



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 15, 2017 – 02:13 am GMT

PDB ID : 3OR1  
Title : Crystal structure of dissimilatory sulfite reductase I (DsrI)  
Authors : Hsieh, Y.C.; Liu, M.Y.; Wang, V.C.C.; Chiang, Y.L.; Liu, E.H.; Wu, W.G.;  
Chan, S.I.; Chen, C.J.  
Deposited on : 2010-09-06  
Resolution : 1.76 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 : 1.7.2 (RC1), CSD as538be (2017)  
Xtriage (Phenix) : 1.9-1692  
EDS : trunk28620  
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)  
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) : recalc28949

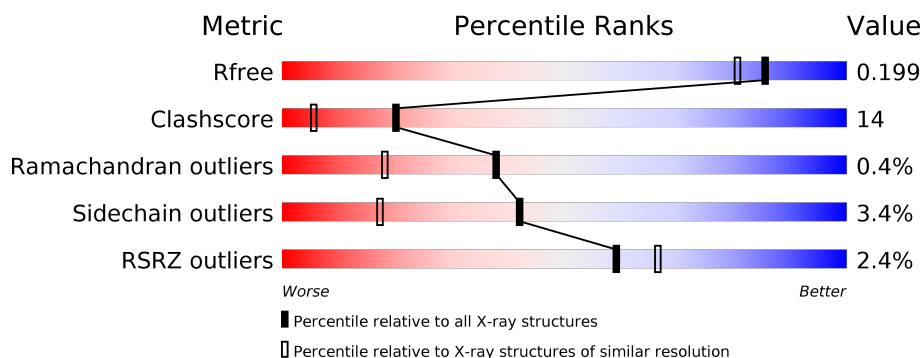
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 1.76 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))
$R_{free}$	100719	1762 (1.76-1.76)
Clashscore	112137	1889 (1.76-1.76)
Ramachandran outliers	110173	1868 (1.76-1.76)
Sidechain outliers	110143	1868 (1.76-1.76)
RSRZ outliers	101464	1770 (1.76-1.76)

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	437	<div> <div>2%</div> <div> <div></div> <div>53%</div> <div>38%</div> <div>8%</div> </div> <div></div> </div>
1	D	437	<div> <div>%</div> <div> <div></div> <div>70%</div> <div>25%</div> <div></div> </div> <div></div> </div>
2	B	386	<div> <div>2%</div> <div> <div></div> <div>69%</div> <div>25%</div> <div>5%</div> </div> <div></div> </div>
2	E	386	<div> <div>2%</div> <div> <div></div> <div>75%</div> <div>22%</div> <div></div> </div> <div></div> </div>
3	C	105	<div> <div>12%</div> <div> <div></div> <div>60%</div> <div>35%</div> <div></div> </div> <div></div> </div>
3	F	105	<div> <div>5%</div> <div> <div></div> <div>68%</div> <div>24%</div> <div>7%</div> </div> <div></div> </div>

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
4	SO3	A	6575	-	-	-	X
4	SO3	D	6576	-	-	-	X
5	SRM	B	581	-	-	-	X

## 2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 15467 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 Sulfite reductase alpha.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	435	Total	C	N	O	S	0	0	0
			3422	2163	585	646	28			
1	D	435	Total	C	N	O	S	0	0	0
			3422	2163	585	646	28			

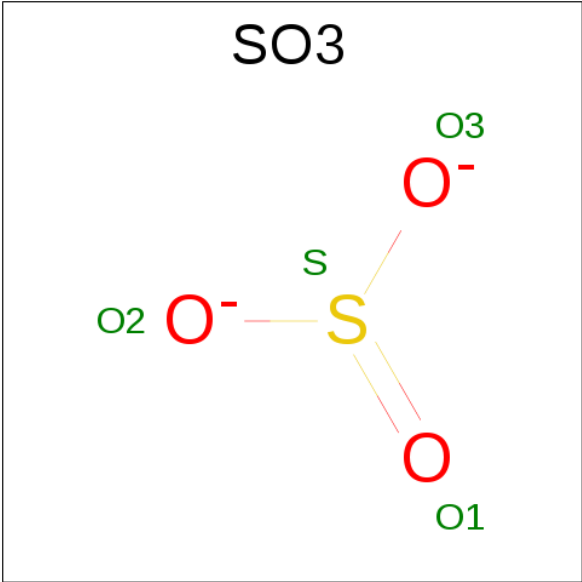
- Molecule 2 is a protein called Sulfite reductase beta.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	385	Total	C	N	O	S	0	0	0
			2999	1912	519	542	26			
2	E	385	Total	C	N	O	S	0	0	0
			2999	1912	519	542	26			

- Molecule 3 is a protein called Sulfite reductase gama.

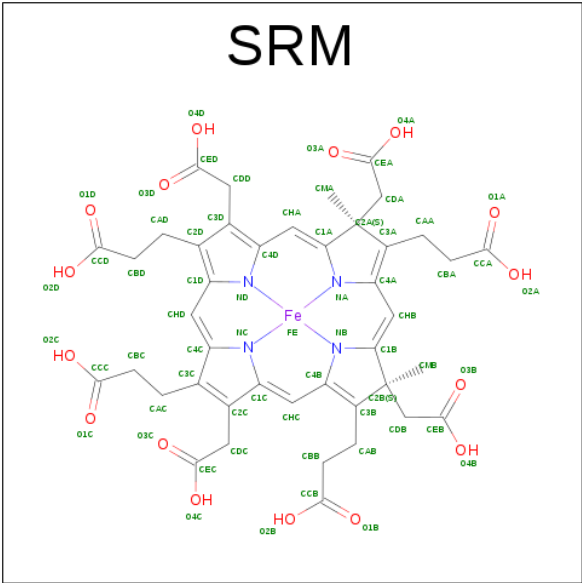
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	104	Total	C	N	O	S	0	0	0
			787	508	125	149	5			
3	F	104	Total	C	N	O	S	0	0	0
			787	508	125	149	5			

- Molecule 4 is SULFITE ION (three-letter code: SO3) (formula: O<sub>3</sub>S).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	O	S	0	0
			4	3	1		
4	D	1	Total	O	S	0	0
			4	3	1		

- Molecule 5 is SIROHEME (three-letter code: SRM) (formula: C<sub>42</sub>H<sub>42</sub>FeN<sub>4</sub>O<sub>16</sub>).



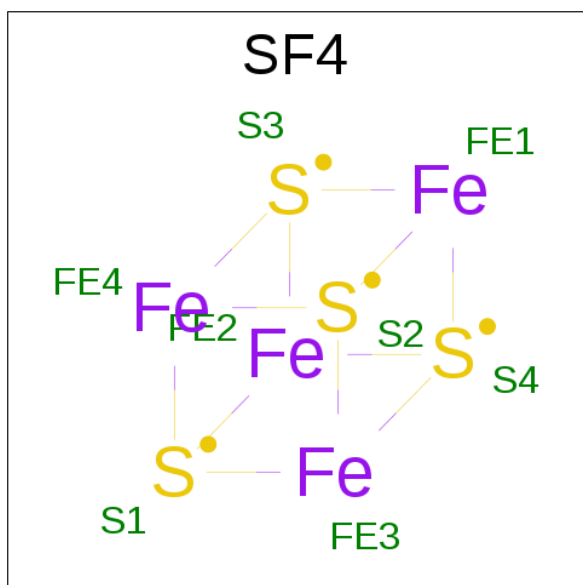
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	A	1	Total	C	Fe	N	O	0
			63	42	1	4	16	
5	B	1	Total	C	N	O	0	0
			62	42	4	16		

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	D	1	Total	C	Fe	N	O	
			63	42	1	4	16	
5	E	1	Total	C	N	O		
			62	42	4	16		

- Molecule 6 is IRON/SULFUR CLUSTER (three-letter code: SF4) (formula: Fe<sub>4</sub>S<sub>4</sub>).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	A	1	Total	Fe	S		
			8	4	4	0	0
6	A	1	Total	Fe	S		
			8	4	4	0	0
6	B	1	Total	Fe	S		
			8	4	4	0	0
6	B	1	Total	Fe	S		
			8	4	4	0	0
6	D	1	Total	Fe	S		
			8	4	4	0	0
6	D	1	Total	Fe	S		
			8	4	4	0	0
6	E	1	Total	Fe	S		
			8	4	4	0	0
6	E	1	Total	Fe	S		
			8	4	4	0	0

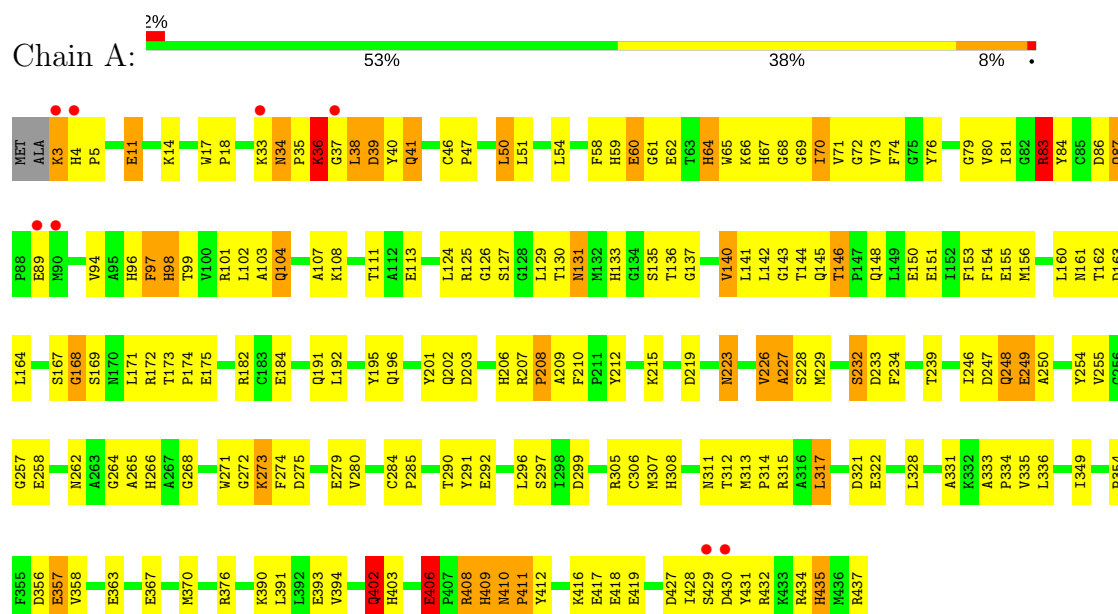
- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	164	Total 164	O 164	0	0
7	B	160	Total 160	O 160	0	0
7	C	12	Total 12	O 12	0	0
7	D	220	Total 220	O 220	0	0
7	E	155	Total 155	O 155	0	0
7	F	18	Total 18	O 18	0	0

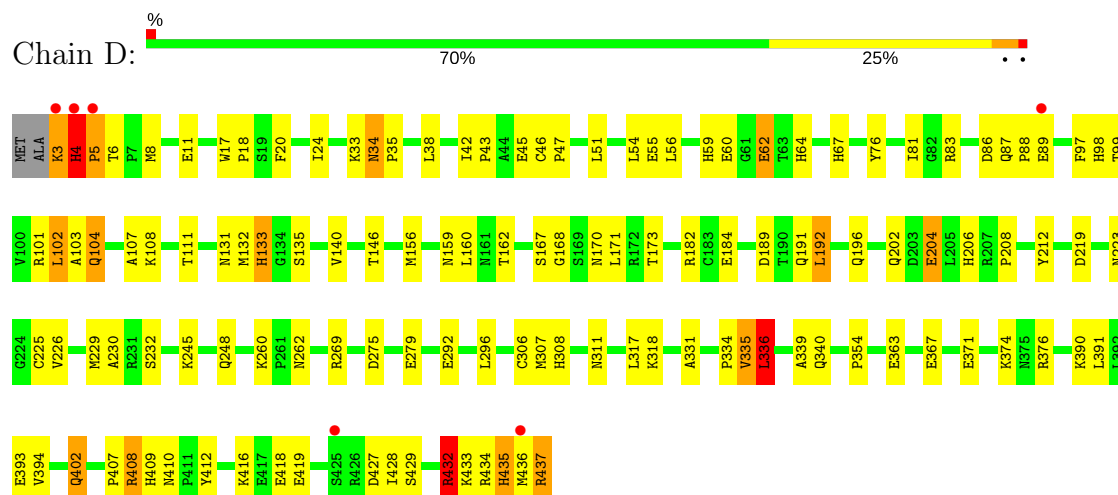
### 3 Residue-property plots

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



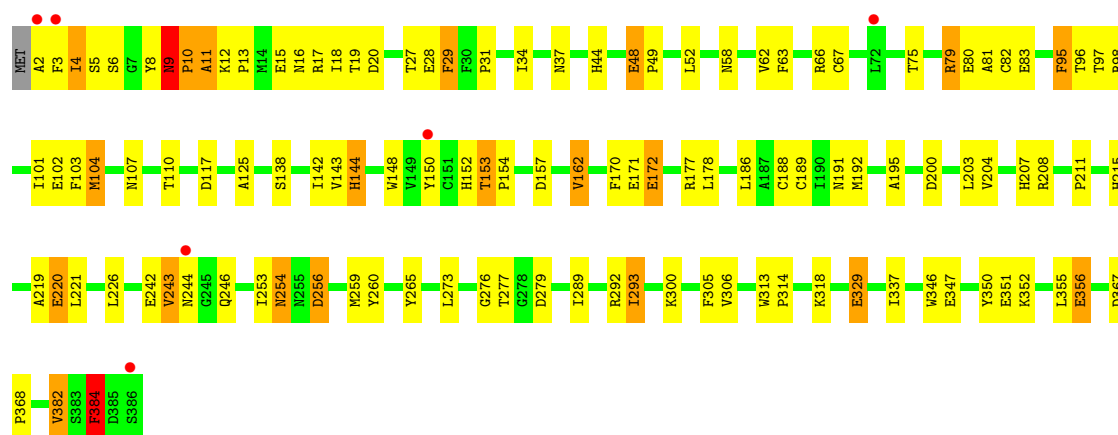
#### • Molecule 1: Sulfite reductase alpha



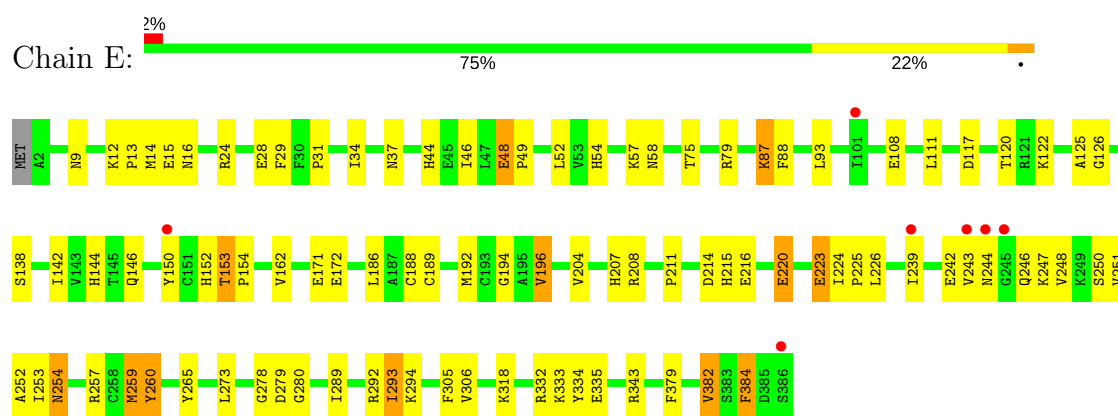
#### • Molecule 2: Sulfite reductase beta



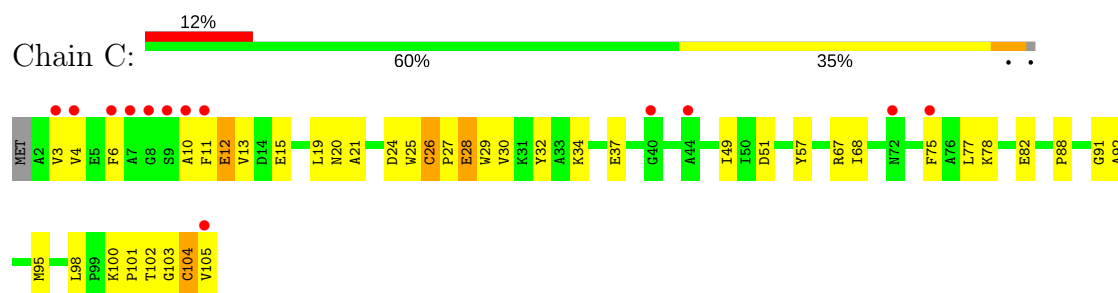




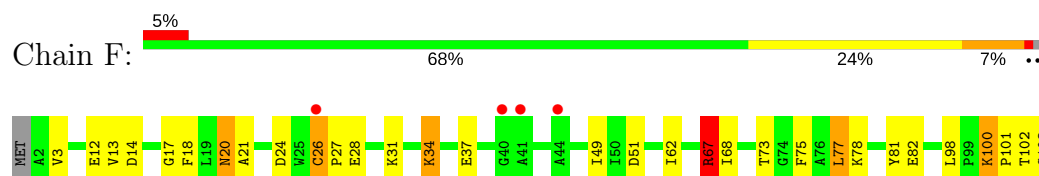
• Molecule 2: Sulfite reductase beta



• Molecule 3: Sulfite reductase gama



• Molecule 3: Sulfite reductase gama



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	114.72Å 60.48Å 132.91Å 90.00° 94.30° 90.00°	Depositor
Resolution (Å)	30.00 – 1.76 29.48 – 1.70	Depositor EDS
% Data completeness (in resolution range)	(Not available) (30.00-1.76) 99.0 (29.48-1.70)	Depositor EDS
$R_{merge}$	0.07	Depositor
$R_{sym}$	0.06	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.96 (at 1.70Å)	Xtriage
Refinement program	CNS	Depositor
R, $R_{free}$	0.193 , 0.212 0.196 , 0.199	Depositor DCC
$R_{free}$ test set	9077 reflections (5.31%)	DCC
Wilson B-factor (Å <sup>2</sup> )	22.0	Xtriage
Anisotropy	0.292	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.36 , 40.0	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.96	EDS
Total number of atoms	15467	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	25.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.43% of the height of the origin peak. No significant pseudotranslation is detected.*

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

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

## 5 Model quality ⓘ

### 5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: SF4, SO3, SRM

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	2.36	257/3512 (7.3%)	1.23	27/4751 (0.6%)
1	D	1.23	58/3512 (1.7%)	1.08	21/4751 (0.4%)
2	B	1.93	133/3076 (4.3%)	0.99	12/4170 (0.3%)
2	E	1.52	67/3076 (2.2%)	0.84	11/4170 (0.3%)
3	C	1.26	9/808 (1.1%)	0.77	1/1090 (0.1%)
3	F	1.60	17/808 (2.1%)	1.27	4/1090 (0.4%)
All	All	1.78	541/14792 (3.7%)	1.05	76/20022 (0.4%)

All (541) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	F	26	CYS	CB-SG	-20.23	1.47	1.82
2	B	384	PHE	CE1-CZ	-19.93	0.99	1.37
2	E	220	GLU	CB-CG	-19.51	1.15	1.52
1	A	406	GLU	CB-CG	-18.91	1.16	1.52
2	B	306	VAL	CB-CG2	-17.20	1.16	1.52
2	B	384	PHE	CD1-CE1	-16.73	1.05	1.39
1	D	335	VAL	CB-CG1	-16.48	1.18	1.52
2	E	28	GLU	CD-OE1	-16.30	1.07	1.25
2	B	243	VAL	CB-CG2	-16.23	1.18	1.52
2	E	220	GLU	CD-OE2	-15.94	1.08	1.25
2	B	28	GLU	CD-OE2	-15.56	1.08	1.25
2	E	48	GLU	CB-CG	-15.35	1.23	1.52
2	E	306	VAL	CB-CG2	-15.27	1.20	1.52
2	E	196	VAL	CB-CG2	-13.45	1.24	1.52
2	B	102	GLU	CD-OE1	-13.26	1.11	1.25
2	B	220	GLU	CB-CG	-12.96	1.27	1.52
2	E	243	VAL	CB-CG2	-12.88	1.25	1.52
1	A	58	PHE	CE1-CZ	-12.33	1.14	1.37
2	E	220	GLU	CG-CD	-11.70	1.34	1.51
2	B	80	GLU	CD-OE1	-11.67	1.12	1.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	E	28	GLU	CB-CG	-11.24	1.30	1.52
2	E	382	VAL	CB-CG2	-11.04	1.29	1.52
2	B	220	GLU	CD-OE1	-11.01	1.13	1.25
3	F	102	THR	CB-OG1	-10.98	1.21	1.43
2	B	220	GLU	CG-CD	-10.89	1.35	1.51
2	E	384	PHE	CE1-CZ	-10.82	1.16	1.37
3	F	103	GLY	C-O	-10.80	1.06	1.23
3	C	103	GLY	C-O	-10.75	1.06	1.23
1	A	209	ALA	CA-CB	-10.70	1.29	1.52
1	A	98	HIS	C-O	-10.65	1.03	1.23
2	B	329	GLU	CD-OE1	-10.54	1.14	1.25
1	A	58	PHE	CD2-CE2	-10.51	1.18	1.39
1	A	315	ARG	CZ-NH2	-10.45	1.19	1.33
1	A	68	GLY	C-O	-10.43	1.06	1.23
3	F	102	THR	C-O	-10.41	1.03	1.23
3	F	67	ARG	CZ-NH2	-10.38	1.19	1.33
1	A	83	ARG	CD-NE	-10.36	1.28	1.46
3	C	26	CYS	CB-SG	-10.25	1.64	1.82
2	B	384	PHE	CE2-CZ	-10.22	1.18	1.37
2	B	52	LEU	C-O	-10.14	1.04	1.23
1	D	11	GLU	CD-OE1	-10.14	1.14	1.25
1	A	229	MET	CB-CG	-10.11	1.19	1.51
1	D	432	ARG	CD-NE	-10.05	1.29	1.46
1	A	50	LEU	CG-CD1	-10.03	1.14	1.51
1	A	290	THR	C-O	-9.90	1.04	1.23
2	E	48	GLU	CD-OE1	-9.89	1.14	1.25
1	A	232	SER	CB-OG	-9.83	1.29	1.42
2	B	204	VAL	CB-CG1	-9.80	1.32	1.52
1	D	260	LYS	CE-NZ	-9.74	1.24	1.49
1	A	418	GLU	CB-CG	-9.71	1.33	1.52
1	D	42	ILE	C-O	-9.70	1.04	1.23
2	E	384	PHE	CG-CD2	-9.67	1.24	1.38
2	B	102	GLU	CD-OE2	-9.66	1.15	1.25
1	A	393	GLU	CD-OE1	-9.65	1.15	1.25
1	A	74	PHE	CE2-CZ	-9.64	1.19	1.37
1	D	269	ARG	CZ-NH2	-9.62	1.20	1.33
2	E	384	PHE	CE2-CZ	-9.62	1.19	1.37
2	B	204	VAL	CB-CG2	-9.47	1.32	1.52
1	A	406	GLU	CG-CD	-9.40	1.37	1.51
1	A	249	GLU	CB-CG	-9.38	1.34	1.52
1	A	103	ALA	C-O	-9.38	1.05	1.23
2	B	15	GLU	CD-OE2	-9.37	1.15	1.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	162	THR	C-O	-9.34	1.05	1.23
1	D	171	LEU	C-O	-9.32	1.05	1.23
1	D	374	LYS	CD-CE	-9.31	1.27	1.51
1	D	269	ARG	CZ-NH1	-9.28	1.21	1.33
2	B	95	PHE	CG-CD1	-9.26	1.24	1.38
1	A	264	GLY	C-O	-9.26	1.08	1.23
1	A	234	PHE	CE1-CZ	-9.26	1.19	1.37
2	B	143	VAL	CB-CG1	-9.23	1.33	1.52
1	A	94	VAL	C-O	-9.18	1.05	1.23
2	B	220	GLU	CD-OE2	-9.16	1.15	1.25
2	E	220	GLU	CD-OE1	-9.16	1.15	1.25
1	A	297	SER	CB-OG	-9.13	1.30	1.42
3	C	37	GLU	CD-OE1	-9.11	1.15	1.25
1	A	155	GLU	CD-OE2	-9.10	1.15	1.25
1	A	254	TYR	CD2-CE2	-9.09	1.25	1.39
2	E	57	LYS	CG-CD	-9.08	1.21	1.52
2	B	384	PHE	CG-CD2	-9.08	1.25	1.38
2	B	66	ARG	CZ-NH1	-9.03	1.21	1.33
1	A	154	PHE	C-O	-8.98	1.06	1.23
2	E	384	PHE	CB-CG	-8.98	1.36	1.51
1	A	60	GLU	CD-OE2	-8.97	1.15	1.25
2	B	350	TYR	CG-CD2	-8.94	1.27	1.39
1	A	150	GLU	CD-OE1	-8.89	1.15	1.25
1	A	130	THR	C-O	-8.86	1.06	1.23
1	D	393	GLU	CD-OE1	-8.85	1.16	1.25
2	E	48	GLU	CD-OE2	-8.84	1.16	1.25
2	B	178	LEU	C-O	-8.82	1.06	1.23
1	A	315	ARG	CB-CG	-8.77	1.28	1.52
1	A	125	ARG	C-O	-8.77	1.06	1.23
1	A	201	TYR	CD1-CE1	-8.77	1.26	1.39
2	E	125	ALA	CA-CB	-8.75	1.34	1.52
2	B	27	THR	C-O	-8.74	1.06	1.23
2	B	191	ASN	CG-OD1	-8.73	1.04	1.24
2	E	384	PHE	CD1-CE1	-8.73	1.21	1.39
1	A	249	GLU	CD-OE1	-8.72	1.16	1.25
1	A	124	LEU	C-O	-8.69	1.06	1.23
2	B	66	ARG	CZ-NH2	-8.63	1.21	1.33
1	A	127	SER	CB-OG	-8.62	1.31	1.42
2	E	16	ASN	C-O	-8.61	1.06	1.23
3	F	104	CYS	CB-SG	-8.61	1.67	1.82
2	B	95	PHE	CE1-CZ	-8.58	1.21	1.37
1	A	58	PHE	CG-CD2	-8.58	1.25	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	417	GLU	CD-OE2	-8.57	1.16	1.25
1	A	437	ARG	CB-CG	-8.56	1.29	1.52
1	D	335	VAL	C-O	-8.53	1.07	1.23
2	B	162	VAL	CB-CG1	-8.51	1.34	1.52
2	B	351	GLU	CD-OE1	-8.51	1.16	1.25
1	A	210	PHE	CG-CD1	-8.50	1.26	1.38
1	A	65	TRP	CG-CD1	-8.49	1.24	1.36
1	A	431	TYR	CD2-CE2	-8.48	1.26	1.39
1	A	175	GLU	CD-OE2	-8.47	1.16	1.25
2	B	3	PHE	C-O	-8.46	1.07	1.23
1	D	434	ARG	C-O	-8.46	1.07	1.23
2	B	48	GLU	CG-CD	-8.45	1.39	1.51
1	A	150	GLU	CD-OE2	-8.43	1.16	1.25
3	F	67	ARG	CB-CG	-8.43	1.29	1.52
2	E	243	VAL	CB-CG1	-8.42	1.35	1.52
1	A	175	GLU	CD-OE1	-8.42	1.16	1.25
1	A	141	LEU	C-O	-8.39	1.07	1.23
2	B	329	GLU	CD-OE2	-8.38	1.16	1.25
2	B	20	ASP	CG-OD1	-8.37	1.06	1.25
1	A	89	GLU	CB-CG	-8.36	1.36	1.52
1	A	155	GLU	CD-OE1	-8.35	1.16	1.25
2	E	248	VAL	CB-CG2	-8.35	1.35	1.52
1	A	97	PHE	CG-CD1	-8.35	1.26	1.38
2	B	356	GLU	C-O	-8.32	1.07	1.23
1	A	131	ASN	C-O	-8.31	1.07	1.23
2	E	318	LYS	C-O	-8.28	1.07	1.23
2	B	356	GLU	CB-CG	-8.27	1.36	1.52
1	A	208	PRO	C-O	-8.25	1.06	1.23
1	D	103	ALA	CA-CB	-8.22	1.35	1.52
1	A	209	ALA	C-O	-8.20	1.07	1.23
1	D	245	LYS	C-O	-8.20	1.07	1.23
1	A	151	GLU	CD-OE2	-8.20	1.16	1.25
2	B	29	PHE	CE1-CZ	-8.17	1.21	1.37
2	B	208	ARG	CZ-NH1	-8.16	1.22	1.33
1	A	171	LEU	C-O	-8.15	1.07	1.23
1	A	322	GLU	CD-OE1	-8.09	1.16	1.25
2	E	194	GLY	C-O	-8.09	1.10	1.23
1	D	62	GLU	C-O	-8.06	1.08	1.23
1	A	182	ARG	CZ-NH2	-8.05	1.22	1.33
1	A	129	LEU	C-O	-8.03	1.08	1.23
1	A	268	GLY	C-O	-8.02	1.10	1.23
1	A	406	GLU	CD-OE1	-8.02	1.16	1.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	228	SER	CB-OG	-7.99	1.31	1.42
2	B	243	VAL	CB-CG1	-7.98	1.36	1.52
1	A	431	TYR	C-O	-7.95	1.08	1.23
1	A	146	THR	C-O	-7.95	1.08	1.23
1	D	393	GLU	CD-OE2	-7.94	1.17	1.25
2	B	384	PHE	CB-CG	-7.91	1.38	1.51
1	A	40	TYR	C-O	-7.91	1.08	1.23
2	B	170	PHE	CE2-CZ	-7.90	1.22	1.37
1	A	317	LEU	C-O	-7.87	1.08	1.23
2	B	191	ASN	CG-ND2	-7.87	1.13	1.32
1	A	40	TYR	CD1-CE1	-7.86	1.27	1.39
2	E	28	GLU	CD-OE2	-7.86	1.17	1.25
1	A	87	GLN	CG-CD	-7.85	1.32	1.51
2	B	226	LEU	C-O	-7.84	1.08	1.23
1	A	274	PHE	CD1-CE1	-7.83	1.23	1.39
1	A	393	GLU	C-O	-7.83	1.08	1.23
1	A	192	LEU	C-O	-7.82	1.08	1.23
1	A	333	ALA	C-O	-7.79	1.08	1.23
1	A	357	GLU	C-O	-7.75	1.08	1.23
1	A	328	LEU	C-O	-7.74	1.08	1.23
1	D	103	ALA	C-O	-7.73	1.08	1.23
1	A	160	LEU	CG-CD1	-7.73	1.23	1.51
1	A	36	LYS	CB-CG	-7.67	1.31	1.52
2	E	196	VAL	C-O	-7.64	1.08	1.23
1	D	393	GLU	CB-CG	-7.63	1.37	1.52
1	A	437	ARG	C-O	-7.62	1.08	1.23
3	C	102	THR	C-O	-7.60	1.08	1.23
1	A	168	GLY	C-O	-7.59	1.11	1.23
1	A	144	THR	C-O	-7.58	1.08	1.23
2	B	104	MET	C-O	-7.57	1.08	1.23
1	A	257	GLY	C-O	-7.56	1.11	1.23
1	A	135	SER	CB-OG	-7.55	1.32	1.42
1	D	102	LEU	C-O	-7.54	1.09	1.23
1	A	335	VAL	CB-CG1	-7.52	1.37	1.52
1	D	8	MET	C-O	-7.52	1.09	1.23
1	A	232	SER	C-O	-7.48	1.09	1.23
1	A	417	GLU	CB-CG	-7.48	1.38	1.52
2	B	102	GLU	CG-CD	-7.47	1.40	1.51
2	B	95	PHE	CE2-CZ	-7.47	1.23	1.37
2	B	117	ASP	C-O	-7.47	1.09	1.23
2	E	382	VAL	CB-CG1	-7.46	1.37	1.52
1	A	246	ILE	C-O	-7.45	1.09	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	F	98	LEU	C-O	-7.45	1.09	1.23
2	B	350	TYR	CG-CD1	-7.44	1.29	1.39
1	A	83	ARG	CZ-NH2	-7.41	1.23	1.33
2	E	28	GLU	C-O	-7.41	1.09	1.23
1	A	136	THR	CB-CG2	-7.41	1.27	1.52
2	B	27	THR	CB-CG2	-7.39	1.27	1.52
1	A	127	SER	C-O	-7.38	1.09	1.23
1	A	315	ARG	C-O	-7.37	1.09	1.23
1	D	245	LYS	CD-CE	-7.34	1.32	1.51
2	E	24	ARG	CG-CD	-7.33	1.33	1.51
1	A	431	TYR	CE1-CZ	-7.31	1.29	1.38
1	A	125	ARG	CZ-NH1	-7.30	1.23	1.33
1	D	275	ASP	C-O	-7.30	1.09	1.23
1	A	71	VAL	CB-CG2	-7.26	1.37	1.52
2	B	79	ARG	CZ-NH1	-7.25	1.23	1.33
2	E	306	VAL	C-O	-7.25	1.09	1.23
2	E	9	ASN	C-O	-7.25	1.09	1.23
2	B	215	HIS	C-O	-7.23	1.09	1.23
1	A	356	ASP	C-O	-7.20	1.09	1.23
2	E	382	VAL	C-O	-7.20	1.09	1.23
2	B	6	SER	C-O	-7.19	1.09	1.23
2	B	48	GLU	CB-CG	-7.19	1.38	1.52
1	A	40	TYR	CE1-CZ	-7.18	1.29	1.38
3	F	67	ARG	CD-NE	-7.18	1.34	1.46
1	A	394	VAL	CB-CG2	-7.16	1.37	1.52
1	A	234	PHE	C-O	-7.13	1.09	1.23
1	A	97	PHE	C-O	-7.11	1.09	1.23
1	D	51	LEU	C-O	-7.11	1.09	1.23
1	D	435	HIS	C-O	-7.11	1.09	1.23
1	A	135	SER	C-O	-7.10	1.09	1.23
1	A	145	GLN	C-O	-7.07	1.09	1.23
1	A	210	PHE	C-O	-7.06	1.09	1.23
1	D	391	LEU	C-O	-7.04	1.09	1.23
1	D	437	ARG	CD-NE	-7.04	1.34	1.46
2	B	80	GLU	CD-OE2	-7.04	1.18	1.25
1	D	432	ARG	CZ-NH2	-7.04	1.24	1.33
2	B	204	VAL	C-O	-7.03	1.09	1.23
1	D	275	ASP	CG-OD2	-7.03	1.09	1.25
1	A	155	GLU	C-O	-7.02	1.10	1.23
1	A	265	ALA	C-O	-7.01	1.10	1.23
2	B	20	ASP	CG-OD2	-7.01	1.09	1.25
2	B	81	ALA	C-O	-7.01	1.10	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	60	GLU	CD-OE1	-7.00	1.18	1.25
1	D	408	ARG	CZ-NH2	-6.99	1.24	1.33
2	E	343	ARG	CZ-NH2	-6.99	1.24	1.33
2	E	93	LEU	C-O	-6.98	1.10	1.23
1	A	435	HIS	C-O	-6.98	1.10	1.23
2	B	243	VAL	C-O	-6.97	1.10	1.23
2	B	5	SER	CB-OG	-6.97	1.33	1.42
1	A	96	HIS	C-O	-6.95	1.10	1.23
1	A	74	PHE	CG-CD2	-6.93	1.28	1.38
1	A	249	GLU	CD-OE2	-6.93	1.18	1.25
1	A	192	LEU	CG-CD1	-6.89	1.26	1.51
1	D	374	LYS	CG-CD	-6.88	1.29	1.52
1	A	137	GLY	C-O	-6.88	1.12	1.23
2	B	305	PHE	CE2-CZ	-6.88	1.24	1.37
1	D	11	GLU	CB-CG	-6.88	1.39	1.52
2	B	350	TYR	C-O	-6.88	1.10	1.23
2	E	223	GLU	CD-OE1	-6.87	1.18	1.25
2	B	305	PHE	C-O	-6.85	1.10	1.23
1	A	356	ASP	CG-OD2	-6.84	1.09	1.25
1	A	254	TYR	CD1-CE1	-6.84	1.29	1.39
2	B	29	PHE	CG-CD2	-6.83	1.28	1.38
1	A	59	HIS	C-O	-6.82	1.10	1.23
1	D	269	ARG	C-O	-6.82	1.10	1.23
1	A	417	GLU	C-O	-6.77	1.10	1.23
1	A	83	ARG	NE-CZ	-6.76	1.24	1.33
1	A	70	ILE	C-O	-6.75	1.10	1.23
2	B	203	LEU	C-O	-6.74	1.10	1.23
2	B	11	ALA	CA-CB	-6.73	1.38	1.52
1	A	36	LYS	C-O	-6.73	1.10	1.23
2	B	384	PHE	C-O	-6.73	1.10	1.23
2	B	384	PHE	CG-CD1	-6.72	1.28	1.38
1	A	195	TYR	CG-CD2	-6.71	1.30	1.39
1	A	299	ASP	C-O	-6.71	1.10	1.23
1	A	148	GLN	CD-OE1	-6.71	1.09	1.24
1	A	266	HIS	C-O	-6.70	1.10	1.23
2	B	103	PHE	CE1-CZ	-6.70	1.24	1.37
1	A	41	GLN	C-O	-6.69	1.10	1.23
1	A	4	HIS	C-O	-6.69	1.10	1.23
1	A	411	PRO	C-O	-6.67	1.09	1.23
2	B	178	LEU	CG-CD2	-6.67	1.27	1.51
2	B	171	GLU	CB-CG	-6.66	1.39	1.52
2	E	117	ASP	CG-OD1	-6.66	1.10	1.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	210	PHE	CE2-CZ	-6.66	1.24	1.37
2	B	306	VAL	CB-CG1	-6.64	1.39	1.52
1	A	140	VAL	C-O	-6.63	1.10	1.23
3	C	67	ARG	C-O	-6.63	1.10	1.23
1	A	408	ARG	C-O	-6.63	1.10	1.23
2	B	79	ARG	CZ-NH2	-6.63	1.24	1.33
1	A	434	ARG	CZ-NH1	-6.62	1.24	1.33
1	A	173	THR	C-O	-6.60	1.10	1.23
1	A	148	GLN	C-O	-6.58	1.10	1.23
2	E	87	LYS	C-O	-6.58	1.10	1.23
2	E	125	ALA	C-O	-6.58	1.10	1.23
1	A	234	PHE	CD2-CE2	-6.58	1.26	1.39
1	D	428	ILE	C-O	-6.57	1.10	1.23
1	A	432	ARG	C-O	-6.56	1.10	1.23
1	A	210	PHE	CD2-CE2	-6.54	1.26	1.39
1	A	79	GLY	C-O	-6.54	1.13	1.23
1	A	248	GLN	CB-CG	-6.54	1.34	1.52
2	B	8	TYR	C-O	-6.54	1.10	1.23
1	A	226	VAL	CB-CG2	-6.50	1.39	1.52
1	A	169	SER	CB-OG	-6.48	1.33	1.42
1	A	223	ASN	CG-OD1	-6.48	1.09	1.24
1	A	35	PRO	C-O	-6.47	1.10	1.23
1	A	201	TYR	CE1-CZ	-6.46	1.30	1.38
1	D	340	GLN	CD-OE1	-6.46	1.09	1.24
2	B	143	VAL	CB-CG2	-6.45	1.39	1.52
1	A	182	ARG	C-O	-6.44	1.11	1.23
2	E	24	ARG	CZ-NH2	-6.43	1.24	1.33
1	A	432	ARG	CZ-NH2	-6.42	1.24	1.33
2	B	6	SER	CB-OG	-6.41	1.33	1.42
1	A	142	LEU	C-O	-6.41	1.11	1.23
1	A	431	TYR	CG-CD1	-6.39	1.30	1.39
2	B	3	PHE	CG-CD2	-6.39	1.29	1.38
1	A	357	GLU	CD-OE1	-6.38	1.18	1.25
1	D	5	PRO	CB-CG	-6.38	1.18	1.50
2	E	93	LEU	CG-CD1	-6.37	1.28	1.51
1	A	250	ALA	C-O	-6.36	1.11	1.23
1	A	226	VAL	C-O	-6.35	1.11	1.23
1	A	182	ARG	CZ-NH1	-6.34	1.24	1.33
1	D	408	ARG	C-O	-6.34	1.11	1.23
1	D	101	ARG	CZ-NH1	-6.33	1.24	1.33
1	A	143	GLY	C-O	-6.33	1.13	1.23
2	E	126	GLY	C-O	-6.33	1.13	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	E	223	GLU	C-O	-6.32	1.11	1.23
1	A	101	ARG	C-O	-6.32	1.11	1.23
1	D	62	GLU	CD-OE1	-6.31	1.18	1.25
2	B	208	ARG	CZ-NH2	-6.31	1.24	1.33
1	D	6	THR	C-O	-6.30	1.11	1.23
1	A	431	TYR	CE2-CZ	-6.30	1.30	1.38
1	A	202	GLN	CG-CD	-6.30	1.36	1.51
1	A	321	ASP	C-O	-6.29	1.11	1.23
1	A	291	TYR	CD1-CE1	-6.28	1.29	1.39
1	A	80	VAL	C-O	-6.27	1.11	1.23
1	A	174	PRO	C-O	-6.27	1.10	1.23
2	B	221	LEU	C-O	-6.26	1.11	1.23
1	A	201	TYR	C-O	-6.25	1.11	1.23
1	A	154	PHE	CE2-CZ	-6.24	1.25	1.37
1	A	328	LEU	CG-CD1	-6.24	1.28	1.51
1	A	37	GLY	C-O	-6.24	1.13	1.23
1	A	84	TYR	C-O	-6.22	1.11	1.23
2	B	48	GLU	CD-OE2	-6.21	1.18	1.25
2	B	171	GLU	C-O	-6.21	1.11	1.23
2	B	16	ASN	C-O	-6.21	1.11	1.23
2	E	108	GLU	CB-CG	-6.21	1.40	1.52
2	E	16	ASN	CG-OD1	-6.20	1.10	1.24
1	A	164	LEU	CG-CD1	-6.20	1.28	1.51
1	A	248	GLN	CD-NE2	-6.20	1.17	1.32
1	A	36	LYS	CG-CD	-6.18	1.31	1.52
2	B	18	ILE	C-O	-6.18	1.11	1.23
2	B	10	PRO	C-O	-6.17	1.10	1.23
1	A	50	LEU	C-O	-6.17	1.11	1.23
1	A	156	MET	C-O	-6.16	1.11	1.23
1	A	394	VAL	CB-CG1	-6.16	1.40	1.52
2	B	177	ARG	C-O	-6.16	1.11	1.23
2	E	57	LYS	CB-CG	-6.15	1.35	1.52
1	A	273	LYS	C-O	-6.15	1.11	1.23
2	B	277	THR	C-O	-6.14	1.11	1.23
1	D	4	HIS	C-O	-6.14	1.11	1.23
2	E	220	GLU	C-O	-6.14	1.11	1.23
1	A	64	HIS	C-O	-6.14	1.11	1.23
2	B	17	ARG	CZ-NH1	-6.14	1.25	1.33
2	B	17	ARG	CZ-NH2	-6.13	1.25	1.33
2	B	244	ASN	C-O	-6.12	1.11	1.23
1	A	233	ASP	C-O	-6.12	1.11	1.23
1	A	140	VAL	CB-CG1	-6.10	1.40	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	82	CYS	C-O	-6.09	1.11	1.23
1	A	161	ASN	CG-ND2	-6.08	1.17	1.32
1	A	201	TYR	CD2-CE2	-6.07	1.30	1.39
3	C	15	GLU	CD-OE2	-6.07	1.19	1.25
1	A	437	ARG	N-CA	-6.06	1.34	1.46
2	B	219	ALA	C-O	-6.05	1.11	1.23
1	A	274	PHE	CD2-CE2	-6.05	1.27	1.39
1	D	336	LEU	C-O	-6.04	1.11	1.23
3	F	37	GLU	CD-OE1	-6.02	1.19	1.25
1	A	250	ALA	CA-CB	-6.02	1.39	1.52
1	A	229	MET	C-O	-6.01	1.11	1.23
1	D	437	ARG	CB-CG	-6.01	1.36	1.52
1	A	402	GLN	C-O	-6.00	1.11	1.23
2	B	20	ASP	C-O	-6.00	1.11	1.23
2	E	111	LEU	C-O	-6.00	1.11	1.23
1	A	182	ARG	CB-CG	-5.99	1.36	1.52
2	B	355	LEU	C-O	-5.98	1.11	1.23
2	E	122	LYS	CD-CE	-5.98	1.36	1.51
1	A	254	TYR	CE2-CZ	-5.97	1.30	1.38
1	A	201	TYR	CG-CD2	-5.96	1.31	1.39
1	D	317	LEU	C-O	-5.96	1.12	1.23
1	A	402	GLN	CD-NE2	-5.95	1.18	1.32
1	A	97	PHE	CE2-CZ	-5.95	1.26	1.37
2	E	14	MET	C-O	-5.95	1.12	1.23
1	A	336	LEU	CG-CD2	-5.94	1.29	1.51
1	A	210	PHE	CE1-CZ	-5.93	1.26	1.37
2	B	79	ARG	C-O	-5.93	1.12	1.23
2	B	103	PHE	C-O	-5.91	1.12	1.23
1	A	201	TYR	CG-CD1	-5.91	1.31	1.39
2	B	144	HIS	C-O	-5.91	1.12	1.23
2	B	8	TYR	CG-CD2	-5.90	1.31	1.39
1	A	97	PHE	CD1-CE1	-5.89	1.27	1.39
3	F	100	LYS	C-O	-5.89	1.12	1.23
2	B	382	VAL	CB-CG2	-5.88	1.40	1.52
1	A	83	ARG	C-O	-5.87	1.12	1.23
1	A	334	PRO	CB-CG	-5.87	1.20	1.50
1	A	226	VAL	CB-CG1	-5.86	1.40	1.52
1	A	315	ARG	CZ-NH1	-5.84	1.25	1.33
1	A	406	GLU	CA-CB	-5.84	1.41	1.53
1	A	234	PHE	CG-CD2	-5.83	1.29	1.38
1	A	153	PHE	CE2-CZ	-5.83	1.26	1.37
1	A	271	TRP	CG-CD1	-5.82	1.28	1.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	408	ARG	CZ-NH1	-5.82	1.25	1.33
3	C	13	VAL	CB-CG2	-5.80	1.40	1.52
1	A	150	GLU	CG-CD	5.80	1.60	1.51
2	B	352	LYS	C-O	-5.80	1.12	1.23
1	A	66	LYS	C-O	-5.79	1.12	1.23
2	B	98	ARG	C-O	-5.77	1.12	1.23
1	A	248	GLN	C-O	-5.77	1.12	1.23
1	A	434	ARG	C-O	-5.77	1.12	1.23
1	A	393	GLU	CB-CG	-5.76	1.41	1.52
1	A	210	PHE	CD1-CE1	-5.76	1.27	1.39
1	A	14	LYS	CE-NZ	5.75	1.63	1.49
3	F	100	LYS	CD-CE	-5.75	1.36	1.51
1	A	94	VAL	CB-CG1	-5.75	1.40	1.52
1	A	409	HIS	C-O	-5.74	1.12	1.23
1	A	61	GLY	C-O	-5.74	1.14	1.23
1	A	228	SER	C-O	-5.74	1.12	1.23
1	A	394	VAL	C-O	-5.73	1.12	1.23
2	B	170	PHE	C-O	-5.72	1.12	1.23
2	E	251	VAL	CB-CG2	-5.72	1.40	1.52
2	B	103	PHE	CE2-CZ	-5.70	1.26	1.37
1	A	72	GLY	C-O	-5.70	1.14	1.23
2	B	195	ALA	CA-CB	-5.70	1.40	1.52
2	B	226	LEU	CG-CD2	-5.70	1.30	1.51
1	A	271	TRP	CD1-NE1	-5.69	1.28	1.38
2	E	15	GLU	C-O	-5.68	1.12	1.23
1	A	5	PRO	C-O	-5.68	1.11	1.23
2	B	162	VAL	C-O	-5.67	1.12	1.23
1	A	150	GLU	C-O	-5.66	1.12	1.23
2	B	97	THR	C-O	-5.66	1.12	1.23
1	A	317	LEU	CG-CD2	-5.65	1.30	1.51
1	D	434	ARG	CZ-NH2	-5.65	1.25	1.33
1	A	65	TRP	CD2-CE2	-5.65	1.34	1.41
1	A	406	GLU	C-O	-5.64	1.12	1.23
1	D	56	LEU	CG-CD1	-5.64	1.30	1.51
1	A	11	GLU	C-O	-5.64	1.12	1.23
1	A	151	GLU	CB-CG	-5.63	1.41	1.52
2	B	384	PHE	CD2-CE2	-5.63	1.27	1.39
1	A	255	VAL	C-O	-5.63	1.12	1.23
3	F	98	LEU	CG-CD1	-5.62	1.31	1.51
1	D	43	PRO	CB-CG	-5.62	1.21	1.50
2	E	117	ASP	CG-OD2	-5.61	1.12	1.25
2	B	8	TYR	CG-CD1	-5.60	1.31	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	40	TYR	CZ-OH	-5.59	1.28	1.37
1	D	317	LEU	CG-CD2	-5.58	1.31	1.51
2	B	80	GLU	C-O	-5.58	1.12	1.23
2	B	83	GLU	C-O	-5.58	1.12	1.23
1	A	223	ASN	C-O	-5.58	1.12	1.23
2	E	343	ARG	CZ-NH1	-5.58	1.25	1.33
1	D	318	LYS	C-O	-5.57	1.12	1.23
2	B	276	GLY	C-O	-5.55	1.14	1.23
1	A	73	VAL	CB-CG2	-5.55	1.41	1.52
1	A	403	HIS	C-O	-5.54	1.12	1.23
3	F	100	LYS	CB-CG	-5.52	1.37	1.52
2	E	318	LYS	CE-NZ	-5.51	1.35	1.49
1	A	195	TYR	CB-CG	-5.51	1.43	1.51
2	B	19	THR	C-O	-5.50	1.12	1.23
2	B	350	TYR	CD1-CE1	-5.50	1.31	1.39
1	D	275	ASP	CG-OD1	-5.50	1.12	1.25
2	B	9	ASN	C-O	-5.50	1.12	1.23
2	E	122	LYS	C-O	-5.49	1.12	1.23
1	D	394	VAL	CB-CG2	-5.49	1.41	1.52
2	B	28	GLU	CD-OE1	-5.48	1.19	1.25
2	B	98	ARG	CZ-NH1	-5.48	1.25	1.33
1	A	38	LEU	C-O	-5.47	1.12	1.23
2	B	103	PHE	CD1-CE1	-5.47	1.28	1.39
1	D	62	GLU	CD-OE2	-5.46	1.19	1.25
2	B	220	GLU	N-CA	-5.46	1.35	1.46
2	B	170	PHE	CD1-CE1	-5.45	1.28	1.39
3	C	13	VAL	CB-CG1	-5.45	1.41	1.52
1	A	40	TYR	CE2-CZ	-5.45	1.31	1.38
1	A	160	LEU	CG-CD2	-5.44	1.31	1.51
1	A	272	GLY	C-O	-5.44	1.15	1.23
2	B	350	TYR	CE1-CZ	-5.44	1.31	1.38
2	E	243	VAL	C-O	-5.43	1.13	1.23
1	A	432	ARG	C-N	-5.41	1.21	1.34
2	E	343	ARG	C-O	-5.40	1.13	1.23
1	A	418	GLU	C-O	-5.39	1.13	1.23
1	A	174	PRO	CA-C	5.37	1.63	1.52
2	B	103	PHE	CD2-CE2	-5.36	1.28	1.39
1	A	434	ARG	CZ-NH2	-5.35	1.26	1.33
1	A	74	PHE	CG-CD1	-5.35	1.30	1.38
1	A	80	VAL	CB-CG2	-5.33	1.41	1.52
2	E	384	PHE	C-O	-5.33	1.13	1.23
2	B	350	TYR	CD2-CE2	-5.33	1.31	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	292	GLU	CD-OE1	-5.31	1.19	1.25
1	A	40	TYR	CD2-CE2	-5.31	1.31	1.39
1	D	436	MET	C-O	-5.30	1.13	1.23
1	A	51	LEU	CG-CD2	-5.30	1.32	1.51
1	A	370	MET	CB-CG	-5.28	1.34	1.51
2	B	191	ASN	C-O	-5.26	1.13	1.23
1	A	227	ALA	CA-CB	-5.26	1.41	1.52
1	A	249	GLU	C-O	-5.25	1.13	1.23
2	E	244	ASN	C-O	-5.25	1.13	1.23
2	E	343	ARG	NE-CZ	-5.25	1.26	1.33
1	A	71	VAL	C-O	-5.24	1.13	1.23
2	B	67	CYS	C-O	-5.24	1.13	1.23
1	D	204	GLU	CD-OE2	-5.23	1.19	1.25
1	A	203	ASP	C-O	-5.23	1.13	1.23
2	E	120	THR	C-O	-5.22	1.13	1.23
2	E	57	LYS	CD-CE	-5.22	1.38	1.51
2	B	66	ARG	NE-CZ	-5.21	1.26	1.33
1	D	318	LYS	CE-NZ	-5.20	1.36	1.49
2	E	384	PHE	CG-CD1	-5.20	1.30	1.38
1	D	133	HIS	C-O	-5.19	1.13	1.23
1	A	175	GLU	CG-CD	5.18	1.59	1.51
1	A	126	GLY	C-O	-5.18	1.15	1.23
1	A	203	ASP	CG-OD1	-5.18	1.13	1.25
1	A	292	GLU	CD-OE2	-5.17	1.20	1.25
2	B	83	GLU	C-N	-5.17	1.22	1.34
1	A	102	LEU	C-O	-5.16	1.13	1.23
3	C	15	GLU	CB-CG	-5.16	1.42	1.52
1	A	271	TRP	C-O	-5.16	1.13	1.23
1	A	195	TYR	C-O	-5.15	1.13	1.23
2	B	306	VAL	C-O	-5.15	1.13	1.23
2	B	117	ASP	CG-OD1	-5.14	1.13	1.25
1	A	163	ASP	C-O	-5.14	1.13	1.23
2	B	220	GLU	CA-CB	-5.12	1.42	1.53
1	A	356	ASP	CG-OD1	-5.12	1.13	1.25
2	E	120	THR	CA-CB	-5.11	1.40	1.53
1	A	358	VAL	CB-CG2	-5.11	1.42	1.52
1	A	275	ASP	C-O	-5.11	1.13	1.23
1	A	154	PHE	CD1-CE1	-5.10	1.29	1.39
1	A	273	LYS	CB-CG	-5.10	1.38	1.52
2	E	194	GLY	N-CA	-5.10	1.38	1.46
1	A	101	ARG	CZ-NH1	-5.10	1.26	1.33
1	A	84	TYR	CD2-CE2	-5.09	1.31	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	246	ILE	CB-CG2	-5.08	1.37	1.52
2	B	329	GLU	C-O	-5.07	1.13	1.23
3	F	104	CYS	N-CA	-5.07	1.36	1.46
3	F	105	VAL	C-O	-5.06	1.13	1.23
1	A	151	GLU	CD-OE1	-5.06	1.20	1.25
2	B	8	TYR	CE2-CZ	-5.05	1.31	1.38
1	A	291	TYR	CD2-CE2	-5.04	1.31	1.39
2	B	102	GLU	C-O	-5.04	1.13	1.23
1	D	336	LEU	CG-CD1	-5.04	1.33	1.51
2	B	351	GLU	CB-CG	-5.04	1.42	1.52
3	F	37	GLU	CD-OE2	-5.04	1.20	1.25
1	A	299	ASP	CG-OD1	-5.03	1.13	1.25
1	A	65	TRP	CB-CG	-5.03	1.41	1.50
1	A	153	PHE	CD1-CE1	-5.03	1.29	1.39
1	A	410	ASN	C-O	-5.03	1.13	1.23
2	B	18	ILE	CB-CG2	-5.03	1.37	1.52
2	E	248	VAL	C-O	-5.01	1.13	1.23

All (76) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	83	ARG	NE-CZ-NH2	-28.06	106.27	120.30
3	F	67	ARG	NE-CZ-NH1	25.12	132.86	120.30
1	D	432	ARG	NE-CZ-NH2	-22.41	109.09	120.30
1	D	437	ARG	NE-CZ-NH2	-18.76	110.92	120.30
3	F	67	ARG	NE-CZ-NH2	-17.91	111.34	120.30
1	D	432	ARG	NE-CZ-NH1	16.75	128.68	120.30
1	A	315	ARG	NE-CZ-NH2	15.66	128.13	120.30
1	D	269	ARG	NE-CZ-NH2	15.48	128.04	120.30
1	A	83	ARG	NE-CZ-NH1	14.31	127.46	120.30
1	D	102	LEU	CB-CG-CD1	-14.18	86.89	111.00
2	B	20	ASP	CB-CG-OD1	12.51	129.56	118.30
1	A	315	ARG	NE-CZ-NH1	-12.20	114.20	120.30
1	D	437	ARG	NE-CZ-NH1	12.14	126.37	120.30
1	D	434	ARG	NE-CZ-NH1	12.04	126.32	120.30
1	D	427	ASP	CB-CG-OD1	11.17	128.35	118.30
2	B	329	GLU	OE1-CD-OE2	-11.08	110.01	123.30
1	D	269	ARG	NE-CZ-NH1	-10.77	114.91	120.30
1	A	356	ASP	CB-CG-OD1	10.50	127.75	118.30
2	B	256	ASP	CB-CG-OD2	-10.21	109.11	118.30
2	E	24	ARG	NE-CZ-NH1	10.18	125.39	120.30
3	F	67	ARG	CD-NE-CZ	9.70	137.19	123.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	39	ASP	CB-CG-OD1	9.25	126.62	118.30
1	D	275	ASP	CB-CG-OD1	9.01	126.41	118.30
1	D	434	ARG	NE-CZ-NH2	-8.24	116.18	120.30
2	E	117	ASP	CB-CG-OD1	8.05	125.54	118.30
1	D	101	ARG	NE-CZ-NH2	8.03	124.31	120.30
1	A	102	LEU	CA-CB-CG	7.89	133.45	115.30
2	B	256	ASP	CB-CG-OD1	7.75	125.27	118.30
1	D	432	ARG	CD-NE-CZ	7.67	134.34	123.60
1	D	427	ASP	CB-CG-OD2	-7.63	111.43	118.30
2	E	257	ARG	NE-CZ-NH1	7.61	124.11	120.30
1	A	408	ARG	NE-CZ-NH1	-7.33	116.63	120.30
1	A	182	ARG	NE-CZ-NH2	7.32	123.96	120.30
1	A	356	ASP	OD1-CG-OD2	-7.23	109.57	123.30
2	E	220	GLU	CG-CD-OE2	-7.18	103.95	118.30
1	A	36	LYS	CD-CE-NZ	6.93	127.63	111.70
1	A	160	LEU	CB-CG-CD2	6.90	122.73	111.00
2	B	192	MET	CG-SD-CE	6.90	111.24	100.20
2	B	117	ASP	CB-CG-OD1	6.77	124.39	118.30
2	B	384	PHE	CD1-CE1-CZ	6.62	128.04	120.10
3	C	104	CYS	O-C-N	6.58	133.22	122.70
1	D	437	ARG	CD-NE-CZ	6.49	132.68	123.60
1	A	406	GLU	CB-CA-C	-6.43	97.55	110.40
1	A	273	LYS	CD-CE-NZ	6.42	126.45	111.70
2	E	117	ASP	OD1-CG-OD2	-6.41	111.11	123.30
2	E	220	GLU	CB-CA-C	-6.34	97.71	110.40
2	E	220	GLU	CG-CD-OE1	6.27	130.85	118.30
1	A	321	ASP	CB-CG-OD1	6.22	123.89	118.30
1	A	83	ARG	CD-NE-CZ	6.20	132.28	123.60
2	E	120	THR	OG1-CB-CG2	6.08	123.99	110.00
2	B	384	PHE	CG-CD2-CE2	-5.97	114.23	120.80
1	D	101	ARG	NE-CZ-NH1	-5.89	117.35	120.30
1	A	299	ASP	CB-CG-OD1	5.79	123.51	118.30
2	B	220	GLU	OE1-CD-OE2	5.71	130.15	123.30
1	D	408	ARG	NE-CZ-NH2	5.69	123.15	120.30
1	A	247	ASP	CB-CG-OD1	5.63	123.37	118.30
2	E	120	THR	CA-CB-OG1	5.61	120.79	109.00
2	E	117	ASP	CB-CG-OD2	5.59	123.33	118.30
1	D	4	HIS	CB-CA-C	5.58	121.55	110.40
3	F	104	CYS	C-N-CA	5.55	135.59	121.70
1	D	4	HIS	N-CA-CB	5.43	120.37	110.60
2	B	352	LYS	CD-CE-NZ	5.40	124.12	111.70
2	E	257	ARG	NH1-CZ-NH2	-5.37	113.49	119.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	163	ASP	CB-CG-OD1	5.35	123.11	118.30
2	B	143	VAL	CG1-CB-CG2	-5.33	102.37	110.90
1	A	125	ARG	NE-CZ-NH1	5.31	122.96	120.30
1	A	247	ASP	CB-CG-OD2	-5.30	113.53	118.30
1	A	83	ARG	NH1-CZ-NH2	5.25	125.18	119.40
1	A	334	PRO	CA-N-CD	-5.25	104.15	111.50
1	D	391	LEU	CB-CG-CD2	5.22	119.87	111.00
1	A	317	LEU	CB-CG-CD1	5.21	119.86	111.00
1	A	432	ARG	NE-CZ-NH2	5.16	122.88	120.30
1	D	269	ARG	CB-CG-CD	5.10	124.87	111.60
1	A	207	ARG	NE-CZ-NH2	5.09	122.85	120.30
1	A	275	ASP	CB-CG-OD1	5.07	122.86	118.30
2	B	52	LEU	CA-CB-CG	5.04	126.88	115.30

There are no chirality outliers.

There are no planarity outliers.

## 5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3422	0	3275	99	0
1	D	3422	0	3275	113	0
2	B	2999	0	2963	79	0
2	E	2999	0	2963	78	0
3	C	787	0	757	49	0
3	F	787	0	758	46	0
4	A	4	0	0	0	0
4	D	4	0	0	0	0
5	A	63	0	33	12	0
5	B	62	0	35	8	0
5	D	63	0	35	10	0
5	E	62	0	34	5	0
6	A	16	0	0	0	0
6	B	16	0	0	0	0
6	D	16	0	0	0	0
6	E	16	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
7	A	164	0	0	10	0
7	B	160	0	0	4	0
7	C	12	0	0	1	0
7	D	220	0	0	8	0
7	E	155	0	0	3	0
7	F	18	0	0	0	0
All	All	15467	0	14128	408	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 14.

All (408) 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)
5:A:580:SRM:HHA	3:C:104:CYS:SG	1.36	1.62
5:D:582:SRM:HHA	3:F:104:CYS:SG	1.47	1.51
5:A:580:SRM:CHA	3:C:104:CYS:SG	2.10	1.39
7:A:6631:HOH:O	3:C:105:VAL:CG2	1.75	1.34
5:D:582:SRM:CHA	3:F:104:CYS:SG	2.20	1.29
1:A:427:ASP:OD2	1:A:429:SER:HB3	1.38	1.24
1:D:3:LYS:HA	1:D:4:HIS:HB3	1.14	1.12
1:A:3:LYS:O	1:A:3:LYS:HG3	1.41	1.07
1:D:167:SER:HB2	3:F:105:VAL:HG21	1.33	1.06
2:E:382:VAL:CG2	2:E:384:PHE:HD1	1.68	1.06
3:F:13:VAL:HG11	3:F:17:GLY:HA2	1.40	1.04
5:B:581:SRM:HBA1	5:B:581:SRM:HMA3	1.36	1.02
3:C:3:VAL:HG22	3:C:12:GLU:OE2	1.61	0.99
7:A:6631:HOH:O	3:C:105:VAL:HG21	1.39	0.99
1:D:3:LYS:O	1:D:3:LYS:HD3	1.63	0.98
7:D:6726:HOH:O	3:F:105:VAL:HG23	1.63	0.97
2:E:196:VAL:HG11	2:E:204:VAL:HG22	1.47	0.97
1:A:39:ASP:OD1	2:B:2:ALA:HA	1.65	0.96
5:B:581:SRM:CBA	5:B:581:SRM:HMA3	1.92	0.94
1:D:3:LYS:CA	1:D:4:HIS:HB3	1.97	0.94
2:B:382:VAL:CG2	2:B:384:PHE:HD1	1.80	0.94
1:A:70:ILE:HG12	3:C:100:LYS:HD2	1.49	0.94
5:E:583:SRM:HMA3	5:E:583:SRM:HBA1	1.48	0.93
3:C:26:CYS:SG	3:C:28:GLU:HG2	2.10	0.91
2:B:382:VAL:HG23	2:B:384:PHE:HD1	1.34	0.91
2:E:196:VAL:HG11	2:E:204:VAL:CG2	2.01	0.90
2:E:382:VAL:HG23	2:E:384:PHE:HD1	1.36	0.90

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:104:GLN:HE21	1:D:104:GLN:H	1.20	0.89
3:C:3:VAL:CG2	3:C:12:GLU:OE2	2.21	0.88
1:A:69:GLY:O	1:A:70:ILE:HD13	1.74	0.86
1:D:97:PHE:O	2:E:150:TYR:HE1	1.59	0.86
2:E:382:VAL:HG21	2:E:384:PHE:HD1	1.40	0.85
1:D:34:ASN:HD21	1:D:38:LEU:H	1.23	0.85
1:A:97:PHE:O	2:B:150:TYR:CE1	2.30	0.84
1:A:104:GLN:HE21	1:A:104:GLN:H	1.25	0.83
1:A:97:PHE:O	2:B:150:TYR:HE1	1.61	0.83
1:D:104:GLN:NE2	1:D:104:GLN:H	1.77	0.82
5:B:581:SRM:HBA1	5:B:581:SRM:CMA	2.10	0.81
7:D:6726:HOH:O	3:F:105:VAL:CG2	2.21	0.80
7:A:6631:HOH:O	3:C:105:VAL:HG23	1.52	0.80
1:D:3:LYS:HA	1:D:4:HIS:CB	2.02	0.80
1:D:402:GLN:H	1:D:402:GLN:HE21	1.29	0.80
1:D:3:LYS:O	1:D:3:LYS:CG	2.30	0.80
3:F:26:CYS:SG	3:F:28:GLU:OE2	2.41	0.79
1:D:3:LYS:O	1:D:3:LYS:CD	2.30	0.79
2:B:382:VAL:CG2	2:B:384:PHE:CD1	2.65	0.79
1:D:97:PHE:O	2:E:150:TYR:CE1	2.36	0.79
3:C:105:VAL:OXT	3:C:105:VAL:HG12	1.82	0.78
2:B:37:ASN:HD21	2:B:58:ASN:HD21	1.29	0.78
2:E:37:ASN:HD21	2:E:58:ASN:HD21	1.28	0.78
1:D:170:ASN:ND2	1:D:208:PRO:HG3	1.99	0.78
1:A:104:GLN:H	1:A:104:GLN:NE2	1.82	0.77
1:D:131:ASN:HB2	1:D:140:VAL:HB	1.66	0.77
1:D:416:LYS:HB2	1:D:419:GLU:HG3	1.66	0.77
2:E:382:VAL:CG2	2:E:384:PHE:CD1	2.61	0.77
1:A:34:ASN:HD21	1:A:38:LEU:H	1.32	0.76
2:E:382:VAL:HG23	2:E:384:PHE:CD1	2.20	0.76
3:F:28:GLU:HA	3:F:31:LYS:HE2	1.67	0.76
2:E:382:VAL:HG21	2:E:384:PHE:CD1	2.21	0.76
3:C:49:ILE:HD11	3:C:75:PHE:HD1	1.50	0.75
1:D:308:HIS:HD2	2:E:292:ARG:HE	1.35	0.75
3:F:13:VAL:HG11	3:F:17:GLY:CA	2.15	0.74
2:E:208:ARG:HD2	2:E:305:PHE:CE1	2.23	0.73
1:D:262:ASN:ND2	2:E:292:ARG:HH22	1.86	0.73
1:A:69:GLY:C	1:A:70:ILE:HD13	2.09	0.73
3:F:13:VAL:HG12	3:F:14:ASP:N	2.02	0.73
1:D:5:PRO:HG2	1:D:5:PRO:O	1.88	0.72
1:A:83:ARG:CD	2:B:150:TYR:O	2.38	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:382:VAL:HG21	2:B:384:PHE:CD1	2.24	0.72
1:D:402:GLN:H	1:D:402:GLN:NE2	1.88	0.72
1:D:408:ARG:HH11	1:D:410:ASN:HD21	1.38	0.71
1:A:402:GLN:HE21	1:A:402:GLN:H	1.37	0.71
1:A:46:CYS:HB3	1:A:47:PRO:HD3	1.72	0.71
1:D:104:GLN:HE22	1:D:173:THR:HG21	1.54	0.71
1:A:83:ARG:HD3	2:B:150:TYR:O	1.91	0.70
1:A:3:LYS:O	1:A:3:LYS:CG	2.30	0.70
3:C:49:ILE:HD11	3:C:75:PHE:CD1	2.26	0.70
1:A:167:SER:HB2	3:C:105:VAL:HG21	1.73	0.70
1:A:308:HIS:HD2	2:B:292:ARG:HE	1.37	0.70
1:D:184:GLU:OE1	2:E:44:HIS:HD2	1.75	0.69
5:D:582:SRM:O1A	2:E:150:TYR:HD2	1.74	0.69
2:B:9:ASN:C	2:B:9:ASN:HD22	1.93	0.69
1:D:81:ILE:CD1	3:F:105:VAL:HG22	2.22	0.69
1:A:427:ASP:OD2	1:A:429:SER:CB	2.29	0.69
1:A:70:ILE:HG12	3:C:100:LYS:CD	2.23	0.69
3:F:105:VAL:HG12	3:F:105:VAL:OXT	1.91	0.69
1:D:104:GLN:N	1:D:104:GLN:HE21	1.90	0.69
1:D:83:ARG:H	1:D:98:HIS:HD2	1.40	0.69
1:A:285:PRO:HG3	2:B:293:ILE:HA	1.75	0.68
3:F:26:CYS:SG	3:F:28:GLU:HG2	2.33	0.68
1:A:427:ASP:CG	1:A:429:SER:HB3	2.12	0.68
1:A:427:ASP:OD2	1:A:430:ASP:OD1	2.12	0.67
1:A:248:GLN:HE22	1:A:296:LEU:H	1.42	0.67
1:A:83:ARG:H	1:A:98:HIS:HD2	1.40	0.67
1:D:3:LYS:HG3	1:D:3:LYS:O	1.93	0.67
1:D:170:ASN:HD22	1:D:208:PRO:HG3	1.60	0.67
1:D:223:ASN:HD21	1:D:311:ASN:HD21	1.40	0.67
5:B:581:SRM:HBA1	5:B:581:SRM:C1A	2.24	0.66
2:E:293:ILE:HG22	2:E:294:LYS:HD2	1.78	0.66
1:A:167:SER:OG	3:C:105:VAL:HG11	1.95	0.66
3:F:13:VAL:CG1	3:F:17:GLY:HA2	2.23	0.66
2:E:208:ARG:HD3	2:E:278:GLY:O	1.96	0.66
2:E:224:ILE:HB	2:E:225:PRO:HD3	1.78	0.66
2:B:9:ASN:ND2	2:B:11:ALA:H	1.94	0.65
1:A:408:ARG:HH11	1:A:410:ASN:HD21	1.44	0.65
2:B:4:ILE:O	2:B:4:ILE:HG13	1.95	0.65
1:A:411:PRO:HG3	2:E:192:MET:CE	2.26	0.64
5:D:582:SRM:HMA2	3:F:104:CYS:SG	2.38	0.64
1:D:376:ARG:NH1	1:D:376:ARG:HB3	2.14	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:3:VAL:HG22	3:C:12:GLU:HG3	1.81	0.63
1:D:46:CYS:HB3	1:D:47:PRO:HD3	1.81	0.63
2:E:239:ILE:HG12	2:E:252:ALA:HB2	1.79	0.63
5:B:581:SRM:C1A	5:B:581:SRM:CBA	2.76	0.62
1:A:104:GLN:HE21	1:A:104:GLN:N	1.97	0.62
1:D:3:LYS:HE2	1:D:4:HIS:ND1	2.14	0.62
1:A:223:ASN:HD21	1:A:311:ASN:HD21	1.48	0.61
1:A:36:LYS:HB2	7:A:6638:HOH:O	1.99	0.61
1:A:402:GLN:NE2	1:A:402:GLN:H	1.97	0.61
3:F:3:VAL:HG22	3:F:12:GLU:HG2	1.82	0.61
2:B:142:ILE:O	2:B:144:HIS:HD2	1.84	0.61
3:F:78:LYS:O	3:F:82:GLU:HG3	2.00	0.61
2:B:207:HIS:HD2	2:B:279:ASP:OD1	1.83	0.61
3:C:78:LYS:O	3:C:82:GLU:HG3	2.01	0.61
5:A:580:SRM:C1A	3:C:104:CYS:SG	2.84	0.61
1:D:418:GLU:H	1:D:418:GLU:CD	2.03	0.61
3:C:11:PHE:HE2	3:C:26:CYS:HG	1.48	0.60
2:B:107:ASN:ND2	2:B:110:THR:H	1.99	0.60
3:C:26:CYS:HB2	3:C:27:PRO:CD	2.31	0.60
5:D:582:SRM:C1A	3:F:104:CYS:SG	2.88	0.60
2:E:247:LYS:HZ3	2:E:247:LYS:HB3	1.65	0.60
1:A:410:ASN:HD22	1:A:412:TYR:H	1.50	0.60
1:D:156:MET:HE3	1:D:162:THR:HB	1.83	0.60
1:A:435:HIS:HD2	1:D:86:ASP:OD2	1.85	0.59
5:B:581:SRM:NA	5:B:581:SRM:HBA2	2.17	0.59
2:B:11:ALA:C	2:B:13:PRO:HD3	2.22	0.59
3:F:13:VAL:CG1	3:F:17:GLY:CA	2.79	0.59
2:B:367:ASP:N	2:B:368:PRO:HD2	2.18	0.59
1:D:230:ALA:HB2	2:E:289:ILE:HD13	1.84	0.59
1:A:206:HIS:HD2	7:A:6580:HOH:O	1.85	0.58
1:D:196:GLN:HE22	1:D:354:PRO:HA	1.68	0.58
1:D:167:SER:OG	3:F:105:VAL:HG11	2.03	0.58
2:B:382:VAL:HG23	2:B:384:PHE:CD1	2.26	0.58
1:A:313:MET:HE3	1:A:317:LEU:HD11	1.84	0.58
1:D:248:GLN:HE22	1:D:296:LEU:H	1.50	0.58
2:B:75:THR:O	2:B:79:ARG:HG3	2.04	0.58
1:A:62:GLU:OE1	1:D:435:HIS:HE1	1.86	0.58
2:E:37:ASN:ND2	2:E:58:ASN:HD21	2.01	0.58
1:A:98:HIS:HA	2:B:150:TYR:OH	2.03	0.58
1:D:45:GLU:H	1:D:45:GLU:CD	2.08	0.58
1:D:34:ASN:ND2	1:D:38:LEU:H	1.97	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:98:HIS:HE1	1:D:146:THR:OG1	1.86	0.57
1:D:363:GLU:O	1:D:367:GLU:HG3	2.04	0.57
3:F:67:ARG:HG3	3:F:68:ILE:N	2.20	0.57
7:B:949:HOH:O	1:D:432:ARG:HD3	2.04	0.57
1:D:416:LYS:HB3	1:D:418:GLU:OE2	2.03	0.57
1:D:3:LYS:C	1:D:3:LYS:HD3	2.24	0.57
3:F:49:ILE:HD11	3:F:75:PHE:HD1	1.69	0.57
1:A:108:LYS:HD3	1:A:133:HIS:CE1	2.40	0.57
2:B:300:LYS:HB3	1:D:407:PRO:HG2	1.87	0.57
2:B:48:GLU:HB3	2:B:49:PRO:CD	2.35	0.56
3:F:13:VAL:HG12	3:F:14:ASP:H	1.70	0.56
1:A:131:ASN:HB2	1:A:140:VAL:HB	1.86	0.56
2:B:153:THR:N	2:B:154:PRO:CD	2.67	0.56
5:D:582:SRM:O1A	2:E:150:TYR:CD2	2.57	0.56
3:C:3:VAL:HG21	3:C:12:GLU:OE2	2.05	0.56
2:B:9:ASN:ND2	2:B:9:ASN:C	2.56	0.56
1:A:184:GLU:OE1	2:B:44:HIS:HD2	1.87	0.56
2:E:247:LYS:NZ	2:E:247:LYS:HB3	2.22	0.55
2:B:200:ASP:HB3	2:B:337:ILE:HD12	1.87	0.55
3:C:4:VAL:O	3:C:10:ALA:HA	2.06	0.55
1:A:33:LYS:HG3	7:A:6734:HOH:O	2.07	0.55
1:A:81:ILE:CD1	3:C:105:VAL:HG22	2.37	0.54
5:A:580:SRM:O1A	2:B:150:TYR:HD2	1.91	0.54
1:A:305:ARG:NH2	2:E:379:PHE:O	2.39	0.54
1:A:376:ARG:HB3	1:A:376:ARG:NH1	2.21	0.54
1:A:227:ALA:CB	2:B:289:ILE:HD13	2.37	0.54
1:D:308:HIS:CD2	2:E:292:ARG:HE	2.21	0.54
3:F:21:ALA:HB3	3:F:24:ASP:OD2	2.06	0.54
1:D:206:HIS:HD2	7:D:6634:HOH:O	1.90	0.54
1:D:229:MET:HB3	2:E:289:ILE:HD11	1.90	0.54
1:A:83:ARG:HD2	2:B:150:TYR:O	2.07	0.54
3:C:3:VAL:HG22	3:C:12:GLU:CD	2.27	0.54
3:C:91:GLY:O	3:C:95:MET:HG3	2.07	0.54
3:F:49:ILE:HD13	3:F:73:THR:HG21	1.90	0.54
1:A:435:HIS:HE1	1:D:62:GLU:OE1	1.91	0.53
1:D:306:CYS:O	1:D:307:MET:HB2	2.08	0.53
1:A:411:PRO:HG3	2:E:192:MET:HE2	1.90	0.53
1:A:306:CYS:O	1:A:307:MET:HB2	2.09	0.53
7:A:6604:HOH:O	2:B:125:ALA:HB3	2.07	0.53
1:D:376:ARG:HB3	1:D:376:ARG:HH11	1.74	0.53
2:B:37:ASN:ND2	2:B:58:ASN:HD21	2.03	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:227:ALA:HB1	2:B:289:ILE:HD13	1.90	0.53
5:A:580:SRM:HMA2	3:C:104:CYS:SG	2.49	0.53
1:D:334:PRO:HD2	7:E:841:HOH:O	2.09	0.53
3:F:13:VAL:HG13	3:F:18:PHE:O	2.09	0.53
1:A:50:LEU:HD13	1:A:50:LEU:C	2.29	0.52
1:D:390:LYS:HD3	1:D:390:LYS:O	2.08	0.52
3:F:13:VAL:CG1	3:F:14:ASP:N	2.72	0.52
3:F:13:VAL:CG1	3:F:17:GLY:C	2.77	0.52
2:B:186:LEU:C	2:B:186:LEU:HD23	2.29	0.52
2:B:300:LYS:CB	1:D:407:PRO:HG2	2.40	0.52
2:E:146:GLN:HE21	2:E:150:TYR:HB3	1.74	0.52
1:D:410:ASN:HD22	1:D:412:TYR:H	1.57	0.52
5:D:582:SRM:HBA1	5:D:582:SRM:HHB	1.91	0.52
2:E:280:GLY:HA3	2:E:305:PHE:CE1	2.45	0.52
2:E:48:GLU:HB2	2:E:49:PRO:CD	2.40	0.52
1:A:349:ILE:HD11	1:A:357:GLU:HB3	1.92	0.52
1:A:70:ILE:HG13	3:C:101:PRO:HD2	1.92	0.52
2:E:153:THR:N	2:E:154:PRO:CD	2.72	0.52
3:C:3:VAL:HG22	3:C:12:GLU:CG	2.40	0.52
2:E:220:GLU:HB3	3:F:20:ASN:O	2.10	0.51
2:B:254:ASN:HD21	2:B:256:ASP:HB2	1.76	0.51
5:E:583:SRM:NA	5:E:583:SRM:HBA2	2.25	0.51
1:D:334:PRO:HG2	2:E:192:MET:CE	2.40	0.51
1:A:67:HIS:HE1	2:B:265:TYR:O	1.93	0.51
3:C:21:ALA:HB3	3:C:24:ASP:OD2	2.11	0.51
1:D:168:GLY:HA2	3:F:105:VAL:HB	1.93	0.51
1:A:280:VAL:HG11	1:A:313:MET:HE1	1.92	0.51
2:B:243:VAL:HG23	2:B:243:VAL:O	2.11	0.50
1:A:67:HIS:CE1	2:B:265:TYR:O	2.64	0.50
3:C:25:TRP:CE3	3:C:26:CYS:HA	2.45	0.50
1:D:34:ASN:N	1:D:35:PRO:HD3	2.26	0.50
1:D:429:SER:O	1:D:433:LYS:HG3	2.12	0.50
1:D:55:GLU:OE2	1:D:59:HIS:HE1	1.94	0.50
2:B:12:LYS:N	2:B:13:PRO:HD3	2.27	0.50
2:B:211:PRO:HB3	2:B:273:LEU:HB3	1.94	0.50
1:A:111:THR:HG23	2:B:29:PHE:HD2	1.75	0.50
1:A:262:ASN:ND2	2:B:292:ARG:HH22	2.09	0.50
1:D:170:ASN:HB3	1:D:208:PRO:HA	1.93	0.50
2:E:211:PRO:HG2	2:E:253:ILE:CD1	2.42	0.50
1:A:390:LYS:O	1:A:390:LYS:HD3	2.11	0.49
1:D:160:LEU:N	1:D:160:LEU:HD12	2.26	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:9:ASN:HD22	2:B:10:PRO:N	2.09	0.49
3:F:49:ILE:HD11	3:F:75:PHE:CD1	2.47	0.49
3:F:77:LEU:HD22	3:F:81:TYR:CD1	2.47	0.49
1:D:279:GLU:O	1:D:308:HIS:HE1	1.96	0.49
2:E:242:GLU:HA	2:E:246:GLN:O	2.12	0.49
5:D:582:SRM:HMA2	3:F:104:CYS:CB	2.43	0.49
1:D:87:GLN:N	1:D:88:PRO:HD3	2.27	0.49
2:E:239:ILE:C	2:E:239:ILE:HD12	2.33	0.49
5:A:580:SRM:HMA2	3:C:104:CYS:CB	2.43	0.48
1:D:168:GLY:N	3:F:105:VAL:HB	2.28	0.48
2:E:293:ILE:HG22	2:E:294:LYS:CD	2.42	0.48
1:A:67:HIS:HA	2:B:152:HIS:CD2	2.48	0.48
1:D:170:ASN:HB2	1:D:204:GLU:O	2.13	0.48
1:D:99:THR:HG23	1:D:140:VAL:HG13	1.96	0.48
2:B:153:THR:N	2:B:154:PRO:HD2	2.29	0.48
2:B:314:PRO:O	2:B:318:LYS:HG2	2.13	0.48
5:B:581:SRM:NA	5:B:581:SRM:CBA	2.74	0.48
3:C:6:PHE:CD2	3:C:32:TYR:HB2	2.48	0.48
1:A:60:GLU:OE1	1:A:64:HIS:HE1	1.96	0.48
2:B:138:SER:HB2	2:B:172:GLU:O	2.14	0.48
3:C:12:GLU:HB3	3:C:20:ASN:HD22	1.78	0.48
1:D:67:HIS:HD2	7:D:6692:HOH:O	1.94	0.48
1:A:196:GLN:HE22	1:A:354:PRO:HA	1.78	0.48
1:A:285:PRO:CG	2:B:293:ILE:HA	2.44	0.48
1:D:159:ASN:C	1:D:160:LEU:HD12	2.34	0.48
2:E:215:HIS:HD2	2:E:250:SER:OG	1.97	0.48
2:E:207:HIS:HD2	2:E:279:ASP:OD1	1.97	0.47
2:B:31:PRO:HG2	2:B:34:ILE:CG1	2.44	0.47
1:D:3:LYS:HE2	1:D:3:LYS:HB2	1.78	0.47
1:D:81:ILE:HD12	3:F:105:VAL:HG22	1.96	0.47
1:A:168:GLY:HA2	3:C:105:VAL:HB	1.96	0.47
1:D:107:ALA:HB3	1:D:191:GLN:HE21	1.78	0.47
1:A:17:TRP:CD2	1:A:18:PRO:HD2	2.49	0.47
1:A:239:THR:OG1	1:A:305:ARG:HD2	2.14	0.47
2:B:9:ASN:HD21	2:B:11:ALA:HB3	1.80	0.47
5:A:580:SRM:C4D	3:C:104:CYS:SG	2.92	0.47
5:A:580:SRM:O1A	2:B:150:TYR:CD2	2.68	0.46
1:A:83:ARG:H	1:A:98:HIS:CD2	2.28	0.46
2:B:254:ASN:HD22	2:B:254:ASN:C	2.18	0.46
1:D:98:HIS:HA	2:E:150:TYR:OH	2.16	0.46
2:E:171:GLU:HG3	7:E:934:HOH:O	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:F:26:CYS:SG	3:F:28:GLU:CG	3.02	0.46
1:A:107:ALA:HB3	1:A:191:GLN:HE21	1.81	0.46
1:A:167:SER:CB	3:C:105:VAL:HG11	2.46	0.46
2:B:242:GLU:HA	2:B:246:GLN:O	2.16	0.46
2:E:142:ILE:O	2:E:144:HIS:HD2	1.98	0.46
5:E:583:SRM:CBA	5:E:583:SRM:C1A	2.93	0.46
1:D:104:GLN:N	1:D:104:GLN:NE2	2.54	0.46
2:E:211:PRO:HB3	2:E:273:LEU:HB3	1.97	0.46
1:A:363:GLU:O	1:A:367:GLU:HG3	2.14	0.46
3:C:105:VAL:CG1	3:C:105:VAL:OXT	2.55	0.46
1:A:313:MET:N	1:A:314:PRO:HD3	2.31	0.46
2:B:144:HIS:CG	2:B:162:VAL:HG21	2.50	0.46
3:C:11:PHE:CE2	3:C:29:TRP:HB2	2.51	0.46
1:A:279:GLU:O	1:A:308:HIS:HE1	1.99	0.46
1:D:168:GLY:CA	3:F:105:VAL:HB	2.46	0.46
1:D:76:TYR:CD1	1:D:206:HIS:HB3	2.51	0.46
1:A:406:GLU:HG3	7:A:6681:HOH:O	2.16	0.45
1:A:411:PRO:HG3	2:E:192:MET:HE1	1.96	0.45
2:B:172:GLU:HA	2:B:172:GLU:OE1	2.14	0.45
2:B:382:VAL:HG22	1:D:402:GLN:OE1	2.16	0.45
1:D:20:PHE:O	1:D:24:ILE:HG13	2.16	0.45
1:D:189:ASP:CG	1:D:192:LEU:HB2	2.37	0.45
2:E:186:LEU:HD23	2:E:186:LEU:C	2.36	0.45
7:D:6726:HOH:O	3:F:105:VAL:HG21	2.03	0.45
2:B:96:THR:HB	5:B:581:SRM:HAB1	1.98	0.45
1:A:113:GLU:HG3	7:A:6608:HOH:O	2.16	0.45
5:A:580:SRM:HDD1	3:C:104:CYS:SG	2.57	0.45
1:D:371:GLU:HG2	7:D:6743:HOH:O	2.15	0.45
1:A:416:LYS:HB2	1:A:419:GLU:HG3	1.97	0.45
1:A:97:PHE:O	2:B:150:TYR:CZ	2.68	0.45
1:D:34:ASN:HD21	1:D:38:LEU:N	2.02	0.45
2:B:62:VAL:O	2:B:62:VAL:HG13	2.17	0.45
1:D:104:GLN:HE22	1:D:173:THR:CG2	2.25	0.45
2:E:214:ASP:OD1	2:E:216:GLU:HG2	2.17	0.45
1:A:232:SER:O	1:A:331:ALA:HB3	2.15	0.45
3:F:26:CYS:SG	3:F:27:PRO:N	2.89	0.45
2:B:48:GLU:HB3	2:B:49:PRO:HD2	1.99	0.45
2:B:63:PHE:O	2:B:104:MET:HA	2.17	0.44
1:D:3:LYS:CD	1:D:3:LYS:C	2.82	0.44
2:B:211:PRO:HG2	2:B:253:ILE:CD1	2.47	0.44
1:D:225:CYS:HA	5:E:583:SRM:C1C	2.48	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:98:HIS:HE1	1:A:146:THR:OG1	2.01	0.44
1:A:64:HIS:HD2	1:A:86:ASP:OD1	2.00	0.44
1:A:60:GLU:OE1	1:A:64:HIS:CE1	2.70	0.44
1:D:170:ASN:HD22	1:D:208:PRO:CG	2.29	0.44
1:D:45:GLU:N	1:D:45:GLU:CD	2.71	0.44
2:E:333:LYS:O	2:E:334:TYR:HB2	2.18	0.44
2:E:223:GLU:HB3	3:F:62:ILE:HG22	1.99	0.44
3:C:57:TYR:CD1	3:C:98:LEU:HD22	2.53	0.43
7:D:6620:HOH:O	2:E:44:HIS:HE1	2.00	0.43
3:F:100:LYS:HG3	3:F:101:PRO:HD2	1.99	0.43
1:D:219:ASP:OD1	1:D:226:VAL:HG12	2.18	0.43
2:E:138:SER:HB2	2:E:172:GLU:O	2.18	0.43
2:E:208:ARG:HD2	2:E:305:PHE:CD1	2.53	0.43
2:E:75:THR:O	2:E:79:ARG:HG3	2.18	0.43
3:F:13:VAL:HG13	3:F:18:PHE:N	2.34	0.43
2:B:346:TRP:CE2	1:D:407:PRO:HD2	2.53	0.43
1:D:308:HIS:HD2	2:E:292:ARG:NE	2.10	0.43
2:E:48:GLU:HB2	2:E:49:PRO:HD2	2.00	0.43
1:A:41:GLN:NE2	2:B:4:ILE:HG23	2.34	0.43
3:C:4:VAL:HG11	3:C:32:TYR:CE2	2.54	0.43
1:D:232:SER:O	1:D:331:ALA:HB3	2.18	0.43
2:E:246:GLN:HA	2:E:246:GLN:OE1	2.18	0.43
1:A:86:ASP:OD1	1:A:87:GLN:HG2	2.17	0.43
1:A:83:ARG:NH1	5:A:580:SRM:O1A	2.52	0.43
1:A:308:HIS:CD2	2:B:292:ARG:HE	2.25	0.43
1:D:334:PRO:HG3	1:D:339:ALA:HB2	2.00	0.43
2:B:148:TRP:CE3	2:B:157:ASP:HB2	2.53	0.43
2:B:347:GLU:HG2	7:B:814:HOH:O	2.17	0.43
1:D:67:HIS:CE1	2:E:265:TYR:O	2.72	0.43
2:E:12:LYS:N	2:E:13:PRO:HD3	2.34	0.43
1:D:67:HIS:HE1	2:E:265:TYR:O	2.01	0.43
2:B:152:HIS:C	2:B:154:PRO:HD2	2.39	0.42
1:D:135:SER:HB2	5:D:582:SRM:HHC	2.01	0.42
1:A:312:THR:C	1:A:314:PRO:HD3	2.39	0.42
1:A:76:TYR:CD1	1:A:206:HIS:HB3	2.55	0.42
3:C:19:LEU:HD21	3:C:29:TRP:CE3	2.54	0.42
1:D:17:TRP:CD2	1:D:18:PRO:HD2	2.53	0.42
2:B:44:HIS:HE1	7:B:837:HOH:O	2.03	0.42
1:D:156:MET:SD	1:D:160:LEU:HD22	2.60	0.42
1:D:335:VAL:HA	1:D:336:LEU:HA	1.85	0.42
3:F:77:LEU:HD22	3:F:81:TYR:CE1	2.55	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:367:ASP:N	2:B:368:PRO:CD	2.82	0.42
3:C:11:PHE:HB3	3:C:19:LEU:CD2	2.49	0.42
1:D:416:LYS:HB2	1:D:419:GLU:CG	2.44	0.42
2:E:254:ASN:HD22	2:E:254:ASN:C	2.21	0.42
5:E:583:SRM:C1A	5:E:583:SRM:HBA2	2.50	0.42
1:A:81:ILE:HD11	3:C:105:VAL:HG22	2.00	0.42
2:B:384:PHE:N	2:B:384:PHE:CD1	2.84	0.42
1:D:182:ARG:HD3	2:E:54:HIS:CE1	2.54	0.42
3:F:13:VAL:HG13	3:F:17:GLY:C	2.39	0.42
2:E:87:LYS:HD3	2:E:88:PHE:CE1	2.55	0.42
1:A:219:ASP:OD1	1:A:226:VAL:HG12	2.20	0.41
1:A:428:ILE:HD13	2:E:214:ASP:HB2	2.02	0.41
5:D:582:SRM:CCA	2:E:150:TYR:HD2	2.32	0.41
2:E:211:PRO:HG2	2:E:253:ILE:HD13	2.01	0.41
2:E:332:ARG:O	2:E:335:GLU:HB2	2.20	0.41
1:D:376:ARG:CB	1:D:376:ARG:HH11	2.33	0.41
2:E:223:GLU:HB2	2:E:226:LEU:HD12	2.01	0.41
5:A:580:SRM:CCA	2:B:150:TYR:HD2	2.34	0.41
2:B:31:PRO:HG2	2:B:34:ILE:HG12	2.01	0.41
3:C:30:VAL:HG13	3:C:95:MET:HE3	2.02	0.41
1:D:111:THR:HG23	2:E:29:PHE:HD2	1.84	0.41
1:D:202:GLN:OE1	1:D:206:HIS:HE1	2.04	0.41
1:A:284:CYS:HA	1:A:285:PRO:HD3	1.92	0.41
1:D:83:ARG:H	1:D:98:HIS:CD2	2.29	0.41
2:E:152:HIS:C	2:E:154:PRO:HD2	2.40	0.41
1:A:428:ILE:CD1	2:E:214:ASP:HB2	2.50	0.41
2:B:95:PHE:CE2	2:B:101:ILE:HG12	2.56	0.41
1:A:11:GLU:O	1:A:11:GLU:HG3	2.20	0.41
3:C:68:ILE:HD12	7:C:514:HOH:O	2.19	0.41
1:D:132:MET:HA	1:D:133:HIS:HA	1.88	0.41
1:A:99:THR:N	2:B:150:TYR:OH	2.53	0.41
1:D:102:LEU:HA	1:D:102:LEU:HD12	1.80	0.41
7:B:949:HOH:O	1:D:437:ARG:HD2	2.20	0.41
2:E:239:ILE:O	2:E:239:ILE:HD12	2.20	0.41
1:D:408:ARG:HH11	1:D:410:ASN:ND2	2.13	0.41
1:D:409:HIS:HD2	7:D:6621:HOH:O	2.03	0.41
2:E:207:HIS:HE1	7:E:954:HOH:O	2.03	0.41
1:A:172:ARG:HB2	1:A:215:LYS:HG2	2.03	0.41
1:A:409:HIS:HD2	7:A:6614:HOH:O	2.04	0.41
1:D:108:LYS:HD3	1:D:133:HIS:CE1	2.56	0.41
1:D:60:GLU:OE1	1:D:64:HIS:CE1	2.74	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:46:ILE:HG12	2:E:52:LEU:HD22	2.03	0.41
1:A:427:ASP:CG	1:A:429:SER:H	2.25	0.41
2:B:313:TRP:N	2:B:314:PRO:HD3	2.35	0.41
1:A:376:ARG:HB3	1:A:376:ARG:HH11	1.85	0.40
3:C:57:TYR:CG	3:C:98:LEU:HD22	2.57	0.40
2:E:144:HIS:CG	2:E:162:VAL:HG21	2.56	0.40
2:E:259:MET:C	2:E:260:TYR:CG	2.93	0.40
2:E:31:PRO:HG2	2:E:34:ILE:CG1	2.51	0.40
3:F:13:VAL:CG1	3:F:14:ASP:H	2.34	0.40
3:F:26:CYS:SG	3:F:28:GLU:CD	2.99	0.40
5:A:580:SRM:CDD	3:C:104:CYS:SG	3.09	0.40
3:C:88:PRO:O	3:C:92:ALA:HB3	2.22	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles [i](#)

### 5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	433/437 (99%)	418 (96%)	15 (4%)	0	100	100
1	D	433/437 (99%)	422 (98%)	10 (2%)	1 (0%)	51	31
2	B	383/386 (99%)	365 (95%)	16 (4%)	2 (0%)	32	13
2	E	383/386 (99%)	369 (96%)	12 (3%)	2 (0%)	32	13
3	C	102/105 (97%)	98 (96%)	3 (3%)	1 (1%)	18	4
3	F	102/105 (97%)	99 (97%)	2 (2%)	1 (1%)	18	4
All	All	1836/1856 (99%)	1771 (96%)	58 (3%)	7 (0%)	38	18

All (7) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	4	HIS

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Mol	Chain	Res	Type
3	C	34	LYS
3	F	34	LYS
2	E	293	ILE
2	E	153	THR
2	B	153	THR
2	B	293	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	364/365 (100%)	350 (96%)	14 (4%)	38	14
1	D	364/365 (100%)	352 (97%)	12 (3%)	43	18
2	B	324/325 (100%)	312 (96%)	12 (4%)	39	14
2	E	324/325 (100%)	319 (98%)	5 (2%)	70	53
3	C	79/80 (99%)	75 (95%)	4 (5%)	28	7
3	F	79/80 (99%)	74 (94%)	5 (6%)	21	4
All	All	1534/1540 (100%)	1482 (97%)	52 (3%)	42	17

All (52) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	3	LYS
1	A	34	ASN
1	A	36	LYS
1	A	54	LEU
1	A	83	ARG
1	A	104	GLN
1	A	208	PRO
1	A	212	TYR
1	A	249	GLU
1	A	258	GLU
1	A	273	LYS
1	A	391	LEU

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Mol	Chain	Res	Type
1	A	402	GLN
1	A	406	GLU
2	B	4	ILE
2	B	9	ASN
2	B	172	GLU
2	B	188	CYS
2	B	189	CYS
2	B	220	GLU
2	B	254	ASN
2	B	259	MET
2	B	260	TYR
2	B	329	GLU
2	B	356	GLU
2	B	384	PHE
3	C	12	GLU
3	C	28	GLU
3	C	51	ASP
3	C	77	LEU
1	D	3	LYS
1	D	4	HIS
1	D	33	LYS
1	D	34	ASN
1	D	54	LEU
1	D	89	GLU
1	D	104	GLN
1	D	192	LEU
1	D	212	TYR
1	D	336	LEU
1	D	402	GLN
1	D	432	ARG
2	E	188	CYS
2	E	189	CYS
2	E	254	ASN
2	E	259	MET
2	E	260	TYR
3	F	20	ASN
3	F	34	LYS
3	F	51	ASP
3	F	67	ARG
3	F	77	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (54) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	34	ASN
1	A	64	HIS
1	A	67	HIS
1	A	98	HIS
1	A	104	GLN
1	A	161	ASN
1	A	196	GLN
1	A	206	HIS
1	A	248	GLN
1	A	262	ASN
1	A	308	HIS
1	A	311	ASN
1	A	402	GLN
1	A	409	HIS
1	A	410	ASN
1	A	435	HIS
2	B	9	ASN
2	B	37	ASN
2	B	44	HIS
2	B	107	ASN
2	B	144	HIS
2	B	191	ASN
2	B	207	HIS
2	B	215	HIS
2	B	254	ASN
2	B	263	ASN
1	D	34	ASN
1	D	64	HIS
1	D	67	HIS
1	D	98	HIS
1	D	104	GLN
1	D	161	ASN
1	D	170	ASN
1	D	196	GLN
1	D	206	HIS
1	D	248	GLN
1	D	262	ASN
1	D	308	HIS
1	D	311	ASN
1	D	375	ASN
1	D	402	GLN
1	D	409	HIS
1	D	410	ASN

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Mol	Chain	Res	Type
1	D	435	HIS
2	E	37	ASN
2	E	44	HIS
2	E	144	HIS
2	E	146	GLN
2	E	191	ASN
2	E	207	HIS
2	E	215	HIS
2	E	254	ASN
2	E	263	ASN
3	F	47	GLN

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

14 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	$\# Z  > 2$
5	SRM	A	580	2,4	34,70,70	1.62	5 (14%)	34,112,112	3.11	7 (20%)
4	SO3	A	6575	5	1,3,3	0.48	0	0,3,3	0.00	-
6	SF4	A	803	1	0,12,12	0.00	-	0,24,24	0.00	-

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
6	SF4	A	804	1	0,12,12	0.00	-	0,24,24	0.00	-
5	SRM	B	581	-	28,66,70	1.34	3 (10%)	35,98,112	6.34	10 (28%)
6	SF4	B	801	2	0,12,12	0.00	-	0,24,24	0.00	-
6	SF4	B	802	2	0,12,12	0.00	-	0,24,24	0.00	-
5	SRM	D	582	2,4	34,70,70	1.52	4 (11%)	34,112,112	2.40	9 (26%)
4	SO3	D	6576	5	1,3,3	1.25	0	0,3,3	0.00	-
6	SF4	D	807	1	0,12,12	0.00	-	0,24,24	0.00	-
6	SF4	D	808	1	0,12,12	0.00	-	0,24,24	0.00	-
5	SRM	E	583	-	28,66,70	1.51	3 (10%)	35,98,112	5.23	9 (25%)
6	SF4	E	805	2	0,12,12	0.00	-	0,24,24	0.00	-
6	SF4	E	806	2	0,12,12	0.00	-	0,24,24	0.00	-

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
5	SRM	A	580	2,4	-	0/22/126/126	0/0/8/8
4	SO3	A	6575	5	-	0/0/0/0	0/0/0/0
6	SF4	A	803	1	-	0/0/48/48	0/6/5/5
6	SF4	A	804	1	-	0/0/48/48	0/6/5/5
5	SRM	B	581	-	-	0/33/94/126	0/0/4/8
6	SF4	B	801	2	-	0/0/48/48	0/6/5/5
6	SF4	B	802	2	-	0/0/48/48	0/6/5/5
5	SRM	D	582	2,4	-	0/22/126/126	0/0/8/8
4	SO3	D	6576	5	-	0/0/0/0	0/0/0/0
6	SF4	D	807	1	-	0/0/48/48	0/6/5/5
6	SF4	D	808	1	-	0/0/48/48	0/6/5/5
5	SRM	E	583	-	-	0/33/94/126	0/0/4/8
6	SF4	E	805	2	-	0/0/48/48	0/6/5/5
6	SF4	E	806	2	-	0/0/48/48	0/6/5/5

All (15) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	E	583	SRM	CBA-CAA	-3.25	1.36	1.52
5	A	580	SRM	CDB-C2B	-2.30	1.52	1.56
5	B	581	SRM	CDA-C2A	2.43	1.59	1.56
5	D	582	SRM	CDA-C2A	3.14	1.60	1.56
5	D	582	SRM	FE-NB	3.36	2.09	1.95
5	E	583	SRM	CMB-C2B	3.45	1.61	1.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	B	581	SRM	CAB-C3B	3.46	1.57	1.51
5	D	582	SRM	CMB-C2B	3.50	1.61	1.54
5	A	580	SRM	CDA-C2A	3.57	1.61	1.56
5	D	582	SRM	FE-NA	3.59	2.09	1.95
5	E	583	SRM	CAB-C3B	3.63	1.57	1.51
5	A	580	SRM	FE-NB	3.67	2.10	1.95
5	A	580	SRM	CMB-C2B	3.71	1.61	1.54
5	B	581	SRM	CMB-C2B	3.76	1.61	1.54
5	A	580	SRM	FE-NA	3.78	2.10	1.95

All (35) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	B	581	SRM	CAA-C3A-C2A	-31.13	88.33	123.52
5	E	583	SRM	CAA-C3A-C2A	-20.37	100.49	123.52
5	E	583	SRM	CAB-C3B-C2B	-15.22	106.31	123.52
5	B	581	SRM	CAB-C3B-C2B	-14.50	107.13	123.52
5	A	580	SRM	CAB-C3B-C2B	-6.94	115.67	123.52
5	D	582	SRM	CAB-C3B-C2B	-6.04	116.70	123.52
5	A	580	SRM	CAA-C3A-C2A	-5.76	117.01	123.52
5	D	582	SRM	CAA-C3A-C2A	-5.35	117.48	123.52
5	E	583	SRM	CBD-CAD-C2D	-4.61	103.66	112.48
5	B	581	SRM	CBD-CAD-C2D	-4.45	103.98	112.48
5	E	583	SRM	CDD-C3D-C4D	-3.06	122.72	127.36
5	E	583	SRM	CDC-C2C-C1C	-2.95	122.94	127.39
5	B	581	SRM	CDD-C3D-C4D	-2.94	122.90	127.36
5	B	581	SRM	CDC-C2C-C1C	-2.71	123.30	127.39
5	D	582	SRM	C3B-C4B-NB	-2.60	107.15	110.12
5	D	582	SRM	CDC-C2C-C1C	-2.11	124.21	127.39
5	B	581	SRM	C2B-C1B-NB	2.05	112.62	109.01
5	D	582	SRM	CBC-CAC-C3C	2.22	116.70	112.47
5	E	583	SRM	C3A-C4A-NA	2.30	110.82	107.59
5	A	580	SRM	CBC-CAC-C3C	2.45	117.14	112.47
5	D	582	SRM	C2A-CDA-CEA	2.60	119.24	115.39
5	E	583	SRM	CAD-CBD-CCD	2.80	117.45	112.66
5	A	580	SRM	C2A-CDA-CEA	3.02	119.86	115.39
5	B	581	SRM	C3A-C4A-NA	3.03	111.85	107.59
5	B	581	SRM	CAD-CBD-CCD	3.19	118.12	112.66
5	B	581	SRM	C2B-CDB-CEB	3.61	120.74	115.39
5	D	582	SRM	C4B-NB-C1B	3.80	108.93	106.37
5	A	580	SRM	C4B-NB-C1B	3.93	109.02	106.37
5	E	583	SRM	C2B-CDB-CEB	4.27	121.71	115.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	580	SRM	C4A-NA-C1A	4.93	109.69	106.37
5	D	582	SRM	C4A-NA-C1A	5.28	109.93	106.37
5	D	582	SRM	CAB-CBB-CCB	6.63	123.99	112.66
5	B	581	SRM	CAA-CBA-CCA	11.54	132.38	112.66
5	A	580	SRM	CAB-CBB-CCB	12.73	134.41	112.66
5	E	583	SRM	CAA-CBA-CCA	14.63	137.67	112.66

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

4 monomers are involved in 35 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	580	SRM	12	0
5	B	581	SRM	8	0
5	D	582	SRM	10	0
5	E	583	SRM	5	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	435/437 (99%)	0.19	8 (1%) 69 77	14, 23, 44, 74	0
1	D	435/437 (99%)	-0.10	6 (1%) 75 83	13, 19, 38, 73	0
2	B	385/386 (99%)	0.13	6 (1%) 72 80	15, 23, 40, 59	0
2	E	385/386 (99%)	0.02	7 (1%) 69 77	13, 21, 36, 78	0
3	C	104/105 (99%)	0.90	13 (12%) 4 6	22, 33, 64, 79	0
3	F	104/105 (99%)	0.33	5 (4%) 31 37	22, 29, 47, 66	0
All	All	1848/1856 (99%)	0.12	45 (2%) 59 66	13, 23, 44, 79	0

All (45) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	C	105	VAL	7.4
3	C	3	VAL	6.2
3	F	105	VAL	5.5
1	D	3	LYS	5.3
2	E	386	SER	5.1
1	D	4	HIS	5.0
3	C	8	GLY	4.9
3	C	4	VAL	4.9
1	A	4	HIS	4.0
3	C	6	PHE	3.9
2	B	2	ALA	3.7
3	C	7	ALA	3.6
1	A	3	LYS	3.2
1	A	430	ASP	3.1
2	E	244	ASN	3.0
3	C	9	SER	3.0
3	C	40	GLY	2.9
2	B	150	TYR	2.9
3	C	10	ALA	2.9

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Mol	Chain	Res	Type	RSRZ
1	A	33	LYS	2.8
3	C	11	PHE	2.7
1	D	89	GLU	2.6
2	E	239	ILE	2.6
3	F	41	ALA	2.6
2	E	243	VAL	2.5
1	A	37	GLY	2.5
2	B	72	LEU	2.4
2	B	244	ASN	2.4
3	C	44	ALA	2.4
3	C	72	ASN	2.4
1	D	425	SER	2.3
2	B	386	SER	2.3
1	A	89	GLU	2.3
2	E	150	TYR	2.2
3	F	26	CYS	2.2
3	F	40	GLY	2.2
2	B	3	PHE	2.2
1	A	90	MET	2.1
3	C	75	PHE	2.1
2	E	101	ILE	2.1
2	E	245	GLY	2.1
1	D	5	PRO	2.1
1	D	436	MET	2.0
3	F	44	ALA	2.0
1	A	429	SER	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( $\text{\AA}^2$ )	Q<0.9
4	SO3	D	6576	4/4	0.96	0.11	2.34	34,35,36,36	0
5	SRM	B	581	62/63	0.90	0.17	2.28	19,21,24,25	0
4	SO3	A	6575	4/4	0.93	0.14	2.25	39,40,40,40	0
5	SRM	E	583	62/63	0.92	0.15	1.47	14,17,20,23	0
5	SRM	D	582	63/63	0.93	0.13	0.54	18,21,28,31	0
5	SRM	A	580	63/63	0.93	0.13	0.27	20,24,31,33	0
6	SF4	D	808	8/8	0.96	0.10	0.14	13,18,21,22	0
6	SF4	D	807	8/8	0.97	0.07	-0.44	17,21,22,22	0
6	SF4	A	804	8/8	0.96	0.11	-0.46	17,20,23,23	0
6	SF4	A	803	8/8	0.95	0.08	-0.46	22,23,25,26	0
6	SF4	E	806	8/8	0.95	0.08	-0.66	22,23,25,25	0
6	SF4	B	802	8/8	0.98	0.07	-0.70	21,22,22,24	0
6	SF4	E	805	8/8	0.95	0.08	-0.89	18,21,24,24	0
6	SF4	B	801	8/8	0.95	0.08	-1.31	17,23,24,24	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.