3	SO4	E	801	-	4,4,4	0.48	0	6,6,6	0.35	0
3	SO4	A	801	-	4,4,4	0.44	0	6,6,6	0.44	0
3	SO4	B	801	-	4,4,4	0.45	0	6,6,6	0.42	0
3	SO4	F	801	-	4,4,4	0.51	0	6,6,6	0.48	0
3	SO4	D	801	-	4,4,4	0.44	0	6,6,6	0.28	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 [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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	634/668 (94%)	-0.90	0 100 100	39, 65, 123, 163	0
1	B	637/668 (95%)	-0.61	1 (0%) 91 83	39, 81, 154, 190	0
1	C	634/668 (94%)	-0.83	0 100 100	46, 75, 113, 163	0
1	D	634/668 (94%)	-0.64	0 100 100	40, 88, 143, 191	0
1	E	634/668 (94%)	-0.71	0 100 100	51, 87, 133, 177	0
1	F	634/668 (94%)	-0.68	0 100 100	49, 99, 143, 179	0
All	All	3807/4008 (94%)	-0.73	1 (0%) 100 100	39, 82, 140, 191	0

All (1) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	214	ALA	2.1

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
3	SO4	C	801	5/5	0.92	0.08	64,66,75,87	0
3	SO4	B	801	5/5	0.94	0.12	77,78,82,90	0
3	SO4	F	801	5/5	0.95	0.09	84,94,102,102	0
3	SO4	E	801	5/5	0.97	0.06	72,74,75,81	0
3	SO4	D	801	5/5	0.97	0.08	76,77,81,88	0
3	SO4	A	801	5/5	0.99	0.04	53,55,59,60	0
2	ZN	C	700	1/1	0.99	0.05	68,68,68,68	0
2	ZN	D	701	1/1	0.99	0.02	80,80,80,80	0
2	ZN	E	700	1/1	1.00	0.01	73,73,73,73	0
2	ZN	E	701	1/1	1.00	0.03	68,68,68,68	0
2	ZN	F	700	1/1	1.00	0.03	80,80,80,80	0
2	ZN	F	701	1/1	1.00	0.04	84,84,84,84	0
2	ZN	B	700	1/1	1.00	0.02	64,64,64,64	0
2	ZN	B	701	1/1	1.00	0.02	70,70,70,70	0
2	ZN	A	700	1/1	1.00	0.04	53,53,53,53	0
2	ZN	C	701	1/1	1.00	0.04	50,50,50,50	0
2	ZN	D	700	1/1	1.00	0.03	85,85,85,85	0
2	ZN	A	701	1/1	1.00	0.03	47,47,47,47	0

6.5 Other polymers ⓘ

There are no such residues in this entry.