



# Full wwPDB X-ray Structure Validation Report ⓘ

Jan 31, 2016 – 10:24 PM GMT

PDB ID : 1TD9  
Title : Crystal Structure of a Phosphotransacetylase from *Bacillus subtilis*  
Authors : Xu, Q.S.; Jancarik, J.; Yokota, H.; Kim, R.; Kim, S.-H.; Berkeley Structural Genomics Center (BSGC)  
Deposited on : 2004-05-21  
Resolution : 2.75 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  
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>  
with specific help available everywhere you see the ⓘ symbol.

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

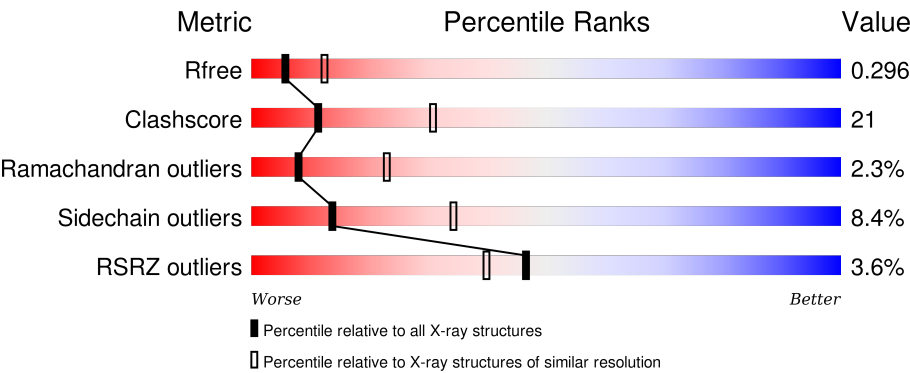
# 1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.75 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	91344	3340 (2.80-2.72)
Clashscore	102246	3829 (2.80-2.72)
Ramachandran outliers	100387	3767 (2.80-2.72)
Sidechain outliers	100360	3770 (2.80-2.72)
RSRZ outliers	91569	3352 (2.80-2.72)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions  $\leq 5\%$ . The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	329	<div><div>2%</div><div>63%31%5%.</div></div>
1	B	329	<div><div>2%</div><div>60%33%6%.</div></div>
1	C	329	<div><div>2%</div><div>61%33%5%.</div></div>
1	D	329	<div><div>2%</div><div>57%36%6%.</div></div>
1	E	329	<div><div>2%</div><div>61%31%6%.</div></div>

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Mol	Chain	Length	Quality of chain
1	F	329	

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	SO4	A	408	-	-	-	X
2	SO4	D	413	-	-	-	X
2	SO4	E	422	-	-	-	X

## 2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 14916 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 Phosphate acetyltransferase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	323	Total	C	N	O	S	0	0	0
			2445	1545	407	484	9			
1	B	324	Total	C	N	O	S	0	0	0
			2449	1547	408	485	9			
1	C	323	Total	C	N	O	S	0	0	0
			2445	1545	407	484	9			
1	D	325	Total	C	N	O	S	0	0	0
			2453	1549	409	486	9			
1	E	323	Total	C	N	O	S	0	0	0
			2445	1545	407	484	9			
1	F	323	Total	C	N	O	S	0	0	0
			2445	1545	407	484	9			

There are 42 discrepancies between the modelled and reference sequences:

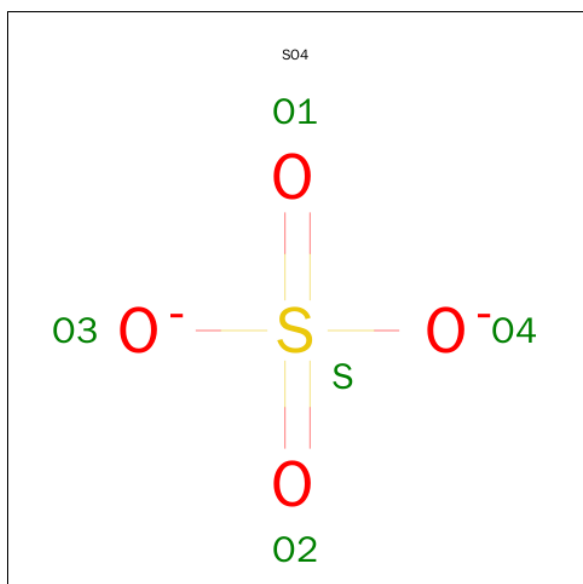
Chain	Residue	Modelled	Actual	Comment	Reference
A	-5	GLY	-	CLONING ARTIFACT	UNP P39646
A	-4	GLY	-	CLONING ARTIFACT	UNP P39646
A	-3	GLY	-	CLONING ARTIFACT	UNP P39646
A	-2	GLY	-	CLONING ARTIFACT	UNP P39646
A	-1	GLY	-	CLONING ARTIFACT	UNP P39646
A	0	GLY	-	CLONING ARTIFACT	UNP P39646
A	1	MET	-	INITIATING MET	UNP P39646
B	-5	GLY	-	CLONING ARTIFACT	UNP P39646
B	-4	GLY	-	CLONING ARTIFACT	UNP P39646
B	-3	GLY	-	CLONING ARTIFACT	UNP P39646
B	-2	GLY	-	CLONING ARTIFACT	UNP P39646
B	-1	GLY	-	CLONING ARTIFACT	UNP P39646
B	0	GLY	-	CLONING ARTIFACT	UNP P39646
B	1	MET	-	INITIATING MET	UNP P39646
C	-5	GLY	-	CLONING ARTIFACT	UNP P39646
C	-4	GLY	-	CLONING ARTIFACT	UNP P39646
C	-3	GLY	-	CLONING ARTIFACT	UNP P39646

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Chain	Residue	Modelled	Actual	Comment	Reference
C	-2	GLY	-	CLONING ARTIFACT	UNP P39646
C	-1	GLY	-	CLONING ARTIFACT	UNP P39646
C	0	GLY	-	CLONING ARTIFACT	UNP P39646
C	1	MET	-	INITIATING MET	UNP P39646
D	-5	GLY	-	CLONING ARTIFACT	UNP P39646
D	-4	GLY	-	CLONING ARTIFACT	UNP P39646
D	-3	GLY	-	CLONING ARTIFACT	UNP P39646
D	-2	GLY	-	CLONING ARTIFACT	UNP P39646
D	-1	GLY	-	CLONING ARTIFACT	UNP P39646
D	0	GLY	-	CLONING ARTIFACT	UNP P39646
D	1	MET	-	INITIATING MET	UNP P39646
E	-5	GLY	-	CLONING ARTIFACT	UNP P39646
E	-4	GLY	-	CLONING ARTIFACT	UNP P39646
E	-3	GLY	-	CLONING ARTIFACT	UNP P39646
E	-2	GLY	-	CLONING ARTIFACT	UNP P39646
E	-1	GLY	-	CLONING ARTIFACT	UNP P39646
E	0	GLY	-	CLONING ARTIFACT	UNP P39646
E	1	MET	-	INITIATING MET	UNP P39646
F	-5	GLY	-	CLONING ARTIFACT	UNP P39646
F	-4	GLY	-	CLONING ARTIFACT	UNP P39646
F	-3	GLY	-	CLONING ARTIFACT	UNP P39646
F	-2	GLY	-	CLONING ARTIFACT	UNP P39646
F	-1	GLY	-	CLONING ARTIFACT	UNP P39646
F	0	GLY	-	CLONING ARTIFACT	UNP P39646
F	1	MET	-	INITIATING MET	UNP P39646

- Molecule 2 is SULFATE ION (three-letter code: SO4) (formula: O<sub>4</sub>S).



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

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

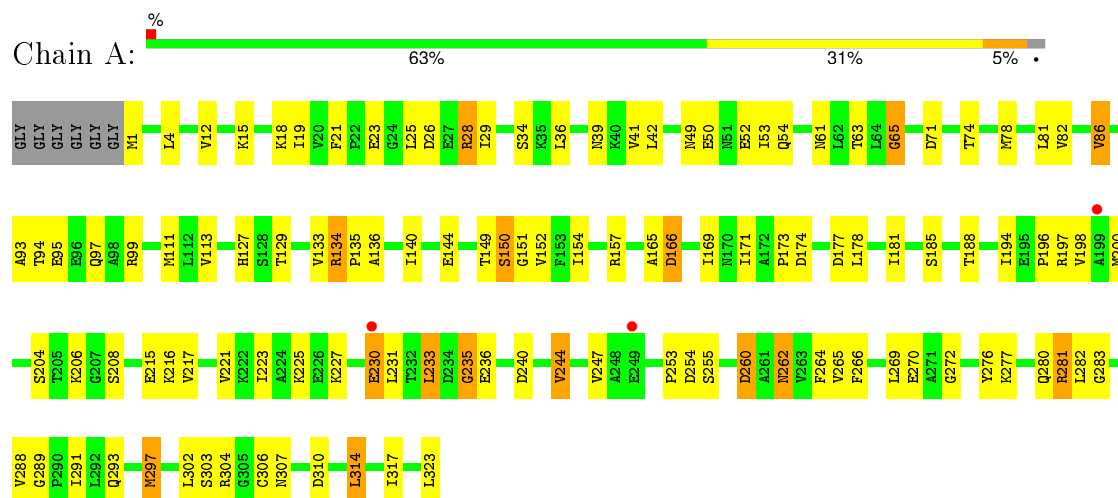
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	25	Total	O	0	0
			25	25		
3	B	18	Total	O	0	0
			18	18		
3	C	26	Total	O	0	0
			26	26		
3	D	18	Total	O	0	0
			18	18		
3	E	20	Total	O	0	0
			20	20		
3	F	7	Total	O	0	0
			7	7		

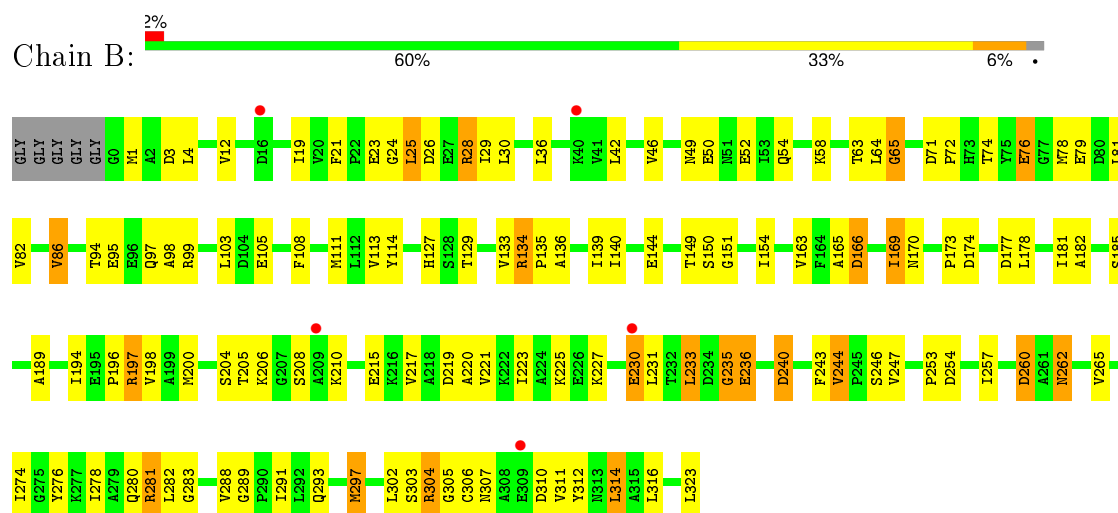
### 3 Residue-property plots

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

#### • Molecule 1: Phosphate acetyltransferase



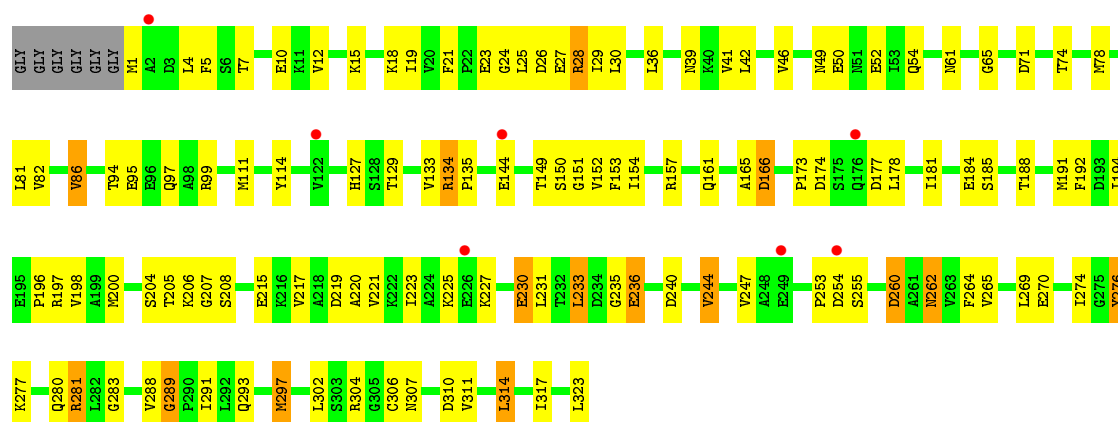
#### • Molecule 1: Phosphate acetyltransferase



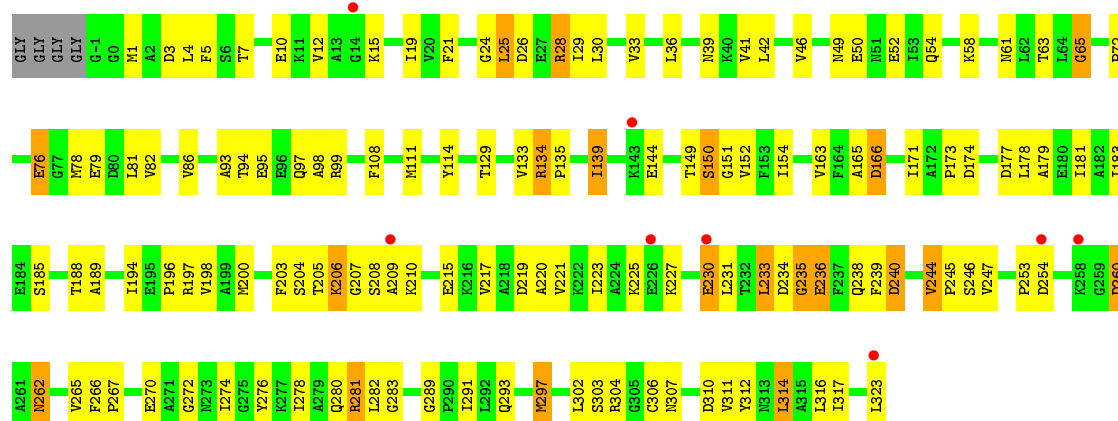
#### • Molecule 1: Phosphate acetyltransferase



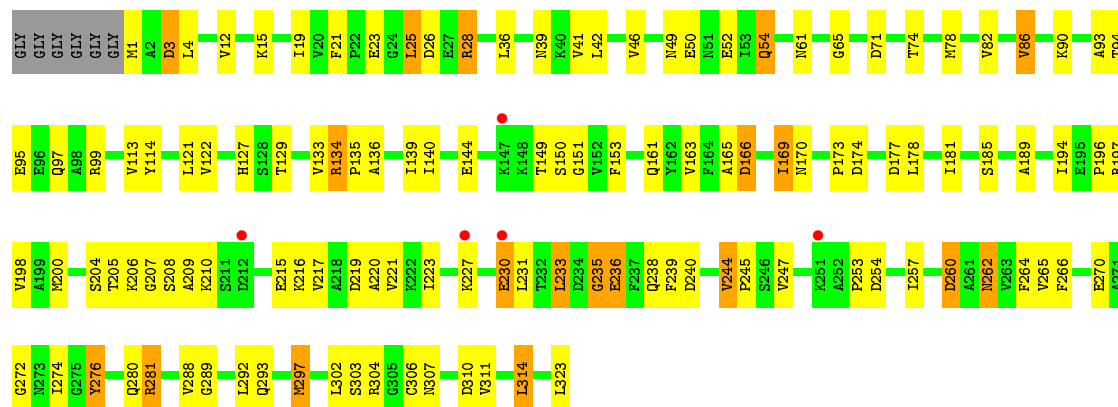




• Molecule 1: Phosphate acetyltransferase

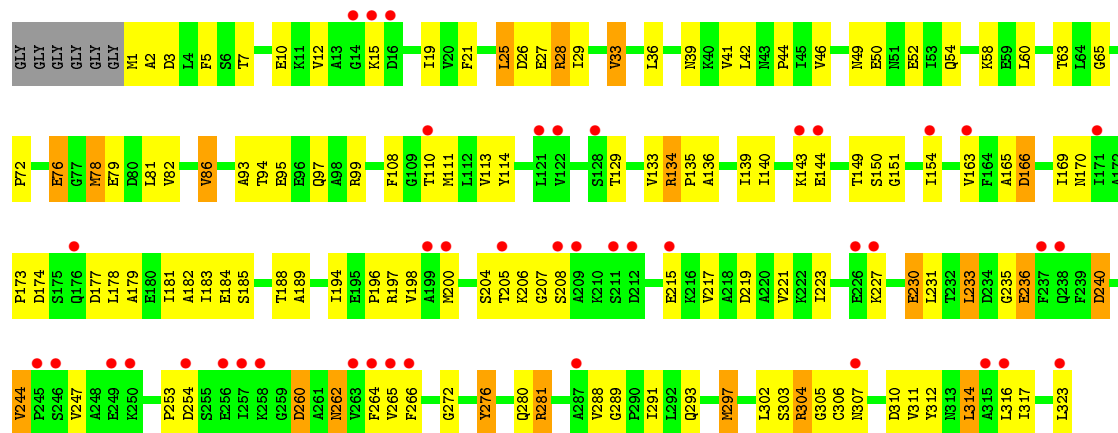


• Molecule 1: Phosphate acetyltransferase



• Molecule 1: Phosphate acetyltransferase





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 64 2 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	185.21Å 185.21Å 259.41Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	19.99 – 2.75 19.99 – 2.75	Depositor EDS
% Data completeness (in resolution range)	94.5 (19.99-2.75) 94.6 (19.99-2.75)	Depositor EDS
$R_{merge}$	0.12	Depositor
$R_{sym}$	0.12	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.29 (at 2.75Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, $R_{free}$	0.268 , 0.297 0.267 , 0.296	Depositor DCC
$R_{free}$ test set	1958 reflections (3.03%)	DCC
Wilson B-factor (Å <sup>2</sup> )	45.6	Xtriage
Anisotropy	0.695	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.32 , 56.4	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtriage
Outliers	6 of 64636 reflections (0.009%)	Xtriage
$F_o, F_c$ correlation	0.92	EDS
Total number of atoms	14916	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	53.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 53.77 % of the origin peak, indicating pseudo translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo translational symmetry is equal to 4.0172e-05. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

<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, 0.375 respectively for untwinned datasets, and 0.333, 0.2 for perfectly twinned datasets.

## 5 Model quality ⓘ

### 5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: 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	0.48	0/2479	0.75	2/3346 (0.1%)
1	B	0.45	0/2483	0.75	3/3351 (0.1%)
1	C	0.47	0/2479	0.74	1/3346 (0.0%)
1	D	0.44	0/2487	0.74	3/3356 (0.1%)
1	E	0.48	0/2479	0.74	2/3346 (0.1%)
1	F	0.45	0/2479	0.72	2/3346 (0.1%)
All	All	0.46	0/14886	0.74	13/20091 (0.1%)

There are no bond length outliers.

All (13) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	260	ASP	CB-CG-OD2	6.96	124.57	118.30
1	D	260	ASP	CB-CG-OD2	6.94	124.55	118.30
1	F	260	ASP	CB-CG-OD2	6.58	124.22	118.30
1	E	260	ASP	CB-CG-OD2	6.54	124.19	118.30
1	C	260	ASP	CB-CG-OD2	6.15	123.83	118.30
1	B	197	ARG	NE-CZ-NH1	5.84	123.22	120.30
1	A	260	ASP	CB-CG-OD2	5.76	123.48	118.30
1	B	235	GLY	N-CA-C	5.56	127.00	113.10
1	E	235	GLY	N-CA-C	5.36	126.49	113.10
1	A	235	GLY	N-CA-C	5.31	126.39	113.10
1	D	235	GLY	N-CA-C	5.27	126.27	113.10
1	F	29	ILE	CG1-CB-CG2	-5.03	100.33	111.40
1	D	238	GLN	N-CA-C	-5.00	97.50	111.00

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	2445	0	2468	97	0
1	B	2449	0	2471	112	0
1	C	2445	0	2468	104	0
1	D	2453	0	2474	117	0
1	E	2445	0	2468	106	0
1	F	2445	0	2468	104	0
2	A	25	0	0	0	0
2	B	20	0	0	0	0
2	C	25	0	0	0	0
2	D	20	0	0	1	0
2	E	20	0	0	0	0
2	F	10	0	0	0	0
3	A	25	0	0	2	0
3	B	18	0	0	4	0
3	C	26	0	0	3	0
3	D	18	0	0	2	0
3	E	20	0	0	0	0
3	F	7	0	0	1	0
All	All	14916	0	14817	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 21.

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:A:165:ALA:HB3	1:A:265:VAL:HA	1.30	1.14
1:C:165:ALA:HB3	1:C:265:VAL:HA	1.30	1.13
1:D:165:ALA:HB3	1:D:265:VAL:HA	1.32	1.11
1:B:165:ALA:HB3	1:B:265:VAL:HA	1.34	1.08
1:E:165:ALA:HB3	1:E:265:VAL:HA	1.33	1.07
1:F:165:ALA:HB3	1:F:265:VAL:HA	1.37	1.03
1:A:204:SER:HB2	1:A:208:SER:HB2	1.49	0.95
1:C:204:SER:HB2	1:C:208:SER:HB2	1.50	0.93
1:B:204:SER:HB2	1:B:208:SER:HB2	1.51	0.93

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:221:VAL:HG21	1:E:235:GLY:HA3	1.51	0.92
1:B:221:VAL:HG21	1:B:235:GLY:HA3	1.51	0.92
1:A:94:THR:OG1	1:A:97:GLN:HG3	1.72	0.90
1:E:204:SER:HB2	1:E:208:SER:HB2	1.53	0.90
1:D:204:SER:HB2	1:D:208:SER:HB2	1.57	0.87
1:C:231:LEU:HD12	1:C:233:LEU:HD23	1.55	0.86
1:A:198:VAL:HB	1:A:233:LEU:HB2	1.58	0.86
1:F:204:SER:HB2	1:F:208:SER:HB2	1.59	0.84
1:C:198:VAL:HB	1:C:233:LEU:HB2	1.60	0.84
1:C:49:ASN:HD22	1:C:52:GLU:H	1.24	0.83
1:C:94:THR:OG1	1:C:97:GLN:HG3	1.79	0.83
1:E:165:ALA:CB	1:E:265:VAL:HA	2.10	0.82
1:E:231:LEU:HD12	1:E:233:LEU:HD23	1.61	0.82
1:B:94:THR:OG1	1:B:97:GLN:HG3	1.80	0.82
1:B:198:VAL:O	1:B:257:ILE:HD11	1.80	0.82
1:A:49:ASN:HD22	1:A:52:GLU:H	1.29	0.81
1:E:280:GLN:HG2	1:E:281:ARG:HD2	1.63	0.81
1:F:198:VAL:HB	1:F:233:LEU:HB2	1.62	0.81
1:E:198:VAL:HB	1:E:233:LEU:HB2	1.61	0.81
1:D:198:VAL:HB	1:D:233:LEU:HB2	1.62	0.80
1:F:165:ALA:CB	1:F:265:VAL:HA	2.11	0.80
1:F:49:ASN:HD22	1:F:52:GLU:H	1.27	0.80
1:D:94:THR:OG1	1:D:97:GLN:HG3	1.82	0.79
1:F:280:GLN:HG2	1:F:281:ARG:HD2	1.63	0.79
1:E:198:VAL:O	1:E:257:ILE:HD11	1.81	0.79
1:B:198:VAL:HB	1:B:233:LEU:HB2	1.64	0.79
1:C:244:VAL:HG22	1:C:247:VAL:HG23	1.64	0.79
1:E:200:MET:HG3	1:E:221:VAL:HG22	1.65	0.78
1:E:94:THR:OG1	1:E:97:GLN:HG3	1.83	0.78
1:F:244:VAL:HG22	1:F:247:VAL:HG23	1.65	0.77
1:C:280:GLN:HG2	1:C:281:ARG:HD2	1.66	0.77
1:F:302:LEU:HD23	1:F:314:LEU:HD12	1.65	0.76
1:A:165:ALA:CB	1:A:265:VAL:HA	2.13	0.76
1:E:240:ASP:HB3	1:E:247:VAL:HG11	1.68	0.76
1:B:165:ALA:CB	1:B:265:VAL:HA	2.15	0.75
1:F:94:THR:OG1	1:F:97:GLN:HG3	1.86	0.75
1:B:221:VAL:CG2	1:B:235:GLY:HA3	2.16	0.75
1:E:221:VAL:CG2	1:E:235:GLY:HA3	2.17	0.74
3:B:515:HOH:O	1:F:58:LYS:HE3	1.88	0.74
1:E:169:ILE:HD11	1:E:292:LEU:CD2	2.18	0.74
1:C:165:ALA:CB	1:C:265:VAL:HA	2.13	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:231:LEU:HD12	1:A:233:LEU:HD23	1.70	0.73
1:B:197:ARG:H	1:B:262:ASN:HD21	1.35	0.73
1:E:49:ASN:HD22	1:E:52:GLU:H	1.33	0.73
1:B:280:GLN:HG2	1:B:281:ARG:HD2	1.71	0.72
1:D:165:ALA:CB	1:D:265:VAL:HA	2.15	0.72
1:F:154:ILE:HD12	1:F:154:ILE:N	2.04	0.72
1:F:36:LEU:HD13	1:F:42:LEU:HD11	1.73	0.71
1:E:244:VAL:HG22	1:E:247:VAL:HG23	1.73	0.71
1:D:231:LEU:HD12	1:D:233:LEU:HD23	1.71	0.70
1:A:61:ASN:CA	1:D:63:THR:HB	2.22	0.70
1:B:200:MET:HG3	1:B:221:VAL:HG22	1.74	0.70
1:D:221:VAL:HG21	1:D:235:GLY:HA3	1.72	0.70
1:B:49:ASN:HD22	1:B:52:GLU:H	1.40	0.69
1:E:1:MET:O	1:E:4:LEU:HB3	1.92	0.69
1:A:173:PRO:HB2	1:A:178:LEU:HD22	1.75	0.69
1:D:114:TYR:HA	1:D:297:MET:HE2	1.72	0.69
1:B:72:PRO:HG3	1:B:108:PHE:CD1	2.27	0.69
1:F:302:LEU:CD2	1:F:314:LEU:HD12	2.23	0.69
1:F:307:ASN:HB3	1:F:310:ASP:OD2	1.93	0.69
1:E:177:ASP:O	1:E:181:ILE:HG12	1.93	0.68
1:A:28:ARG:HH12	1:A:306:CYS:H	1.42	0.68
1:C:200:MET:HG3	1:C:221:VAL:HG22	1.74	0.68
1:B:114:TYR:HA	1:B:297:MET:HE2	1.75	0.68
1:E:197:ARG:NH1	1:E:260:ASP:O	2.25	0.68
1:F:58:LYS:HD2	3:F:552:HOH:O	1.93	0.67
1:A:36:LEU:HD13	1:A:42:LEU:HD11	1.76	0.67
1:C:231:LEU:CD1	1:C:233:LEU:HD23	2.23	0.67
1:D:303:SER:O	1:D:306:CYS:HB3	1.94	0.67
1:D:49:ASN:HD22	1:D:52:GLU:H	1.41	0.67
1:F:197:ARG:H	1:F:262:ASN:HD21	1.43	0.67
1:B:231:LEU:HD12	1:B:233:LEU:HD23	1.75	0.67
1:B:219:ASP:O	1:B:223:ILE:HG12	1.94	0.67
1:E:173:PRO:HB2	1:E:178:LEU:HD22	1.77	0.66
1:C:157:ARG:NH2	1:D:282:LEU:O	2.28	0.66
1:F:173:PRO:HB2	1:F:178:LEU:HD22	1.78	0.66
1:D:154:ILE:N	1:D:154:ILE:HD12	2.10	0.66
1:D:36:LEU:HD13	1:D:42:LEU:HD11	1.77	0.66
1:D:200:MET:HG3	1:D:221:VAL:HG22	1.79	0.65
1:F:231:LEU:HD12	1:F:233:LEU:HD23	1.78	0.65
1:B:173:PRO:HB2	1:B:178:LEU:HD22	1.79	0.65
1:A:280:GLN:HG2	1:A:281:ARG:HD2	1.79	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:200:MET:HG3	1:F:221:VAL:HG22	1.79	0.65
1:A:244:VAL:HG22	1:A:247:VAL:HG23	1.77	0.65
1:C:1:MET:O	1:C:4:LEU:HB3	1.97	0.65
1:B:240:ASP:HB3	1:B:247:VAL:HG11	1.78	0.64
1:F:154:ILE:HD13	1:F:288:VAL:HG11	1.78	0.64
1:D:280:GLN:HG2	1:D:281:ARG:HD2	1.78	0.64
1:A:221:VAL:HG21	1:A:235:GLY:HA3	1.79	0.64
1:E:36:LEU:HD13	1:E:42:LEU:HD11	1.79	0.64
1:D:1:MET:CE	1:D:4:LEU:HD23	2.27	0.64
1:A:240:ASP:HB3	1:A:247:VAL:HG11	1.78	0.64
1:F:28:ARG:HH12	1:F:306:CYS:H	1.44	0.64
1:D:114:TYR:HA	1:D:297:MET:CE	2.27	0.64
1:D:307:ASN:HB3	1:D:310:ASP:OD2	1.97	0.64
1:D:197:ARG:NH1	1:D:260:ASP:O	2.27	0.63
1:F:72:PRO:HG3	1:F:108:PHE:CD1	2.33	0.63
1:E:197:ARG:H	1:E:262:ASN:HD21	1.45	0.63
1:F:197:ARG:N	1:F:262:ASN:HD21	1.96	0.63
1:F:219:ASP:O	1:F:223:ILE:HG13	1.99	0.62
1:D:221:VAL:CG2	1:D:235:GLY:HA3	2.29	0.62
1:C:127:HIS:HB2	3:C:558:HOH:O	1.98	0.62
1:B:58:LYS:HD2	3:B:605:HOH:O	1.98	0.62
1:C:198:VAL:HB	1:C:233:LEU:CB	2.29	0.62
1:B:303:SER:O	1:B:306:CYS:HB3	1.99	0.62
1:D:270:GLU:O	1:D:274:ILE:HG12	2.00	0.62
1:C:240:ASP:HB3	1:C:247:VAL:HG11	1.82	0.62
1:D:173:PRO:HB2	1:D:178:LEU:HD22	1.82	0.62
1:B:197:ARG:N	1:B:262:ASN:HD21	1.98	0.61
1:C:129:THR:O	1:C:133:VAL:HG12	2.00	0.61
1:A:177:ASP:O	1:A:181:ILE:HG12	2.00	0.61
1:C:173:PRO:HB2	1:C:178:LEU:HD22	1.81	0.61
1:C:197:ARG:H	1:C:262:ASN:HD21	1.48	0.61
1:B:36:LEU:HD13	1:B:42:LEU:HD11	1.81	0.61
1:A:302:LEU:HD23	1:A:314:LEU:HD12	1.81	0.61
1:A:221:VAL:CG2	1:A:235:GLY:HA3	2.31	0.61
1:D:152:VAL:HG22	1:D:291:ILE:HB	1.82	0.61
1:A:154:ILE:N	1:A:154:ILE:HD12	2.16	0.60
1:D:231:LEU:CD1	1:D:233:LEU:HD23	2.31	0.60
1:A:174:ASP:O	1:A:178:LEU:HD23	2.01	0.60
1:A:28:ARG:HH12	1:A:306:CYS:N	1.98	0.60
1:C:5:PHE:HE2	1:C:317:ILE:HD11	1.65	0.60
1:D:28:ARG:HH12	1:D:306:CYS:H	1.48	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:197:ARG:NH1	1:A:260:ASP:O	2.29	0.60
1:A:134:ARG:HB3	1:A:135:PRO:CD	2.31	0.60
1:F:49:ASN:ND2	1:F:52:GLU:H	1.99	0.60
1:B:114:TYR:HA	1:B:297:MET:CE	2.31	0.60
1:A:113:VAL:O	1:A:297:MET:HE2	2.02	0.60
1:C:36:LEU:HD13	1:C:42:LEU:HD11	1.83	0.60
1:A:291:ILE:HD12	1:A:317:ILE:HG21	1.83	0.60
1:B:63:THR:HB	1:C:61:ASN:CA	2.32	0.60
1:C:49:ASN:ND2	1:C:52:GLU:H	1.98	0.60
1:D:177:ASP:O	1:D:181:ILE:HG12	2.03	0.59
1:B:1:MET:O	1:B:4:LEU:HB3	2.02	0.59
1:C:152:VAL:HG22	1:C:291:ILE:HB	1.83	0.59
1:C:177:ASP:O	1:C:181:ILE:HG12	2.03	0.59
1:B:302:LEU:HD23	1:B:314:LEU:HD12	1.84	0.59
1:E:39:ASN:HB2	1:E:41:VAL:HG23	1.85	0.59
1:E:169:ILE:HD11	1:E:292:LEU:HD23	1.84	0.59
1:F:233:LEU:HD12	1:F:233:LEU:C	2.23	0.58
1:C:23:GLU:OE1	1:C:127:HIS:HD2	1.86	0.58
1:B:307:ASN:HB3	1:B:310:ASP:OD2	2.04	0.58
1:F:221:VAL:HG21	1:F:235:GLY:HA3	1.85	0.58
1:A:19:ILE:HG22	1:A:21:PHE:CE1	2.38	0.58
1:E:198:VAL:HB	1:E:233:LEU:CB	2.30	0.58
1:A:61:ASN:C	1:D:63:THR:HB	2.23	0.58
1:B:194:ILE:O	1:B:196:PRO:HD3	2.03	0.58
1:C:244:VAL:CG2	1:C:247:VAL:HG23	2.32	0.58
1:C:197:ARG:N	1:C:262:ASN:HD21	2.01	0.58
1:F:82:VAL:O	1:F:86:VAL:HG13	2.03	0.58
1:E:217:VAL:O	1:E:221:VAL:HG23	2.04	0.58
1:E:174:ASP:O	1:E:178:LEU:HD23	2.03	0.58
1:D:151:GLY:O	1:D:166:ASP:HA	2.03	0.58
1:B:233:LEU:C	1:B:233:LEU:HD12	2.25	0.57
1:B:197:ARG:NH1	1:B:260:ASP:O	2.34	0.57
1:A:1:MET:O	1:A:4:LEU:HB3	2.04	0.57
1:E:134:ARG:HB3	1:E:135:PRO:CD	2.34	0.57
1:D:240:ASP:HB3	1:D:247:VAL:HG11	1.85	0.57
1:D:244:VAL:HG22	1:D:247:VAL:HG23	1.86	0.57
1:F:81:LEU:HD22	1:F:111:MET:HB3	1.86	0.57
1:C:95:GLU:HG2	1:C:99:ARG:NH2	2.19	0.57
1:E:113:VAL:O	1:E:297:MET:HE2	2.05	0.57
1:A:233:LEU:HD12	1:A:233:LEU:C	2.23	0.57
1:E:231:LEU:CD1	1:E:233:LEU:HD23	2.32	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:303:SER:O	1:F:306:CYS:HB3	2.05	0.57
1:E:61:ASN:OD1	1:F:63:THR:HG22	2.04	0.57
1:A:1:MET:CE	1:A:288:VAL:HG23	2.35	0.57
1:E:135:PRO:O	1:E:139:ILE:HG12	2.05	0.57
1:A:23:GLU:OE1	1:A:127:HIS:HD2	1.86	0.57
1:F:114:TYR:HA	1:F:297:MET:HE2	1.86	0.57
1:D:129:THR:O	1:D:133:VAL:HG12	2.05	0.56
1:C:114:TYR:HA	1:C:297:MET:HE2	1.87	0.56
1:F:165:ALA:HB1	1:F:181:ILE:HG22	1.87	0.56
1:F:198:VAL:HB	1:F:233:LEU:CB	2.35	0.56
1:E:197:ARG:N	1:E:262:ASN:HD21	2.02	0.56
1:B:134:ARG:HB3	1:B:135:PRO:CD	2.34	0.56
1:F:188:THR:OG1	1:F:293:GLN:NE2	2.39	0.56
1:A:200:MET:HG3	1:A:221:VAL:HG22	1.88	0.56
1:D:72:PRO:HG3	1:D:108:PHE:CD1	2.41	0.56
1:D:194:ILE:O	1:D:196:PRO:HD3	2.06	0.56
1:F:163:VAL:HG21	1:F:189:ALA:HB2	1.87	0.56
1:C:134:ARG:HB3	1:C:135:PRO:CD	2.35	0.56
1:C:12:VAL:HA	1:C:323:LEU:HD11	1.86	0.56
1:E:136:ALA:O	1:E:140:ILE:O	2.25	0.55
1:A:151:GLY:O	1:A:166:ASP:HA	2.07	0.55
1:D:198:VAL:HB	1:D:233:LEU:CB	2.35	0.55
1:A:61:ASN:HA	1:D:63:THR:HB	1.88	0.55
1:A:240:ASP:CB	1:A:247:VAL:HG11	2.37	0.55
1:B:26:ASP:OD2	1:B:28:ARG:HB2	2.07	0.55
1:B:28:ARG:HH12	1:B:306:CYS:H	1.53	0.55
1:C:82:VAL:O	1:C:86:VAL:HG13	2.05	0.55
1:B:231:LEU:CD1	1:B:233:LEU:HD23	2.36	0.55
1:F:244:VAL:CG2	1:F:247:VAL:HG23	2.36	0.55
1:D:179:ALA:O	1:D:183:ILE:HG12	2.06	0.55
1:E:270:GLU:O	1:E:274:ILE:HG12	2.07	0.55
1:F:94:THR:HG1	1:F:97:GLN:HG3	1.72	0.55
1:D:188:THR:OG1	1:D:293:GLN:NE2	2.40	0.55
1:C:23:GLU:HB2	1:C:29:ILE:HD12	1.88	0.54
1:B:63:THR:HB	1:C:61:ASN:HA	1.89	0.54
1:B:29:ILE:HD13	1:B:311:VAL:HG11	1.90	0.54
1:E:28:ARG:HH12	1:E:306:CYS:H	1.53	0.54
1:A:277:LYS:NZ	1:B:240:ASP:OD2	2.40	0.54
1:D:197:ARG:N	1:D:262:ASN:HD21	2.05	0.54
1:B:151:GLY:O	1:B:166:ASP:HA	2.07	0.54
1:F:197:ARG:NH1	1:F:260:ASP:O	2.38	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:233:LEU:C	1:E:233:LEU:HD12	2.28	0.54
1:C:281:ARG:HG3	1:C:281:ARG:HH11	1.71	0.54
1:F:28:ARG:HG2	1:F:28:ARG:HH11	1.72	0.54
1:D:174:ASP:O	1:D:178:LEU:HD23	2.07	0.54
1:D:135:PRO:O	1:D:139:ILE:HG12	2.08	0.54
1:D:12:VAL:HA	1:D:323:LEU:HD11	1.90	0.54
1:A:129:THR:O	1:A:133:VAL:HG12	2.08	0.54
1:B:198:VAL:HB	1:B:233:LEU:CB	2.36	0.53
1:F:19:ILE:HG22	1:F:21:PHE:CE1	2.43	0.53
1:D:154:ILE:H	1:D:154:ILE:HD12	1.72	0.53
1:C:1:MET:HE1	1:C:288:VAL:HG23	1.90	0.53
1:C:151:GLY:O	1:C:166:ASP:HA	2.09	0.53
1:C:28:ARG:HH12	1:C:306:CYS:H	1.56	0.53
1:A:198:VAL:HB	1:A:233:LEU:CB	2.31	0.53
1:B:244:VAL:HG22	1:B:247:VAL:HG23	1.90	0.53
1:F:205:THR:HA	1:F:236:GLU:O	2.09	0.53
1:A:152:VAL:HG22	1:A:291:ILE:HB	1.90	0.53
1:D:185:SER:HA	1:D:293:GLN:HE22	1.72	0.53
1:C:302:LEU:HD21	1:C:311:VAL:HA	1.90	0.53
1:B:177:ASP:O	1:B:181:ILE:HG13	2.08	0.53
1:F:221:VAL:CG2	1:F:235:GLY:HA3	2.39	0.53
1:C:174:ASP:O	1:C:178:LEU:HD23	2.08	0.53
1:B:302:LEU:CD2	1:B:314:LEU:HD12	2.38	0.53
1:A:302:LEU:CD2	1:A:314:LEU:HD12	2.38	0.53
1:B:136:ALA:O	1:B:140:ILE:O	2.26	0.53
1:B:12:VAL:HA	1:B:323:LEU:HD11	1.90	0.53
1:B:81:LEU:HD22	1:B:111:MET:HB3	1.91	0.53
1:E:23:GLU:OE1	1:E:127:HIS:HD2	1.92	0.53
1:C:205:THR:HA	1:C:236:GLU:O	2.09	0.53
1:D:217:VAL:O	1:D:221:VAL:HG23	2.09	0.53
1:F:154:ILE:HD13	1:F:288:VAL:CG1	2.38	0.52
1:A:1:MET:HE1	1:A:288:VAL:HG23	1.91	0.52
1:A:307:ASN:HB3	1:A:310:ASP:OD2	2.09	0.52
1:D:29:ILE:HD13	1:D:311:VAL:HG11	1.89	0.52
1:D:134:ARG:HG2	1:D:134:ARG:HH11	1.73	0.52
1:C:283:GLY:HA2	1:D:283:GLY:HA2	1.90	0.52
1:A:157:ARG:NH2	1:B:282:LEU:O	2.42	0.52
1:C:270:GLU:O	1:C:274:ILE:HG12	2.09	0.52
1:A:169:ILE:N	1:A:169:ILE:HD12	2.24	0.52
1:D:81:LEU:HD22	1:D:111:MET:HB3	1.91	0.52
1:B:82:VAL:O	1:B:86:VAL:HG13	2.09	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:197:ARG:NH1	1:C:260:ASP:O	2.36	0.52
1:A:197:ARG:N	1:A:262:ASN:HD21	2.08	0.52
1:D:233:LEU:C	1:D:233:LEU:HD12	2.30	0.52
1:A:197:ARG:H	1:A:262:ASN:HD21	1.58	0.52
1:C:240:ASP:CB	1:C:247:VAL:HG11	2.40	0.52
1:D:26:ASP:OD2	1:D:28:ARG:HB2	2.09	0.52
1:C:233:LEU:HD12	1:C:233:LEU:C	2.30	0.51
1:A:150:SER:HB3	1:A:181:ILE:HD12	1.91	0.51
1:B:185:SER:HA	1:B:293:GLN:HE22	1.75	0.51
1:E:134:ARG:HH11	1:E:134:ARG:HG2	1.75	0.51
1:D:1:MET:HE1	1:D:4:LEU:HD23	1.92	0.51
1:F:217:VAL:O	1:F:221:VAL:HG23	2.11	0.51
1:F:12:VAL:HA	1:F:323:LEU:HD11	1.92	0.51
1:F:253:PRO:O	1:F:254:ASP:HB2	2.10	0.51
1:F:165:ALA:HB1	1:F:181:ILE:CG2	2.41	0.51
1:D:58:LYS:HD2	3:D:512:HOH:O	2.10	0.51
1:A:231:LEU:CD1	1:A:233:LEU:HD23	2.38	0.51
1:F:266:PHE:CD2	1:F:272:GLY:HA2	2.46	0.51
1:B:23:GLU:OE1	1:B:127:HIS:HD2	1.93	0.51
1:E:19:ILE:HG22	1:E:21:PHE:CE1	2.46	0.51
1:F:93:ALA:HA	1:F:97:GLN:OE1	2.11	0.51
1:D:1:MET:O	1:D:4:LEU:HB3	2.11	0.51
1:E:71:ASP:HB3	1:E:74:THR:HB	1.93	0.51
1:F:177:ASP:O	1:F:181:ILE:HG13	2.11	0.50
1:F:129:THR:O	1:F:133:VAL:HG12	2.11	0.50
1:F:76:GLU:HA	1:F:76:GLU:OE1	2.11	0.50
1:A:15:LYS:N	1:A:15:LYS:HD2	2.26	0.50
1:A:26:ASP:OD2	1:A:28:ARG:HB2	2.12	0.50
1:E:82:VAL:O	1:E:86:VAL:HG13	2.12	0.50
1:A:61:ASN:HD21	1:D:65:GLY:HA3	1.76	0.50
1:E:307:ASN:HB3	1:E:310:ASP:OD2	2.12	0.50
1:C:5:PHE:CE2	1:C:317:ILE:HD11	2.47	0.50
1:C:114:TYR:HA	1:C:297:MET:CE	2.41	0.50
1:A:39:ASN:HB2	1:A:41:VAL:HG23	1.93	0.50
1:D:197:ARG:H	1:D:262:ASN:HD21	1.58	0.50
1:C:194:ILE:O	1:C:196:PRO:HD3	2.12	0.50
1:C:302:LEU:HD23	1:C:314:LEU:HD12	1.93	0.50
1:D:253:PRO:O	1:D:254:ASP:HB2	2.12	0.50
1:D:93:ALA:HA	1:D:97:GLN:OE1	2.12	0.49
1:E:1:MET:CE	1:E:288:VAL:HG23	2.43	0.49
1:E:240:ASP:CB	1:E:247:VAL:HG11	2.41	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:307:ASN:HB3	1:B:310:ASP:CG	2.32	0.49
1:C:219:ASP:O	1:C:223:ILE:HG13	2.12	0.49
1:E:50:GLU:O	1:E:54:GLN:HB2	2.13	0.49
1:F:7:THR:O	1:F:10:GLU:HB3	2.12	0.49
1:C:253:PRO:O	1:C:254:ASP:HB2	2.12	0.49
1:A:94:THR:HG1	1:A:97:GLN:HG3	1.76	0.49
1:C:94:THR:HG1	1:C:97:GLN:HG3	1.75	0.49
1:A:23:GLU:HB2	1:A:29:ILE:HD12	1.94	0.49
1:C:262:ASN:HD22	1:C:262:ASN:H	1.61	0.49
1:C:277:LYS:HD2	3:C:534:HOH:O	2.11	0.49
1:E:244:VAL:CG2	1:E:247:VAL:HG23	2.40	0.49
1:B:165:ALA:HB1	1:B:181:ILE:HG22	1.94	0.49
1:B:225:LYS:HE3	1:B:233:LEU:O	2.13	0.49
1:C:39:ASN:HB2	1:C:41:VAL:HG23	1.95	0.49
1:C:307:ASN:HB3	1:C:310:ASP:OD2	2.13	0.48
1:F:230:GLU:H	1:F:230:GLU:CD	2.15	0.48
1:A:82:VAL:O	1:A:86:VAL:HG13	2.13	0.48
1:E:219:ASP:O	1:E:223:ILE:HG13	2.13	0.48
1:E:12:VAL:HA	1:E:323:LEU:HD11	1.94	0.48
1:E:28:ARG:HH12	1:E:306:CYS:N	2.09	0.48
1:E:302:LEU:HD23	1:E:314:LEU:HD12	1.95	0.48
1:F:240:ASP:HB3	1:F:247:VAL:HG11	1.95	0.48
1:D:1:MET:SD	1:D:4:LEU:HD23	2.53	0.48
1:A:134:ARG:HB3	1:A:135:PRO:HD2	1.94	0.48
1:C:28:ARG:HH12	1:C:306:CYS:N	2.11	0.48
1:C:277:LYS:HB3	1:D:239:PHE:HB3	1.96	0.48
1:A:185:SER:HA	1:A:293:GLN:HE22	1.77	0.48
1:B:235:GLY:O	1:B:236:GLU:HB3	2.13	0.48
1:D:94:THR:HG1	1:D:97:GLN:HG3	1.74	0.48
1:B:230:GLU:N	1:B:230:GLU:OE1	2.46	0.48
1:D:7:THR:O	1:D:10:GLU:HB3	2.14	0.48
1:E:151:GLY:O	1:E:166:ASP:HA	2.14	0.48
1:E:194:ILE:O	1:E:196:PRO:HD3	2.14	0.48
1:C:221:VAL:HG21	1:C:235:GLY:HA3	1.96	0.48
1:F:262:ASN:HD22	1:F:262:ASN:H	1.62	0.48
1:E:114:TYR:HA	1:E:297:MET:HE2	1.95	0.48
3:A:573:HOH:O	1:B:274:ILE:HG12	2.13	0.48
1:D:5:PHE:HE2	1:D:317:ILE:HD11	1.78	0.48
1:A:262:ASN:HD22	1:A:262:ASN:H	1.61	0.48
1:B:134:ARG:HH11	1:B:134:ARG:HG2	1.78	0.48
1:A:231:LEU:HD13	1:A:233:LEU:HB3	1.96	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:134:ARG:HH11	1:A:134:ARG:HG2	1.78	0.47
1:B:135:PRO:O	1:B:139:ILE:HG12	2.13	0.47
1:B:169:ILE:HG22	1:B:170:ASN:N	2.29	0.47
1:E:61:ASN:CA	1:F:63:THR:HB	2.44	0.47
1:C:19:ILE:HG22	1:C:21:PHE:CE1	2.49	0.47
1:D:205:THR:HA	1:D:236:GLU:O	2.13	0.47
1:D:28:ARG:HG2	1:D:28:ARG:HH11	1.78	0.47
1:F:114:TYR:HA	1:F:297:MET:CE	2.44	0.47
1:F:134:ARG:HB3	1:F:135:PRO:CD	2.43	0.47
1:B:113:VAL:O	1:B:297:MET:HE2	2.14	0.47
1:F:28:ARG:HH12	1:F:306:CYS:N	2.10	0.47
1:D:307:ASN:HB3	1:D:310:ASP:CG	2.34	0.47
1:F:134:ARG:HG2	1:F:134:ARG:HH11	1.79	0.47
1:A:71:ASP:HB3	1:A:74:THR:HB	1.97	0.47
1:D:163:VAL:HG21	1:D:189:ALA:HB2	1.96	0.47
1:E:114:TYR:HA	1:E:297:MET:CE	2.44	0.47
1:B:129:THR:O	1:B:133:VAL:HG12	2.15	0.47
1:A:136:ALA:O	1:A:140:ILE:O	2.32	0.47
1:B:217:VAL:O	1:B:221:VAL:HG23	2.15	0.47
1:C:134:ARG:HB3	1:C:135:PRO:HD2	1.96	0.47
1:D:49:ASN:ND2	1:D:52:GLU:H	2.11	0.47
1:B:303:SER:C	1:B:304:ARG:O	2.49	0.47
1:D:219:ASP:O	1:D:223:ILE:HG13	2.15	0.47
1:E:281:ARG:HH11	1:E:281:ARG:HG3	1.79	0.47
1:F:231:LEU:CD1	1:F:233:LEU:HD23	2.43	0.47
1:D:1:MET:HE3	1:D:4:LEU:HB3	1.96	0.47
1:F:179:ALA:O	1:F:183:ILE:HG12	2.15	0.47
1:E:129:THR:O	1:E:133:VAL:HG12	2.15	0.47
1:F:151:GLY:O	1:F:166:ASP:HA	2.15	0.47
1:B:95:GLU:HG2	1:B:99:ARG:NH2	2.29	0.47
1:D:165:ALA:HB1	1:D:181:ILE:CG2	2.45	0.47
1:D:235:GLY:O	1:D:236:GLU:HB3	2.15	0.47
1:E:1:MET:O	1:E:4:LEU:N	2.46	0.47
1:A:281:ARG:HB3	1:B:243:PHE:HD2	1.80	0.47
1:B:24:GLY:O	1:B:30:LEU:HD21	2.15	0.47
1:B:71:ASP:HB3	1:B:74:THR:HB	1.97	0.47
1:B:29:ILE:HD13	1:B:311:VAL:CG1	2.45	0.46
1:B:246:SER:OG	1:D:3:ASP:OD1	2.32	0.46
1:D:302:LEU:HD23	1:D:314:LEU:HD12	1.96	0.46
1:F:185:SER:HA	1:F:293:GLN:HE22	1.79	0.46
1:A:61:ASN:OD1	1:D:63:THR:HG22	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:113:VAL:O	1:F:297:MET:HE2	2.15	0.46
1:C:307:ASN:O	1:C:311:VAL:HG23	2.14	0.46
1:D:29:ILE:HD13	1:D:311:VAL:CG1	2.46	0.46
1:A:253:PRO:O	1:A:254:ASP:HB2	2.14	0.46
1:C:15:LYS:N	1:C:15:LYS:HD2	2.30	0.46
1:F:244:VAL:HG22	1:F:244:VAL:O	2.14	0.46
1:A:266:PHE:CD2	1:A:272:GLY:HA2	2.51	0.46
1:B:28:ARG:HH11	1:B:28:ARG:HG2	1.79	0.46
1:B:217:VAL:O	1:B:220:ALA:HB3	2.16	0.46
1:D:225:LYS:HE3	1:D:233:LEU:O	2.16	0.46
1:E:134:ARG:HB3	1:E:135:PRO:HD2	1.97	0.46
1:F:50:GLU:O	1:F:54:GLN:HB2	2.16	0.46
1:E:15:LYS:HD2	1:E:15:LYS:N	2.31	0.46
1:A:230:GLU:CD	1:A:230:GLU:H	2.18	0.46
1:B:63:THR:HB	1:C:61:ASN:C	2.36	0.46
1:C:270:GLU:OE2	1:D:267:PRO:HB2	2.15	0.46
1:B:105:GLU:HG3	3:B:602:HOH:O	2.14	0.46
1:F:26:ASP:OD2	1:F:28:ARG:HB2	2.16	0.46
1:B:1:MET:CE	1:B:288:VAL:HG23	2.46	0.46
1:F:230:GLU:N	1:F:230:GLU:OE1	2.48	0.46
1:C:81:LEU:HD22	1:C:111:MET:HB3	1.97	0.46
1:F:154:ILE:HD11	1:F:291:ILE:HD12	1.97	0.46
1:B:253:PRO:O	1:B:254:ASP:HB2	2.16	0.46
1:C:4:LEU:HD21	1:C:154:ILE:HG21	1.97	0.45
1:D:262:ASN:HD22	1:D:262:ASN:H	1.64	0.45
1:E:302:LEU:HD21	1:E:311:VAL:HA	1.97	0.45
1:E:230:GLU:OE1	1:E:230:GLU:N	2.45	0.45
1:E:26:ASP:OD2	1:E:28:ARG:HB2	2.16	0.45
1:F:27:GLU:HB3	1:F:60:LEU:HD11	1.98	0.45
1:A:283:GLY:HA2	1:B:283:GLY:HA2	1.99	0.45
1:C:230:GLU:H	1:C:230:GLU:CD	2.19	0.45
1:B:244:VAL:O	1:B:244:VAL:HG22	2.16	0.45
1:B:86:VAL:HG12	1:B:98:ALA:HB2	1.98	0.45
1:D:82:VAL:O	1:D:86:VAL:HG13	2.16	0.45
1:C:217:VAL:O	1:C:220:ALA:HB3	2.15	0.45
1:E:244:VAL:O	1:E:244:VAL:HG22	2.17	0.45
1:B:19:ILE:HG22	1:B:21:PHE:CE1	2.51	0.45
1:A:194:ILE:O	1:A:196:PRO:HD3	2.17	0.45
1:E:204:SER:HB2	1:E:209:ALA:H	1.81	0.45
1:D:134:ARG:HB3	1:D:135:PRO:CD	2.46	0.45
1:D:302:LEU:CD2	1:D:314:LEU:HD12	2.47	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:121:LEU:HD23	1:E:122:VAL:N	2.31	0.45
1:F:264:PHE:CD1	1:F:264:PHE:N	2.84	0.45
1:E:205:THR:HA	1:E:236:GLU:O	2.17	0.45
1:A:169:ILE:CD1	1:A:169:ILE:N	2.80	0.45
1:A:34:SER:OG	1:D:61:ASN:HB3	2.17	0.45
1:E:221:VAL:HG21	1:E:235:GLY:CA	2.35	0.45
1:D:207:GLY:O	1:D:208:SER:C	2.55	0.45
1:C:134:ARG:HG2	1:C:134:ARG:HH11	1.82	0.45
1:D:165:ALA:HB1	1:D:181:ILE:HG22	1.98	0.44
1:E:262:ASN:HD22	1:E:262:ASN:C	2.20	0.44
1:D:314:LEU:HA	1:D:314:LEU:HD23	1.71	0.44
1:F:194:ILE:O	1:F:196:PRO:HD3	2.17	0.44
1:F:15:LYS:HD2	1:F:15:LYS:N	2.32	0.44
1:C:165:ALA:HB1	1:C:181:ILE:CG2	2.47	0.44
1:E:93:ALA:HA	1:E:97:GLN:OE1	2.17	0.44
1:F:1:MET:CE	1:F:288:VAL:HG23	2.48	0.44
1:F:28:ARG:HG2	1:F:28:ARG:NH1	2.32	0.44
1:A:188:THR:OG1	1:A:293:GLN:NE2	2.51	0.44
1:A:81:LEU:HD22	1:A:111:MET:HB3	1.99	0.44
1:B:205:THR:HA	1:B:236:GLU:O	2.17	0.44
1:E:216:LYS:HE2	1:E:216:LYS:HB3	1.80	0.44
1:C:50:GLU:O	1:C:54:GLN:HB2	2.18	0.44
1:E:217:VAL:O	1:E:220:ALA:HB3	2.18	0.44
1:B:134:ARG:CB	1:B:135:PRO:CD	2.96	0.44
1:D:312:TYR:HE2	1:D:316:LEU:HD11	1.83	0.44
1:B:76:GLU:HA	1:B:76:GLU:OE1	2.17	0.44
1:A:217:VAL:O	1:A:221:VAL:HG23	2.18	0.44
1:E:28:ARG:HH11	1:E:28:ARG:HG2	1.81	0.44
1:F:174:ASP:O	1:F:178:LEU:HD23	2.18	0.44
1:E:253:PRO:O	1:E:254:ASP:HB2	2.17	0.44
1:E:231:LEU:HD13	1:E:233:LEU:HB3	2.00	0.44
1:D:217:VAL:O	1:D:220:ALA:HB3	2.18	0.44
1:B:288:VAL:HG12	1:B:291:ILE:HD11	2.00	0.44
1:E:207:GLY:O	1:E:208:SER:C	2.56	0.44
1:C:244:VAL:O	1:C:244:VAL:HG22	2.17	0.44
1:E:94:THR:HG1	1:E:97:GLN:HG3	1.82	0.44
1:B:197:ARG:H	1:B:262:ASN:ND2	2.10	0.44
1:F:304:ARG:O	1:F:305:GLY:C	2.56	0.44
1:C:264:PHE:CD1	1:C:264:PHE:N	2.86	0.44
1:E:185:SER:HA	1:E:293:GLN:HE22	1.83	0.44
1:D:307:ASN:CB	1:D:310:ASP:OD2	2.64	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:191:MET:HE2	1:C:192:PHE:CE1	2.52	0.43
1:F:312:TYR:HE2	1:F:316:LEU:HD11	1.82	0.43
1:C:165:ALA:HB1	1:C:181:ILE:HG22	1.99	0.43
1:A:225:LYS:HE3	1:A:233:LEU:O	2.18	0.43
1:C:277:LYS:NZ	1:D:240:ASP:OD2	2.51	0.43
1:B:139:ILE:HB	1:B:140:ILE:H	1.65	0.43
1:E:314:LEU:HD23	1:E:314:LEU:HA	1.74	0.43
1:D:291:ILE:HD12	1:D:317:ILE:HG21	1.99	0.43
1:B:307:ASN:CB	1:B:310:ASP:OD2	2.66	0.43
1:A:12:VAL:HA	1:A:323:LEU:HD11	1.99	0.43
1:F:136:ALA:O	1:F:140:ILE:O	2.36	0.43
1:A:264:PHE:N	1:A:264:PHE:CD1	2.86	0.43
1:B:312:TYR:HE2	1:B:316:LEU:HD11	1.84	0.43
1:E:244:VAL:HA	1:E:245:PRO:HD3	1.84	0.43
1:A:262:ASN:HD22	1:A:262:ASN:C	2.22	0.43
1:C:302:LEU:CD2	1:C:314:LEU:HD12	2.48	0.43
1:B:163:VAL:HG21	1:B:189:ALA:HB2	2.00	0.43
1:E:163:VAL:HG21	1:E:189:ALA:HB2	2.00	0.43
1:C:71:ASP:HB3	1:C:74:THR:HB	2.01	0.43
1:B:221:VAL:HG21	1:B:235:GLY:CA	2.35	0.43
1:F:307:ASN:O	1:F:310:ASP:HB2	2.18	0.43
1:D:86:VAL:HG12	1:D:98:ALA:HB2	2.01	0.43
1:E:302:LEU:CD2	1:E:314:LEU:HD12	2.49	0.43
1:C:188:THR:OG1	1:C:293:GLN:NE2	2.51	0.43
1:C:207:GLY:O	1:C:208:SER:C	2.57	0.43
1:E:174:ASP:O	1:E:178:LEU:CD2	2.65	0.43
1:B:134:ARG:HB3	1:B:135:PRO:HD2	1.99	0.43
1:C:185:SER:HA	1:C:293:GLN:HE22	1.83	0.43
1:D:24:GLY:O	1:D:30:LEU:HD21	2.19	0.43
1:D:28:ARG:HH12	1:D:306:CYS:N	2.16	0.43
1:D:278:ILE:O	1:D:282:LEU:HB2	2.19	0.43
1:C:289:GLY:O	1:C:291:ILE:HD12	2.18	0.43
1:D:266:PHE:CD2	1:D:272:GLY:HA2	2.54	0.43
1:F:95:GLU:HG2	1:F:99:ARG:NH2	2.33	0.43
1:E:165:ALA:HB1	1:E:181:ILE:CG2	2.49	0.43
1:F:307:ASN:O	1:F:311:VAL:HG23	2.19	0.43
1:D:95:GLU:HG2	1:D:99:ARG:NH2	2.34	0.43
1:C:24:GLY:O	1:C:30:LEU:HD21	2.18	0.43
1:E:165:ALA:HB1	1:E:181:ILE:HG22	2.01	0.42
1:A:63:THR:HG22	1:A:65:GLY:H	1.83	0.42
1:E:1:MET:O	1:E:4:LEU:CB	2.62	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:244:VAL:HG22	1:A:244:VAL:O	2.19	0.42
1:A:314:LEU:HD23	1:A:314:LEU:HA	1.78	0.42
1:D:29:ILE:O	1:D:33:VAL:HB	2.19	0.42
1:D:230:GLU:N	1:D:230:GLU:OE1	2.47	0.42
1:D:15:LYS:N	1:D:15:LYS:HD2	2.34	0.42
1:B:231:LEU:HD13	1:B:233:LEU:HB3	2.01	0.42
1:A:4:LEU:HD21	1:A:154:ILE:HG21	2.01	0.42
1:E:61:ASN:HA	1:F:63:THR:HB	2.00	0.42
1:E:95:GLU:HG2	1:E:99:ARG:NH2	2.34	0.42
1:B:165:ALA:HB1	1:B:181:ILE:CG2	2.50	0.42
1:B:174:ASP:O	1:B:178:LEU:HD23	2.19	0.42
1:A:134:ARG:CB	1:A:135:PRO:CD	2.95	0.42
1:C:281:ARG:NH1	1:C:281:ARG:HG3	2.34	0.42
1:F:223:ILE:HG13	1:F:223:ILE:H	1.64	0.42
1:A:50:GLU:O	1:A:54:GLN:HB2	2.19	0.42
1:B:182:ALA:HB2	1:B:265:VAL:HG21	2.01	0.42
1:B:94:THR:HG1	1:B:97:GLN:HG3	1.81	0.42
1:C:223:ILE:H	1:C:223:ILE:HG13	1.67	0.42
1:A:171:ILE:HA	1:A:269:LEU:HB2	2.02	0.42
1:F:207:GLY:O	1:F:208:SER:C	2.58	0.42
1:B:307:ASN:O	1:B:310:ASP:HB2	2.19	0.42
1:D:244:VAL:HA	1:D:245:PRO:HD3	1.84	0.42
1:C:166:ASP:HB3	3:C:586:HOH:O	2.19	0.42
1:C:28:ARG:HH11	1:C:28:ARG:HG2	1.84	0.42
1:E:238:GLN:O	1:E:239:PHE:C	2.58	0.42
1:E:153:PHE:CE2	1:E:276:TYR:CZ	3.07	0.42
1:A:223:ILE:HG13	1:A:223:ILE:H	1.69	0.42
1:E:61:ASN:C	1:F:63:THR:HB	2.40	0.42
1:A:270:GLU:HG3	3:A:520:HOH:O	2.20	0.42
1:F:169:ILE:HG22	1:F:170:ASN:N	2.34	0.42
1:C:231:LEU:HD13	1:C:233:LEU:HB3	2.02	0.42
1:C:221:VAL:CG2	1:C:235:GLY:HA3	2.50	0.42
1:B:28:ARG:HH12	1:B:306:CYS:N	2.18	0.42
1:C:262:ASN:HD22	1:C:262:ASN:N	2.16	0.42
1:E:161:GLN:HE21	1:E:194:ILE:HD11	1.85	0.42
1:F:33:VAL:HG22	1:F:44:PRO:HB2	2.01	0.42
1:A:95:GLU:HG2	1:A:99:ARG:NH2	2.35	0.42
1:F:182:ALA:HB2	1:F:265:VAL:HG21	2.01	0.42
1:A:61:ASN:OD1	1:D:63:THR:CG2	2.68	0.42
1:A:282:LEU:HD23	1:B:243:PHE:CE2	2.55	0.42
1:E:303:SER:O	1:E:306:CYS:HB3	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:161:GLN:HE21	1:C:194:ILE:HD11	1.85	0.42
1:D:99:ARG:NH1	3:D:525:HOH:O	2.53	0.42
1:D:19:ILE:HG22	1:D:21:PHE:CE1	2.55	0.42
1:E:235:GLY:O	1:E:236:GLU:HB3	2.19	0.41
1:E:169:ILE:CD1	1:E:292:LEU:CD2	2.95	0.41
1:E:49:ASN:ND2	1:E:52:GLU:H	2.07	0.41
1:F:1:MET:O	1:F:3:ASP:N	2.53	0.41
1:A:281:ARG:HH11	1:A:281:ARG:HG3	1.84	0.41
1:B:262:ASN:HD22	1:B:262:ASN:H	1.68	0.41
1:A:281:ARG:HB3	1:B:243:PHE:CD2	2.55	0.41
1:B:278:ILE:O	1:B:282:LEU:HB2	2.21	0.41
1:D:206:LYS:NZ	1:D:234:ASP:OD1	2.46	0.41
1:D:25:LEU:HD12	1:D:25:LEU:HA	1.91	0.41
1:E:169:ILE:HG22	1:E:170:ASN:N	2.34	0.41
1:C:235:GLY:O	1:C:236:GLU:HB3	2.20	0.41
1:B:314:LEU:HA	1:B:314:LEU:HD23	1.75	0.41
1:F:78:MET:O	1:F:82:VAL:HG23	2.21	0.41
1:F:110:THR:HB	1:F:139:ILE:HD12	2.02	0.41
1:B:50:GLU:O	1:B:54:GLN:HB2	2.21	0.41
1:E:169:ILE:HD11	1:E:292:LEU:HD21	2.00	0.41
1:E:61:ASN:OD1	1:F:63:THR:CG2	2.66	0.41
1:C:134:ARG:CB	1:C:135:PRO:CD	2.98	0.41
1:C:27:GLU:HG2	1:C:27:GLU:H	1.72	0.41
1:D:39:ASN:HB2	1:D:41:VAL:HG23	2.03	0.41
1:C:153:PHE:CE2	1:C:276:TYR:CZ	3.08	0.41
1:F:25:LEU:HD12	1:F:25:LEU:HA	1.85	0.41
1:E:3:ASP:OD2	1:E:3:ASP:N	2.54	0.41
1:B:304:ARG:O	1:B:305:GLY:C	2.59	0.41
1:B:4:LEU:HD21	1:B:154:ILE:HG21	2.02	0.41
1:E:307:ASN:O	1:E:311:VAL:HG23	2.20	0.41
1:D:50:GLU:O	1:D:54:GLN:HB2	2.21	0.41
1:C:225:LYS:HE3	1:C:233:LEU:O	2.21	0.41
1:E:307:ASN:O	1:E:310:ASP:HB2	2.21	0.41
1:C:269:LEU:HD23	1:D:203:PHE:CE2	2.56	0.41
1:B:103:LEU:CD1	1:F:52:GLU:HG3	2.51	0.41
1:F:307:ASN:HB3	1:F:310:ASP:CG	2.41	0.41
1:A:303:SER:O	1:A:306:CYS:HB3	2.21	0.41
1:B:240:ASP:CB	1:B:247:VAL:HG11	2.48	0.41
1:D:270:GLU:O	1:D:274:ILE:CG1	2.69	0.41
1:B:1:MET:SD	1:B:4:LEU:HD23	2.60	0.41
1:C:26:ASP:OD2	1:C:28:ARG:HB2	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:266:PHE:CG	1:F:272:GLY:HA2	2.55	0.41
1:B:23:GLU:HB2	3:B:521:HOH:O	2.21	0.41
1:F:312:TYR:CE2	1:F:316:LEU:HD11	2.56	0.41
1:F:39:ASN:HB2	1:F:41:VAL:HG23	2.03	0.41
1:B:3:ASP:OD1	1:D:246:SER:OG	2.36	0.41
1:C:7:THR:O	1:C:10:GLU:HB3	2.21	0.41
1:C:253:PRO:C	1:C:255:SER:H	2.22	0.41
1:B:64:LEU:O	1:B:65:GLY:O	2.39	0.41
1:E:266:PHE:CD2	1:E:272:GLY:HA2	2.56	0.41
1:D:303:SER:HA	2:D:418:SO4:O2	2.21	0.40
1:B:302:LEU:HD21	1:B:311:VAL:HA	2.03	0.40
1:E:134:ARG:CB	1:E:135:PRO:CD	2.95	0.40
1:E:25:LEU:HA	1:E:25:LEU:HD12	1.85	0.40
1:D:150:SER:HB3	1:D:181:ILE:HD12	2.02	0.40
1:A:93:ALA:HA	1:A:97:GLN:OE1	2.22	0.40
1:D:204:SER:HB2	1:D:209:ALA:H	1.86	0.40
1:D:28:ARG:HG2	1:D:28:ARG:NH1	2.37	0.40
1:C:230:GLU:N	1:C:230:GLU:OE1	2.52	0.40
1:A:262:ASN:N	1:A:262:ASN:HD22	2.16	0.40
1:D:76:GLU:HA	1:D:76:GLU:OE1	2.22	0.40
1:A:253:PRO:C	1:A:255:SER:H	2.25	0.40
1:D:171:ILE:H	1:D:171:ILE:HD12	1.85	0.40
1:F:5:PHE:HE2	1:F:317:ILE:HD11	1.86	0.40
1:A:216:LYS:HE2	1:A:216:LYS:HB3	1.88	0.40
1:E:264:PHE:CD1	1:E:264:PHE:N	2.89	0.40
1:F:276:TYR:C	1:F:276:TYR:CD1	2.95	0.40
1:B:25:LEU:HA	1:B:25:LEU:HD12	1.84	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	321/329 (98%)	289 (90%)	26 (8%)	6 (2%)	10	28
1	B	322/329 (98%)	288 (89%)	26 (8%)	8 (2%)	7	21
1	C	321/329 (98%)	290 (90%)	25 (8%)	6 (2%)	10	28
1	D	323/329 (98%)	287 (89%)	28 (9%)	8 (2%)	7	21
1	E	321/329 (98%)	285 (89%)	28 (9%)	8 (2%)	7	21
1	F	321/329 (98%)	281 (88%)	31 (10%)	9 (3%)	6	18
All	All	1929/1974 (98%)	1720 (89%)	164 (8%)	45 (2%)	8	23

All (45) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	65	GLY
1	B	144	GLU
1	D	144	GLU
1	F	2	ALA
1	F	144	GLU
1	A	65	GLY
1	A	144	GLU
1	A	166	ASP
1	A	289	GLY
1	B	289	GLY
1	C	65	GLY
1	C	144	GLU
1	C	166	ASP
1	C	236	GLU
1	C	289	GLY
1	D	65	GLY
1	D	236	GLU
1	D	289	GLY
1	E	65	GLY
1	E	144	GLU
1	E	166	ASP
1	E	236	GLU
1	E	289	GLY
1	F	65	GLY
1	F	166	ASP
1	F	206	LYS
1	A	206	LYS
1	A	236	GLU
1	B	166	ASP
1	B	206	LYS

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Mol	Chain	Res	Type
1	B	236	GLU
1	C	206	LYS
1	D	166	ASP
1	E	90	LYS
1	F	143	LYS
1	F	236	GLU
1	F	240	ASP
1	D	206	LYS
1	D	240	ASP
1	E	169	ILE
1	F	289	GLY
1	B	240	ASP
1	E	206	LYS
1	D	139	ILE
1	B	169	ILE

### 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	257/257 (100%)	237 (92%)	20 (8%)	16	38
1	B	257/257 (100%)	235 (91%)	22 (9%)	13	33
1	C	257/257 (100%)	236 (92%)	21 (8%)	14	35
1	D	257/257 (100%)	236 (92%)	21 (8%)	14	35
1	E	257/257 (100%)	235 (91%)	22 (9%)	13	33
1	F	257/257 (100%)	234 (91%)	23 (9%)	12	31
All	All	1542/1542 (100%)	1413 (92%)	129 (8%)	14	34

All (129) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	18	LYS
1	A	25	LEU
1	A	28	ARG

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Mol	Chain	Res	Type
1	A	53	ILE
1	A	78	MET
1	A	86	VAL
1	A	134	ARG
1	A	149	THR
1	A	150	SER
1	A	215	GLU
1	A	227	LYS
1	A	230	GLU
1	A	233	LEU
1	A	244	VAL
1	A	262	ASN
1	A	276	TYR
1	A	281	ARG
1	A	297	MET
1	A	304	ARG
1	A	314	LEU
1	B	25	LEU
1	B	28	ARG
1	B	46	VAL
1	B	76	GLU
1	B	78	MET
1	B	79	GLU
1	B	86	VAL
1	B	134	ARG
1	B	149	THR
1	B	150	SER
1	B	210	LYS
1	B	215	GLU
1	B	227	LYS
1	B	230	GLU
1	B	233	LEU
1	B	244	VAL
1	B	262	ASN
1	B	276	TYR
1	B	281	ARG
1	B	297	MET
1	B	304	ARG
1	B	314	LEU
1	C	18	LYS
1	C	25	LEU
1	C	28	ARG

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Mol	Chain	Res	Type
1	C	46	VAL
1	C	78	MET
1	C	86	VAL
1	C	134	ARG
1	C	149	THR
1	C	150	SER
1	C	184	GLU
1	C	215	GLU
1	C	227	LYS
1	C	230	GLU
1	C	233	LEU
1	C	244	VAL
1	C	262	ASN
1	C	276	TYR
1	C	281	ARG
1	C	297	MET
1	C	304	ARG
1	C	314	LEU
1	D	25	LEU
1	D	28	ARG
1	D	46	VAL
1	D	76	GLU
1	D	78	MET
1	D	79	GLU
1	D	134	ARG
1	D	149	THR
1	D	150	SER
1	D	210	LYS
1	D	215	GLU
1	D	227	LYS
1	D	230	GLU
1	D	233	LEU
1	D	244	VAL
1	D	262	ASN
1	D	276	TYR
1	D	281	ARG
1	D	297	MET
1	D	304	ARG
1	D	314	LEU
1	E	3	ASP
1	E	25	LEU
1	E	28	ARG

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Mol	Chain	Res	Type
1	E	46	VAL
1	E	54	GLN
1	E	78	MET
1	E	86	VAL
1	E	134	ARG
1	E	149	THR
1	E	150	SER
1	E	210	LYS
1	E	215	GLU
1	E	227	LYS
1	E	230	GLU
1	E	233	LEU
1	E	244	VAL
1	E	262	ASN
1	E	276	TYR
1	E	281	ARG
1	E	297	MET
1	E	304	ARG
1	E	314	LEU
1	F	25	LEU
1	F	28	ARG
1	F	33	VAL
1	F	46	VAL
1	F	76	GLU
1	F	78	MET
1	F	79	GLU
1	F	86	VAL
1	F	134	ARG
1	F	149	THR
1	F	150	SER
1	F	184	GLU
1	F	215	GLU
1	F	227	LYS
1	F	230	GLU
1	F	233	LEU
1	F	244	VAL
1	F	262	ASN
1	F	276	TYR
1	F	281	ARG
1	F	297	MET
1	F	304	ARG
1	F	314	LEU

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

Mol	Chain	Res	Type
1	A	49	ASN
1	A	127	HIS
1	A	161	GLN
1	A	176	GLN
1	A	262	ASN
1	A	293	GLN
1	B	49	ASN
1	B	127	HIS
1	B	161	GLN
1	B	262	ASN
1	B	293	GLN
1	C	49	ASN
1	C	127	HIS
1	C	161	GLN
1	C	176	GLN
1	C	262	ASN
1	C	293	GLN
1	D	49	ASN
1	D	127	HIS
1	D	161	GLN
1	D	176	GLN
1	D	262	ASN
1	D	293	GLN
1	E	49	ASN
1	E	127	HIS
1	E	161	GLN
1	E	176	GLN
1	E	262	ASN
1	E	293	GLN
1	F	49	ASN
1	F	127	HIS
1	F	161	GLN
1	F	176	GLN
1	F	262	ASN
1	F	293	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 carbohydrates in this entry.

## 5.6 Ligand geometry ⓘ

24 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z  > 2$	Counts	RMSZ	$\# Z  > 2$
2	SO4	A	401	-	4,4,4	3.78	1 (25%)	6,6,6	0.94	1 (16%)
2	SO4	A	402	-	4,4,4	2.89	1 (25%)	6,6,6	1.09	1 (16%)
2	SO4	A	403	-	4,4,4	3.81	1 (25%)	6,6,6	0.86	0
2	SO4	A	405	-	4,4,4	3.35	2 (50%)	6,6,6	0.78	0
2	SO4	A	408	-	4,4,4	3.78	2 (50%)	6,6,6	1.15	1 (16%)
2	SO4	B	404	-	4,4,4	3.77	2 (50%)	6,6,6	0.77	0
2	SO4	B	406	-	4,4,4	3.53	2 (50%)	6,6,6	0.81	0
2	SO4	B	407	-	4,4,4	3.25	1 (25%)	6,6,6	0.98	1 (16%)
2	SO4	B	409	-	4,4,4	3.97	2 (50%)	6,6,6	0.76	0
2	SO4	C	410	-	4,4,4	3.70	2 (50%)	6,6,6	0.87	0
2	SO4	C	411	-	4,4,4	3.12	2 (50%)	6,6,6	1.10	1 (16%)
2	SO4	C	412	-	4,4,4	3.66	2 (50%)	6,6,6	0.82	0
2	SO4	C	414	-	4,4,4	3.89	2 (50%)	6,6,6	0.70	0
2	SO4	C	417	-	4,4,4	3.59	1 (25%)	6,6,6	0.79	0
2	SO4	D	413	-	4,4,4	3.10	1 (25%)	6,6,6	0.88	0
2	SO4	D	415	-	4,4,4	4.04	2 (50%)	6,6,6	0.81	0
2	SO4	D	416	-	4,4,4	3.39	1 (25%)	6,6,6	1.14	1 (16%)
2	SO4	D	418	-	4,4,4	4.21	2 (50%)	6,6,6	0.75	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
2	SO4	E	419	-	4,4,4	3.89	1 (25%)	6,6,6	1.04	1 (16%)
2	SO4	E	420	-	4,4,4	3.31	1 (25%)	6,6,6	1.24	1 (16%)
2	SO4	E	421	-	4,4,4	3.62	1 (25%)	6,6,6	1.21	1 (16%)
2	SO4	E	422	-	4,4,4	3.32	1 (25%)	6,6,6	1.00	1 (16%)
2	SO4	F	423	-	4,4,4	3.52	2 (50%)	6,6,6	0.92	0
2	SO4	F	424	-	4,4,4	3.16	1 (25%)	6,6,6	0.94	1 (16%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the chemical component dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	SO4	A	401	-	-	0/0/0/0	0/0/0/0
2	SO4	A	402	-	-	0/0/0/0	0/0/0/0
2	SO4	A	403	-	-	0/0/0/0	0/0/0/0
2	SO4	A	405	-	-	0/0/0/0	0/0/0/0
2	SO4	A	408	-	-	0/0/0/0	0/0/0/0
2	SO4	B	404	-	-	0/0/0/0	0/0/0/0
2	SO4	B	406	-	-	0/0/0/0	0/0/0/0
2	SO4	B	407	-	-	0/0/0/0	0/0/0/0
2	SO4	B	409	-	-	0/0/0/0	0/0/0/0
2	SO4	C	410	-	-	0/0/0/0	0/0/0/0
2	SO4	C	411	-	-	0/0/0/0	0/0/0/0
2	SO4	C	412	-	-	0/0/0/0	0/0/0/0
2	SO4	C	414	-	-	0/0/0/0	0/0/0/0
2	SO4	C	417	-	-	0/0/0/0	0/0/0/0
2	SO4	D	413	-	-	0/0/0/0	0/0/0/0
2	SO4	D	415	-	-	0/0/0/0	0/0/0/0
2	SO4	D	416	-	-	0/0/0/0	0/0/0/0
2	SO4	D	418	-	-	0/0/0/0	0/0/0/0
2	SO4	E	419	-	-	0/0/0/0	0/0/0/0
2	SO4	E	420	-	-	0/0/0/0	0/0/0/0
2	SO4	E	421	-	-	0/0/0/0	0/0/0/0
2	SO4	E	422	-	-	0/0/0/0	0/0/0/0
2	SO4	F	423	-	-	0/0/0/0	0/0/0/0
2	SO4	F	424	-	-	0/0/0/0	0/0/0/0

All (36) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	418	SO4	O3-S	-3.18	1.36	1.47
2	B	409	SO4	O3-S	-2.92	1.36	1.47
2	B	404	SO4	O3-S	-2.82	1.37	1.47
2	A	405	SO4	O3-S	-2.41	1.38	1.47
2	C	411	SO4	O3-S	-2.38	1.38	1.47
2	C	410	SO4	O3-S	-2.29	1.39	1.47
2	C	414	SO4	O3-S	-2.25	1.39	1.47
2	F	423	SO4	O2-S	2.16	1.54	1.47
2	B	406	SO4	O2-S	2.18	1.54	1.47
2	C	412	SO4	O2-S	2.29	1.55	1.47
2	D	415	SO4	O2-S	2.68	1.56	1.47
2	A	408	SO4	O2-S	2.84	1.56	1.47
2	A	402	SO4	O1-S	5.18	1.64	1.47
2	C	411	SO4	O1-S	5.48	1.65	1.47
2	D	413	SO4	O1-S	5.76	1.66	1.47
2	B	407	SO4	O1-S	5.83	1.67	1.47
2	F	424	SO4	O1-S	5.89	1.67	1.47
2	A	405	SO4	O1-S	5.98	1.67	1.47
2	E	420	SO4	O1-S	6.27	1.68	1.47
2	D	416	SO4	O1-S	6.34	1.68	1.47
2	E	422	SO4	O1-S	6.36	1.68	1.47
2	B	406	SO4	O1-S	6.38	1.69	1.47
2	F	423	SO4	O1-S	6.53	1.69	1.47
2	A	408	SO4	O1-S	6.75	1.70	1.47
2	C	417	SO4	O1-S	6.75	1.70	1.47
2	B	404	SO4	O1-S	6.79	1.70	1.47
2	E	421	SO4	O1-S	6.86	1.70	1.47
2	C	412	SO4	O1-S	6.88	1.70	1.47
2	C	410	SO4	O1-S	6.96	1.71	1.47
2	B	409	SO4	O1-S	7.22	1.71	1.47
2	A	401	SO4	O1-S	7.24	1.71	1.47
2	A	403	SO4	O1-S	7.27	1.72	1.47
2	C	414	SO4	O1-S	7.28	1.72	1.47
2	E	419	SO4	O1-S	7.34	1.72	1.47
2	D	415	SO4	O1-S	7.39	1.72	1.47
2	D	418	SO4	O1-S	7.70	1.73	1.47

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	E	421	SO4	O2-S-O1	-2.41	101.85	109.50
2	F	424	SO4	O4-S-O3	2.02	117.21	108.98
2	A	401	SO4	O4-S-O3	2.13	117.64	108.98

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	407	SO4	O4-S-O3	2.17	117.80	108.98
2	E	422	SO4	O4-S-O3	2.24	118.10	108.98
2	E	419	SO4	O4-S-O3	2.25	118.14	108.98
2	A	402	SO4	O4-S-O3	2.29	118.30	108.98
2	C	411	SO4	O4-S-O3	2.35	118.55	108.98
2	A	408	SO4	O4-S-O3	2.46	118.99	108.98
2	D	416	SO4	O4-S-O3	2.47	119.04	108.98
2	E	420	SO4	O4-S-O3	2.71	119.99	108.98

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	D	418	SO4	1	0

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

## 6 Fit of model and data ⓘ

### 6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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	323/329 (98%)	-0.20	3 (0%) 85 82	21, 42, 70, 90	0
1	B	324/329 (98%)	-0.02	5 (1%) 76 72	22, 48, 78, 95	0
1	C	323/329 (98%)	-0.10	7 (2%) 65 59	18, 43, 78, 99	0
1	D	325/329 (98%)	0.06	8 (2%) 61 54	19, 49, 81, 96	0
1	E	323/329 (98%)	0.05	5 (1%) 76 72	20, 49, 76, 96	0
1	F	323/329 (98%)	0.80	42 (13%) 5 3	34, 75, 99, 106	0
All	All	1941/1974 (98%)	0.10	70 (3%) 46 40	18, 50, 87, 106	0

All (70) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	F	254	ASP	4.2
1	F	199	ALA	3.5
1	F	14	GLY	3.4
1	C	2	ALA	3.4
1	F	287	ALA	3.3
1	F	163	VAL	3.2
1	F	212	ASP	3.1
1	F	209	ALA	3.1
1	F	122	VAL	3.1
1	E	251	LYS	3.0
1	F	211	SER	2.9
1	F	215	GLU	2.9
1	F	265	VAL	2.9
1	D	209	ALA	2.8
1	F	307	ASN	2.8
1	D	226	GLU	2.8
1	F	264	PHE	2.7
1	F	323	LEU	2.7
1	E	227	LYS	2.7

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Mol	Chain	Res	Type	RSRZ
1	F	16	ASP	2.7
1	F	250	LYS	2.6
1	F	237	PHE	2.6
1	F	176	GLN	2.6
1	D	14	GLY	2.6
1	D	230	GLU	2.6
1	F	171	ILE	2.6
1	E	147	LYS	2.6
1	F	208	SER	2.5
1	F	15	LYS	2.5
1	D	254	ASP	2.5
1	F	227	LYS	2.5
1	A	230	GLU	2.4
1	F	226	GLU	2.4
1	F	246	SER	2.4
1	F	263	VAL	2.4
1	B	16	ASP	2.4
1	D	258	LYS	2.4
1	F	143	LYS	2.3
1	F	110	THR	2.3
1	C	144	GLU	2.3
1	D	143	LYS	2.3
1	C	226	GLU	2.3
1	F	128	SER	2.3
1	B	209	ALA	2.3
1	F	257	ILE	2.3
1	E	230	GLU	2.2
1	E	212	ASP	2.2
1	F	200	MET	2.2
1	C	122	VAL	2.2
1	F	316	LEU	2.2
1	B	309	GLU	2.2
1	F	154	ILE	2.2
1	F	121	LEU	2.2
1	B	230	GLU	2.2
1	F	266	PHE	2.1
1	F	205	THR	2.1
1	F	258	LYS	2.1
1	A	199	ALA	2.1
1	B	40	LYS	2.1
1	F	249	GLU	2.1
1	F	245	PRO	2.1

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Mol	Chain	Res	Type	RSRZ
1	A	249	GLU	2.1
1	F	144	GLU	2.1
1	D	323	LEU	2.1
1	F	238	GLN	2.1
1	C	254	ASP	2.1
1	C	249	GLU	2.0
1	C	176	GLN	2.0
1	F	256	GLU	2.0
1	F	315	ALA	2.0

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

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

## 6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 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	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
2	SO4	D	413	5/5	0.92	0.24	2.51	72,74,80,83	0
2	SO4	A	408	5/5	0.92	0.28	2.33	70,71,80,82	0
2	SO4	E	422	5/5	0.91	0.29	2.11	55,69,74,75	0
2	SO4	B	404	5/5	0.94	0.26	1.86	70,76,77,79	0
2	SO4	B	409	5/5	0.90	0.25	1.85	61,66,83,84	0
2	SO4	C	417	5/5	0.94	0.22	1.36	66,78,80,86	0
2	SO4	C	414	5/5	0.89	0.22	1.18	72,72,85,88	0
2	SO4	D	418	5/5	0.92	0.23	1.05	58,62,75,77	0
2	SO4	A	405	5/5	0.95	0.21	0.79	63,67,75,77	0
2	SO4	D	415	5/5	0.92	0.31	-	67,69,84,84	0
2	SO4	B	406	5/5	0.92	0.30	-	76,76,86,88	0
2	SO4	E	421	5/5	0.88	0.29	-	65,66,76,84	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
2	SO4	E	420	5/5	0.88	0.33	-	67,70,75,80	0
2	SO4	F	423	5/5	0.92	0.33	-	74,78,84,86	0
2	SO4	A	403	5/5	0.91	0.30	-	68,71,78,84	0
2	SO4	A	401	5/5	0.94	0.29	-	57,76,76,77	0
2	SO4	D	416	5/5	0.83	0.32	-	66,70,79,83	0
2	SO4	A	402	5/5	0.94	0.26	-	59,63,66,69	0
2	SO4	C	411	5/5	0.94	0.24	-	64,72,76,77	0
2	SO4	E	419	5/5	0.89	0.34	-	60,71,79,83	0
2	SO4	B	407	5/5	0.90	0.36	-	66,76,83,85	0
2	SO4	F	424	5/5	0.92	0.32	-	68,71,83,83	0
2	SO4	C	410	5/5	0.93	0.30	-	62,73,75,76	0
2	SO4	C	412	5/5	0.86	0.42	-	69,77,83,89	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.