



# Full wwPDB X-ray Structure Validation Report ⓘ

Oct 18, 2017 – 12:34 PM EDT

PDB ID : 3BN9  
Title : Crystal Structure of MT-SP1 in complex with Fab Inhibitor E2  
Authors : Farady, C.J.; Schneider, E.L.; Egea, P.F.; Goetz, D.H.; Craik, C.S.  
Deposited on : unknown  
Resolution : 2.17 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 : rb-20030345  
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) : rb-20030345

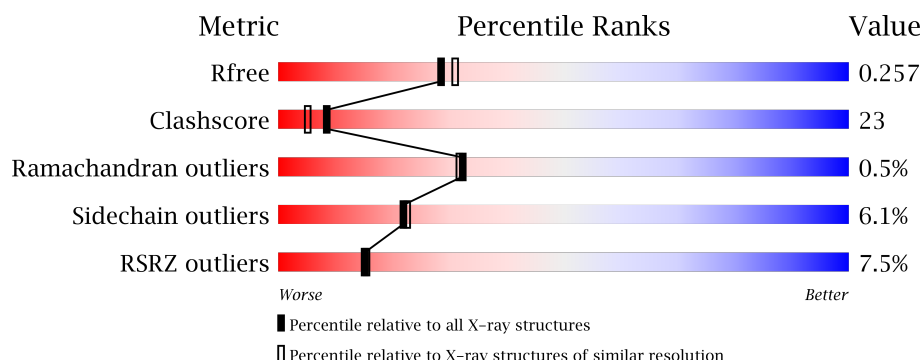
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.17 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	5526 (2.20-2.16)
Clashscore	112137	6386 (2.20-2.16)
Ramachandran outliers	110173	6282 (2.20-2.16)
Sidechain outliers	110143	6282 (2.20-2.16)
RSRZ outliers	101464	5562 (2.20-2.16)

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	241	<div> <div>78%</div> <div>20%</div> <div>.</div> </div>
1	B	241	<div> <div>83%</div> <div>17%</div> <div>.</div> </div>
2	C	214	<div> <div>19%</div> <div>62%</div> <div>35%</div> <div>..</div> </div>
2	E	214	<div> <div>12%</div> <div>64%</div> <div>30%</div> <div>5%</div> <div>.</div> </div>
3	D	257	<div> <div>7%</div> <div>53%</div> <div>26%</div> <div>18%</div> </div>

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Mol	Chain	Length	Quality of chain
3	F	257	

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	EDO	A	13	-	-	X	X
4	EDO	A	2	-	-	X	-
4	EDO	B	1	-	-	-	X
4	EDO	B	6	-	-	X	-
4	EDO	B	7	-	-	X	X
4	EDO	C	216	-	-	X	-
4	EDO	D	243	-	-	-	X
4	EDO	E	216	-	-	-	X

## 2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 11103 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 Membrane-type serine protease 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	B	241	Total	C	N	O	S	2	3	0
			1882	1188	331	352	11			
1	A	241	Total	C	N	O	S	2	4	0
			1891	1194	334	352	11			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	122	SER	CYS	ENGINEERED	UNP Q9Y5Y6
A	122	SER	CYS	ENGINEERED	UNP Q9Y5Y6

- Molecule 2 is a protein called E2 Fab Light Chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	C	210	Total	C	N	O	S	0	0	0
			1593	996	266	326	5			
2	E	211	Total	C	N	O	S	0	1	0
			1609	1007	269	328	5			

- Molecule 3 is a protein called E2 Fab Heavy Chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	D	211	Total	C	N	O	S	0	1	0
			1575	998	267	302	8			
3	F	224	Total	C	N	O	S	0	1	0
			1667	1050	285	325	7			

- Molecule 4 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: C<sub>2</sub>H<sub>6</sub>O<sub>2</sub>).



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

- Molecule 5 is SULFATE ION (three-letter code: SO4) (formula: O<sub>4</sub>S).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	C	1	Total	O	S	0	0
			5	4	1		
5	E	1	Total	O	S	0	0
			5	4	1		

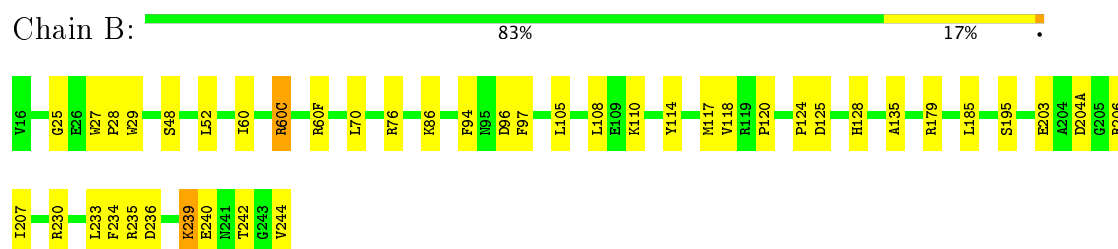
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	B	199	Total	O	0	0
			199	199		
6	C	118	Total	O	0	0
			118	118		
6	D	105	Total	O	0	0
			105	105		
6	A	175	Total	O	0	0
			175	175		
6	E	124	Total	O	0	0
			124	124		
6	F	103	Total	O	0	0
			103	103		

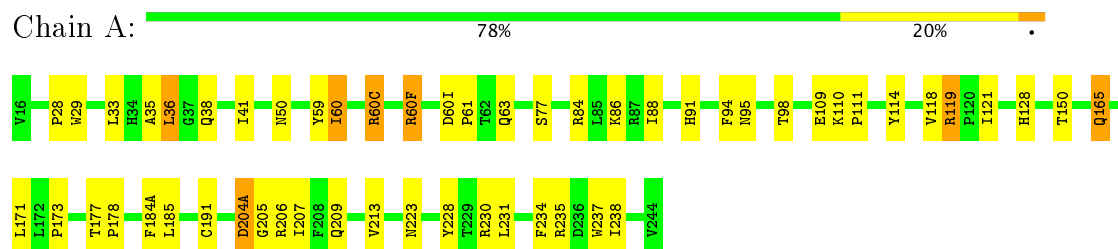
### 3 Residue-property plots

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.

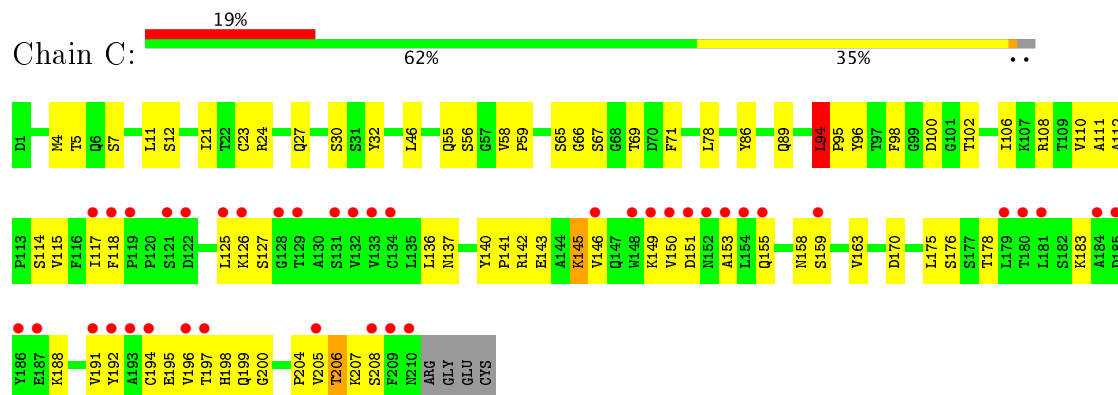
- Molecule 1: Membrane-type serine protease 1



- Molecule 1: Membrane-type serine protease 1

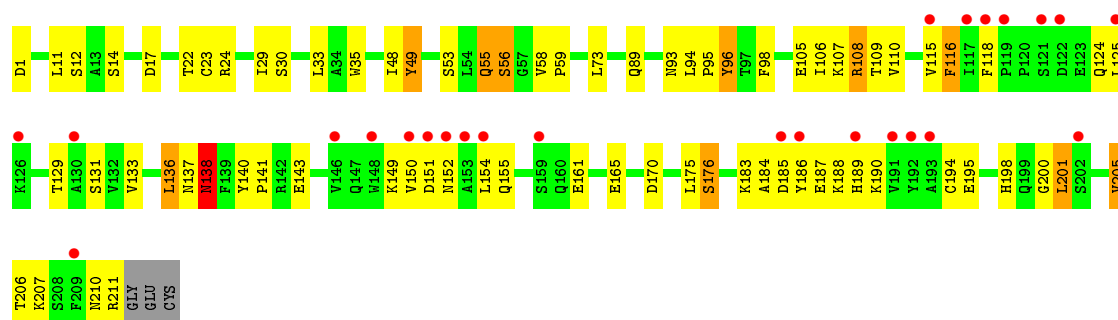


- Molecule 2: E2 Fab Light Chain

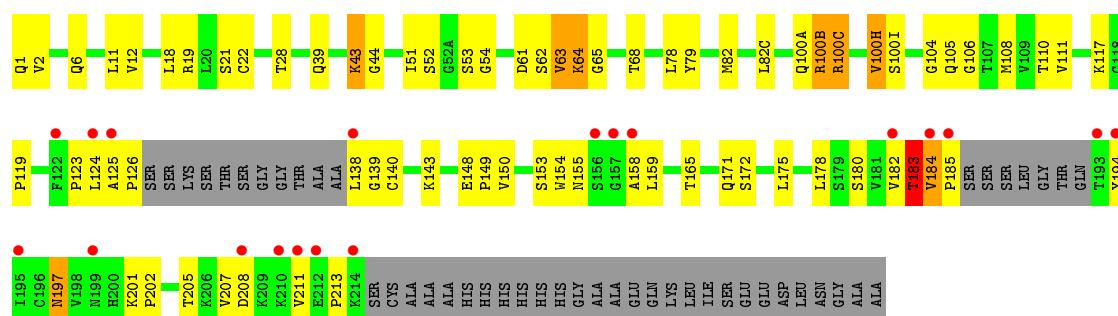


- Molecule 2: E2 Fab Light Chain

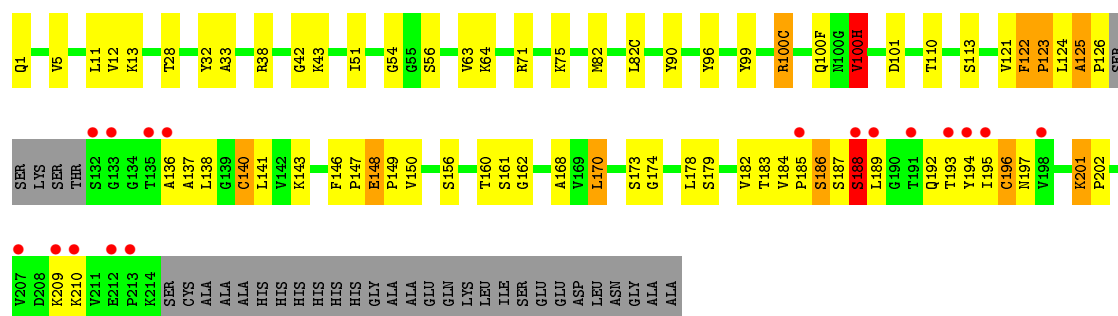




• Molecule 3: E2 Fab Heavy Chain



• Molecule 3: E2 Fab Heavy Chain





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	48.62Å 163.28Å 201.16Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	85.64 – 2.17 85.64 – 2.17	Depositor EDS
% Data completeness (in resolution range)	87.4 (85.64-2.17) 87.4 (85.64-2.17)	Depositor EDS
$R_{merge}$	0.09	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.87 (at 2.18Å)	Xtriage
Refinement program	PHENIX	Depositor
R, $R_{free}$	0.223 , 0.267 0.213 , 0.257	Depositor DCC
$R_{free}$ test set	5776 reflections (7.72%)	DCC
Wilson B-factor (Å <sup>2</sup> )	29.0	Xtriage
Anisotropy	0.731	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.30 , 51.4	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	11103	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	41.0	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 44.76 % 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 1.4561e-04. 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, 0.333 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: SO4, EDO

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	1.10	7/1946 (0.4%)	0.81	2/2647 (0.1%)
1	B	0.96	0/1934	0.66	0/2630
2	C	1.00	3/1627 (0.2%)	0.70	0/2212
2	E	1.00	5/1644 (0.3%)	0.75	2/2235 (0.1%)
3	D	0.71	1/1618 (0.1%)	0.67	0/2207
3	F	0.94	4/1708 (0.2%)	0.80	5/2326 (0.2%)
All	All	0.97	20/10477 (0.2%)	0.73	9/14257 (0.1%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
2	C	0	2
3	D	0	4
3	F	0	2
All	All	0	8

All (20) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	59	TYR	CE1-CZ	-10.47	1.25	1.38
1	A	59	TYR	CE2-CZ	-9.67	1.25	1.38
1	A	59	TYR	CD1-CE1	-9.37	1.25	1.39
3	D	43	LYS	C-N	-7.23	1.20	1.33
1	A	59	TYR	CD2-CE2	-6.19	1.30	1.39
1	A	60	ILE	C-N	6.17	1.48	1.34
2	E	49	TYR	CD2-CE2	-5.94	1.30	1.39
1	A	60	ILE	C-O	-5.65	1.12	1.23
2	C	32	TYR	CD1-CE1	-5.65	1.30	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	E	96	TYR	CD1-CE1	-5.62	1.30	1.39
2	E	49	TYR	CD1-CE1	-5.45	1.31	1.39
2	C	86	TYR	CD1-CE1	-5.31	1.31	1.39
3	F	32	TYR	CD2-CE2	-5.26	1.31	1.39
2	C	32	TYR	CD2-CE2	-5.20	1.31	1.39
2	E	96	TYR	CD2-CE2	-5.17	1.31	1.39
3	F	100(H)	VAL	CB-CG1	-5.17	1.42	1.52
1	A	59	TYR	CG-CD1	-5.12	1.32	1.39
3	F	148	GLU	CG-CD	-5.11	1.44	1.51
3	F	42	GLY	C-N	-5.11	1.22	1.34
2	E	165	GLU	CD-OE2	-5.04	1.20	1.25

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	F	43	LYS	O-C-N	-8.48	108.78	123.20
3	F	43	LYS	CA-C-N	7.07	130.34	116.20
3	F	188	SER	CB-CA-C	-6.64	97.48	110.10
2	E	136	LEU	CA-CB-CG	5.89	128.84	115.30
1	A	204(A)	ASP	CB-CG-OD1	-5.83	113.05	118.30
1	A	204(A)	ASP	CB-CG-OD2	5.73	123.46	118.30
3	F	196	CYS	CA-CB-SG	5.72	124.29	114.00
2	E	205	VAL	CB-CA-C	-5.30	101.32	111.40
3	F	140	CYS	CA-CB-SG	5.20	123.36	114.00

There are no chirality outliers.

All (8) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	C	126	LYS	Peptide
2	C	94	LEU	Peptide
3	D	100(A)	GLN	Peptide
3	D	125	ALA	Peptide
3	D	172	SER	Peptide
3	D	183	THR	Peptide
3	F	125	ALA	Peptide
3	F	188	SER	Peptide

## 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	1891	0	1808	67	0
1	B	1882	0	1793	47	0
2	C	1593	0	1540	85	0
2	E	1609	0	1550	95	0
3	D	1575	0	1526	95	0
3	F	1667	0	1629	91	0
4	A	12	0	18	10	0
4	B	24	0	36	21	0
4	C	8	0	12	8	0
4	D	4	0	6	3	0
4	E	4	0	6	0	0
5	C	5	0	0	0	0
5	E	5	0	0	0	0
6	A	175	0	0	11	0
6	B	199	0	0	8	0
6	C	118	0	0	8	0
6	D	105	0	0	3	0
6	E	124	0	0	2	0
6	F	103	0	0	7	0
All	All	11103	0	9924	463	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 23.

All (463) 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)
3:F:123:PRO:CG	3:F:209:LYS:HE2	1.35	1.54
3:F:123:PRO:HG3	3:F:209:LYS:CE	1.45	1.44
2:C:151:ASP:HA	2:C:191:VAL:CG2	1.46	1.42
2:E:187:GLU:C	2:E:211:ARG:NH1	1.74	1.39
3:F:122:PHE:HA	3:F:209:LYS:NZ	1.27	1.37
3:F:123:PRO:CD	3:F:209:LYS:NZ	1.88	1.36
3:F:123:PRO:HD3	3:F:209:LYS:NZ	1.05	1.36
2:E:195:GLU:CB	2:E:206:THR:HG22	1.56	1.35

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:F:123:PRO:CD	3:F:209:LYS:HZ3	1.44	1.23
2:C:151:ASP:CA	2:C:191:VAL:CG2	2.17	1.22
2:C:150:VAL:O	2:C:153:ALA:HB3	1.42	1.20
2:E:187:GLU:CA	2:E:211:ARG:NH1	2.04	1.20
2:E:195:GLU:HB2	2:E:206:THR:HG22	1.20	1.18
1:A:35:ALA:HB3	1:A:41:ILE:CD1	1.75	1.16
2:E:187:GLU:HA	2:E:211:ARG:NH1	1.62	1.12
2:E:195:GLU:HB2	2:E:206:THR:CG2	1.80	1.12
2:E:195:GLU:HG3	2:E:206:THR:CG2	1.79	1.11
2:E:189:HIS:O	2:E:211:ARG:NE	1.81	1.10
3:D:183:THR:HA	3:D:184:VAL:CG2	1.79	1.10
2:C:151:ASP:HA	2:C:191:VAL:HG22	1.10	1.10
2:E:116:PHE:CE1	3:F:137:ALA:HB2	1.86	1.09
1:A:35:ALA:HB3	1:A:41:ILE:HD11	1.34	1.08
3:F:185:PRO:HG2	3:F:188:SER:OG	1.51	1.08
3:F:140:CYS:SG	3:F:196:CYS:CB	2.42	1.08
3:D:183:THR:CA	3:D:184:VAL:HG23	1.85	1.07
2:E:187:GLU:O	2:E:211:ARG:NH1	1.86	1.06
3:F:122:PHE:CA	3:F:209:LYS:NZ	2.17	1.06
2:C:150:VAL:O	2:C:153:ALA:CB	2.03	1.05
1:A:35:ALA:CB	1:A:41:ILE:HD12	1.86	1.05
1:B:230:ARG:HD3	4:B:6:EDO:H12	1.33	1.04
1:A:91:HIS:NE2	4:A:13:EDO:H22	1.71	1.03
1:A:91:HIS:HE2	4:A:13:EDO:H22	0.88	1.03
2:C:151:ASP:N	2:C:191:VAL:HG23	1.74	1.02
3:F:193:THR:HG23	3:F:210:LYS:HD2	1.06	1.02
2:E:151:ASP:OD2	2:E:189:HIS:CD2	2.14	1.01
2:E:195:GLU:CB	2:E:206:THR:CG2	2.37	1.01
2:C:125:LEU:O	2:C:183:LYS:HD3	1.59	1.01
2:E:205:VAL:HG12	2:E:205:VAL:O	1.56	1.01
3:F:193:THR:CG2	3:F:210:LYS:HD2	1.91	1.00
3:F:123:PRO:CG	3:F:209:LYS:CE	2.19	0.98
1:B:60:ILE:HD11	1:B:94:PHE:HE2	1.28	0.98
2:C:151:ASP:HA	2:C:191:VAL:HG21	1.46	0.97
3:F:122:PHE:CA	3:F:209:LYS:HZ3	1.73	0.97
2:E:195:GLU:CG	2:E:206:THR:CG2	2.43	0.96
2:E:187:GLU:CA	2:E:211:ARG:HH12	1.74	0.96
2:E:187:GLU:C	2:E:211:ARG:HH11	1.59	0.96
1:A:35:ALA:CB	1:A:41:ILE:CD1	2.41	0.96
2:E:195:GLU:CG	2:E:206:THR:HG22	1.96	0.95
2:C:94:LEU:CD2	2:C:96:TYR:CE1	2.50	0.94

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:197:THR:HG22	2:C:204:PRO:HG3	1.50	0.93
2:E:187:GLU:C	2:E:211:ARG:HH12	1.46	0.93
2:C:151:ASP:H	2:C:191:VAL:HG23	1.28	0.92
2:C:100:ASP:HB2	6:C:405:HOH:O	1.68	0.92
1:A:91:HIS:HE2	4:A:13:EDO:C2	1.81	0.92
2:E:116:PHE:CD1	3:F:137:ALA:HB3	2.05	0.91
3:F:193:THR:HG23	3:F:210:LYS:CD	1.99	0.91
3:F:123:PRO:HD3	3:F:209:LYS:CE	2.00	0.91
1:B:230:ARG:HB3	4:B:6:EDO:H11	1.50	0.91
2:C:151:ASP:CA	2:C:191:VAL:HG22	1.90	0.91
2:E:116:PHE:CE1	3:F:137:ALA:CB	2.55	0.90
3:F:123:PRO:N	3:F:209:LYS:HZ3	1.70	0.90
2:E:150:VAL:HG12	2:E:189:HIS:CD2	2.07	0.89
3:F:140:CYS:CB	3:F:196:CYS:SG	2.60	0.89
2:C:198:HIS:CD2	2:C:200:GLY:H	1.91	0.89
3:F:123:PRO:CD	3:F:209:LYS:CE	2.45	0.88
2:E:151:ASP:CG	2:E:189:HIS:CD2	2.47	0.88
2:C:151:ASP:N	2:C:191:VAL:CG2	2.36	0.87
2:C:146:VAL:CG2	2:C:196:VAL:HG22	2.05	0.87
1:B:60:ILE:HD11	1:B:94:PHE:CE2	2.10	0.87
3:D:155:ASN:HD21	3:D:194:TYR:HD1	1.16	0.87
2:E:188:LYS:O	2:E:188:LYS:HG3	1.74	0.86
2:E:195:GLU:HG3	2:E:206:THR:HG23	1.57	0.86
2:C:198:HIS:HD2	2:C:200:GLY:H	1.21	0.86
3:D:6:GLN:HE21	3:D:104:GLY:HA3	1.38	0.86
1:A:84:ARG:HG2	1:A:84:ARG:HH11	1.40	0.86
1:A:35:ALA:HB2	1:A:41:ILE:HD12	1.55	0.86
2:E:108:ARG:HD3	2:E:109:THR:O	1.76	0.85
2:E:116:PHE:CD1	3:F:137:ALA:CB	2.59	0.85
1:A:128:HIS:HD2	6:A:284:HOH:O	1.58	0.85
3:F:122:PHE:HA	3:F:209:LYS:HZ2	1.03	0.84
3:F:122:PHE:C	3:F:209:LYS:HZ3	1.81	0.83
2:E:195:GLU:CA	2:E:206:THR:HG22	2.06	0.83
3:F:136:ALA:CB	3:F:189:LEU:HD11	2.09	0.83
3:F:33:ALA:H	3:F:100(F):GLN:HE22	1.25	0.83
3:D:43:LYS:HE2	6:D:289:HOH:O	1.78	0.82
3:F:96:TYR:HB2	3:F:101:ASP:HB3	1.62	0.82
3:D:138:LEU:HD12	3:D:139:GLY:O	1.79	0.81
2:E:108:ARG:HG2	2:E:109:THR:N	1.95	0.81
3:F:186:SER:O	3:F:189:LEU:HB2	1.80	0.81
3:D:143:LYS:HE3	3:D:171:GLN:HE22	1.46	0.81

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:60(F):ARG:HG2	1:A:60(I):ASP:HB2	1.63	0.81
2:C:94:LEU:HD23	2:C:96:TYR:CE1	2.13	0.81
3:D:117:LYS:HD3	3:D:175:LEU:CD2	2.11	0.80
2:C:146:VAL:HG22	2:C:196:VAL:HA	1.64	0.80
2:C:146:VAL:HG21	2:C:196:VAL:HG22	1.62	0.79
1:A:60:ILE:HD11	1:A:94:PHE:HE2	1.47	0.79
2:C:149:LYS:HA	2:C:153:ALA:O	1.83	0.79
3:F:33:ALA:H	3:F:100(F):GLN:NE2	1.81	0.78
2:E:189:HIS:O	2:E:211:ARG:CD	2.31	0.78
2:E:118:PHE:CD1	3:F:124:LEU:HB3	2.19	0.77
3:D:184:VAL:HB	3:D:185:PRO:HD3	1.65	0.77
3:D:183:THR:HA	3:D:184:VAL:HG23	0.89	0.77
2:C:46:LEU:HD23	2:C:55:GLN:HE21	1.50	0.76
3:D:155:ASN:HB2	3:D:158:ALA:HB3	1.68	0.76
1:A:185:LEU:H	4:A:2:EDO:H22	1.51	0.75
2:E:94:LEU:CD2	2:E:96:TYR:CE1	2.69	0.75
2:C:65:SER:OG	4:C:216:EDO:H12	1.87	0.75
3:F:121:VAL:O	3:F:209:LYS:HD2	1.86	0.75
6:B:346:HOH:O	3:D:100(C):ARG:HD3	1.88	0.74
3:F:185:PRO:CG	3:F:188:SER:OG	2.33	0.74
1:A:185:LEU:H	4:A:2:EDO:C2	2.00	0.74
3:D:124:LEU:HB2	3:D:139:GLY:HA2	1.70	0.73
1:A:119[A]:ARG:HH11	1:A:119[A]:ARG:CG	2.00	0.73
2:E:183:LYS:NZ	2:E:187:GLU:OE2	2.22	0.73
2:E:108:ARG:HG2	2:E:109:THR:H	1.53	0.72
3:D:124:LEU:H	3:D:139:GLY:HA3	1.54	0.72
6:B:346:HOH:O	3:D:100(C):ARG:CD	2.37	0.71
1:B:207:ILE:CD1	4:B:7:EDO:H22	2.21	0.71
1:A:128:HIS:HE1	6:A:269:HOH:O	1.74	0.71
1:A:119[A]:ARG:HG3	1:A:119[A]:ARG:HH11	1.55	0.71
3:F:123:PRO:HD3	3:F:209:LYS:HZ1	0.89	0.70
3:D:82:MET:HB3	3:D:82(C):LEU:HD21	1.73	0.70
3:F:170:LEU:HD21	3:F:174:GLY:HA2	1.72	0.70
3:D:108[A]:MET:SD	3:D:149:PRO:HG3	2.31	0.70
2:E:184:ALA:O	6:E:444:HOH:O	2.10	0.69
1:A:28:PRO:HB2	1:A:119[A]:ARG:HB3	1.75	0.69
1:A:204(A):ASP:C	1:A:204(A):ASP:OD1	2.30	0.69
2:E:210:ASN:O	2:E:211:ARG:C	2.30	0.69
3:F:121:VAL:O	3:F:209:LYS:CD	2.41	0.68
1:B:105:LEU:HD13	1:B:242:THR:CG2	2.23	0.68
2:C:151:ASP:H	2:C:191:VAL:CG2	2.01	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:94:LEU:HD21	2:C:96:TYR:CE1	2.28	0.68
3:D:117:LYS:HD3	3:D:175:LEU:HD22	1.75	0.68
1:B:125:ASP:OD2	6:B:440:HOH:O	2.11	0.68
2:E:151:ASP:HB2	2:E:189:HIS:CD2	2.29	0.67
2:C:118:PHE:CD1	3:D:124:LEU:HB3	2.30	0.67
1:B:204(A):ASP:OD2	1:B:206:ARG:NE	2.27	0.67
1:A:86:LYS:HG2	1:A:86:LYS:O	1.92	0.67
1:B:128:HIS:HE1	6:B:341:HOH:O	1.78	0.67
3:D:119:PRO:HD2	3:D:205:THR:HG21	1.77	0.67
3:F:125:ALA:HA	3:F:126:PRO:C	2.15	0.67
2:C:146:VAL:HG22	2:C:196:VAL:HG22	1.75	0.67
2:E:12[B]:SER:OG	2:E:107:LYS:HB2	1.94	0.66
1:A:28:PRO:HD2	1:A:29:TRP:CZ3	2.31	0.66
1:A:185:LEU:N	4:A:2:EDO:H22	2.09	0.66
3:D:194:TYR:O	3:D:211:VAL:HG22	1.96	0.66
1:A:60(C):ARG:HG2	3:F:28:THR:CG2	2.26	0.66
2:E:149:LYS:HG2	2:E:154:LEU:HD23	1.76	0.66
1:A:150[A]:THR:HG23	6:A:266:HOH:O	1.95	0.66
2:E:149:LYS:CG	2:E:154:LEU:HD23	2.25	0.66
3:F:140:CYS:CB	3:F:196:CYS:HG	2.01	0.66
2:E:198:HIS:HD2	2:E:200:GLY:H	1.43	0.66
3:D:100(C):ARG:CB	3:D:100(C):ARG:HH11	2.10	0.65
2:C:94:LEU:HD21	2:C:96:TYR:HE1	1.60	0.65
3:D:159:LEU:HD13	3:D:182:VAL:HG21	1.78	0.65
3:D:201:LYS:N	3:D:202:PRO:CD	2.60	0.65
3:D:124:LEU:HB2	3:D:139:GLY:CA	2.26	0.65
3:D:19:ARG:NH1	3:D:79:TYR:CD1	2.66	0.64
1:A:178:PRO:HG2	4:A:12:EDO:O2	1.97	0.64
1:A:60:ILE:HD11	1:A:94:PHE:CE2	2.32	0.64
2:E:187:GLU:CA	2:E:211:ARG:HH11	1.95	0.64
2:C:66:GLY:HA2	4:C:216:EDO:H11	1.79	0.64
3:F:100(H):VAL:CG1	3:F:100(H):VAL:O	2.44	0.64
2:E:140:TYR:CG	2:E:141:PRO:HA	2.33	0.64
2:E:151:ASP:CB	2:E:189:HIS:CD2	2.80	0.64
3:D:155:ASN:ND2	3:D:194:TYR:HD1	1.92	0.63
1:B:128:HIS:HD2	6:B:351:HOH:O	1.81	0.63
1:A:84:ARG:HH11	1:A:84:ARG:CG	2.11	0.63
2:C:21:ILE:HG12	2:C:102:THR:HG21	1.81	0.63
1:B:29:TRP:HH2	4:B:7:EDO:H21	1.64	0.62
2:C:115:VAL:HG22	2:C:136:LEU:HD22	1.80	0.62
2:C:150:VAL:O	2:C:153:ALA:HB2	1.94	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:123:PRO:HB3	3:D:211:VAL:HG12	1.81	0.62
2:C:66:GLY:CA	4:C:216:EDO:H11	2.29	0.62
2:E:125:LEU:O	2:E:183:LYS:HD2	2.00	0.62
2:E:195:GLU:HA	2:E:206:THR:HG22	1.82	0.62
3:D:182:VAL:O	3:D:184:VAL:HG22	1.99	0.61
2:E:195:GLU:HB2	2:E:206:THR:HG21	1.78	0.61
3:D:100(C):ARG:HH11	3:D:100(C):ARG:HB2	1.65	0.61
1:B:204(A):ASP:OD2	1:B:206:ARG:NH2	2.33	0.61
3:D:182:VAL:O	3:D:184:VAL:CG2	2.49	0.61
1:B:28:PRO:HD2	1:B:29:TRP:CZ3	2.36	0.60
3:F:121:VAL:HG12	3:F:121:VAL:O	1.99	0.60
3:D:100(I):SER:O	4:D:243:EDO:H12	2.01	0.60
1:A:150[B]:THR:HG22	6:A:266:HOH:O	2.01	0.60
2:C:151:ASP:OD1	2:C:191:VAL:HG22	2.02	0.60
2:E:152:ASN:O	2:E:152:ASN:OD1	2.19	0.60
2:E:189:HIS:O	2:E:211:ARG:HD2	2.00	0.60
3:F:122:PHE:CA	3:F:209:LYS:HZ2	1.96	0.60
2:C:198:HIS:HD2	2:C:200:GLY:N	1.98	0.60
2:E:55:GLN:HE21	2:E:56:SER:H	1.49	0.60
2:C:46:LEU:HD23	2:C:55:GLN:NE2	2.17	0.60
2:E:89:GLN:HE21	2:E:96:TYR:HB3	1.65	0.60
1:A:119[A]:ARG:HH11	1:A:119[A]:ARG:HB2	1.65	0.59
1:B:25:GLY:HA2	4:B:3:EDO:H22	1.83	0.59
2:C:65:SER:OG	4:C:216:EDO:C1	2.50	0.59
1:B:124:PRO:HD2	6:B:349:HOH:O	2.02	0.59
3:D:100(H):VAL:O	3:D:100(H):VAL:CG1	2.51	0.59
1:A:165:GLN:NE2	6:A:346:HOH:O	2.33	0.59
2:C:146:VAL:HG22	2:C:196:VAL:CA	2.32	0.59
1:A:121:ILE:HD13	1:A:209:GLN:HB2	1.83	0.59
1:B:204(A):ASP:CG	1:B:206:ARG:HE	2.06	0.59
1:B:135:ALA:H	4:B:8:EDO:H21	1.67	0.58
3:D:19:ARG:NH1	3:D:79:TYR:CE1	2.70	0.58
3:F:75:LYS:HE2	6:F:334:HOH:O	2.02	0.58
1:A:119[A]:ARG:HB2	1:A:119[A]:ARG:NH1	2.19	0.58
3:F:185:PRO:HG2	3:F:188:SER:HG	1.63	0.58
2:C:195:GLU:O	2:C:195:GLU:HG3	2.04	0.58
1:A:28:PRO:HD2	1:A:29:TRP:CE3	2.39	0.58
1:B:234:PHE:CE1	4:B:1:EDO:H11	2.39	0.57
1:B:230:ARG:CD	4:B:6:EDO:H12	2.23	0.57
1:A:237:TRP:HB2	4:A:13:EDO:O2	2.04	0.57
3:F:51:ILE:HD11	3:F:54:GLY:HA2	1.86	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:124:LEU:HD12	3:D:139:GLY:HA2	1.84	0.57
3:D:126:PRO:O	3:D:138:LEU:HB2	2.04	0.57
3:F:13:LYS:NZ	6:F:309:HOH:O	2.38	0.57
2:E:188:LYS:CG	2:E:188:LYS:O	2.49	0.57
1:A:36:LEU:HD22	1:A:63:GLN:HA	1.87	0.56
3:D:182:VAL:HG22	3:D:183:THR:N	2.20	0.56
3:D:6:GLN:HE21	3:D:104:GLY:CA	2.16	0.56
1:B:233:LEU:HG	4:B:6:EDO:O2	2.06	0.56
2:C:145:LYS:O	2:C:145:LYS:HG3	2.05	0.56
3:D:100(B):ARG:HD2	6:D:259:HOH:O	2.04	0.56
2:C:108:ARG:O	6:C:400:HOH:O	2.17	0.56
1:A:60(C):ARG:HG2	3:F:28:THR:HG23	1.88	0.56
1:B:230:ARG:HB3	4:B:6:EDO:C1	2.29	0.56
3:F:123:PRO:CD	3:F:209:LYS:HZ1	1.85	0.55
2:E:116:PHE:N	2:E:116:PHE:CD2	2.74	0.55
3:F:184:VAL:HB	3:F:185:PRO:HD2	1.88	0.55
2:E:138:ASN:N	2:E:138:ASN:OD1	2.39	0.55
1:A:165:GLN:NE2	1:A:230:ARG:HH21	2.05	0.55
3:D:64:LYS:HD2	3:D:65:GLY:N	2.21	0.55
1:A:119[A]:ARG:HH11	1:A:119[A]:ARG:CB	2.19	0.55
1:B:124:PRO:O	1:B:235:ARG:HD3	2.07	0.55
2:C:11:LEU:HD12	2:C:11:LEU:C	2.27	0.55
3:F:148:GLU:OE2	3:F:168:ALA:HB3	2.05	0.55
2:E:94:LEU:HD21	2:E:96:TYR:CE1	2.42	0.55
1:B:114:TYR:CZ	1:B:120:PRO:HG3	2.42	0.54
1:A:204(A):ASP:OD1	1:A:205:GLY:N	2.40	0.54
1:A:60(C):ARG:HG2	3:F:28:THR:HG21	1.90	0.54
2:E:11:LEU:HD12	2:E:11:LEU:C	2.28	0.54
3:D:100(I):SER:HB2	4:D:243:EDO:C1	2.37	0.54
2:C:150:VAL:HG23	2:C:155:GLN:NE2	2.23	0.54
2:C:191:VAL:HG23	2:C:191:VAL:O	2.08	0.54
3:F:160:THR:HG23	6:F:364:HOH:O	2.08	0.54
1:B:25:GLY:CA	4:B:3:EDO:H22	2.39	0.53
3:F:148:GLU:HG2	3:F:149:PRO:HA	1.90	0.53
3:F:162:GLY:HA3	3:F:182:VAL:HG23	1.90	0.53
3:F:100(H):VAL:HG13	3:F:100(H):VAL:O	2.08	0.53
3:F:140:CYS:HG	3:F:196:CYS:CB	2.03	0.53
3:D:154:TRP:HZ2	3:D:180:SER:O	1.91	0.53
3:D:11:LEU:HD12	3:D:110:THR:O	2.09	0.53
1:A:36:LEU:O	1:A:38:GLN:HG3	2.09	0.53
1:A:165:GLN:HA	1:A:165:GLN:HE21	1.73	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:95:ASN:ND2	3:F:56:SER:OG	2.42	0.52
1:A:77:SER:HB2	6:A:304:HOH:O	2.08	0.52
2:C:151:ASP:CA	2:C:191:VAL:HG21	2.14	0.52
2:C:89:GLN:HE21	2:C:96:TYR:HB3	1.74	0.52
2:E:141:PRO:HB2	2:E:143:GLU:OE1	2.10	0.52
3:D:184:VAL:CB	3:D:185:PRO:HD3	2.33	0.52
2:C:125:LEU:O	2:C:183:LYS:CD	2.48	0.52
2:E:124:GLN:HE22	2:E:131:SER:HB2	1.74	0.51
1:B:105:LEU:HD13	1:B:242:THR:HG23	1.91	0.51
3:F:136:ALA:HB2	3:F:189:LEU:HD11	1.91	0.51
2:C:175:LEU:HD11	6:C:439:HOH:O	2.10	0.51
3:D:159:LEU:CD1	3:D:182:VAL:HG11	2.40	0.51
2:C:143:GLU:OE1	2:C:143:GLU:N	2.30	0.51
3:D:51:ILE:HD11	3:D:54:GLY:HA2	1.92	0.51
2:E:151:ASP:OD2	2:E:189:HIS:CG	2.62	0.51
1:A:185:LEU:N	4:A:2:EDO:C2	2.71	0.51
1:B:70:LEU:HD11	1:B:76:ARG:HG2	1.93	0.51
3:D:68:THR:HG21	3:F:173:SER:HA	1.92	0.51
1:B:234:PHE:CD1	4:B:1:EDO:H11	2.46	0.51
3:D:6:GLN:H	3:D:105:GLN:HE22	1.58	0.51
2:E:190:LYS:HA	2:E:211:ARG:HD2	1.91	0.51
2:E:1:ASP:N	6:E:331:HOH:O	2.44	0.51
1:B:28:PRO:HD2	1:B:29:TRP:CE3	2.46	0.51
2:E:94:LEU:HA	2:E:95:PRO:C	2.30	0.51
2:C:5:THR:HG22	6:C:341:HOH:O	2.12	0.50
3:F:182:VAL:CG2	3:F:183:THR:N	2.74	0.50
3:F:193:THR:CG2	3:F:210:LYS:CD	2.75	0.50
3:F:201:LYS:N	3:F:202:PRO:CD	2.74	0.50
3:D:6:GLN:NE2	3:D:104:GLY:HA3	2.19	0.50
3:D:143:LYS:HE3	3:D:171:GLN:NE2	2.23	0.50
3:D:100(I):SER:HB2	4:D:243:EDO:H11	1.93	0.49
2:E:188:LYS:N	2:E:211:ARG:HH11	2.08	0.49
3:F:122:PHE:O	3:F:141:LEU:N	2.33	0.49
2:C:140:TYR:CG	2:C:141:PRO:HA	2.48	0.49
2:C:146:VAL:HG11	2:C:194:CYS:SG	2.52	0.49
2:E:151:ASP:HB2	2:E:189:HIS:NE2	2.27	0.49
3:D:61:ASP:O	3:D:63:VAL:N	2.46	0.49
2:E:55:GLN:HE21	2:E:56:SER:N	2.10	0.49
3:F:38:ARG:HD3	3:F:90:TYR:CE2	2.47	0.49
3:F:182:VAL:HG22	3:F:183:THR:N	2.28	0.49
1:A:86:LYS:HB2	1:A:109:GLU:HG2	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:111:ALA:HA	4:C:217:EDO:H12	1.93	0.49
2:E:108:ARG:CG	2:E:109:THR:N	2.69	0.49
3:F:178:LEU:HD12	3:F:179:SER:N	2.27	0.49
4:B:4:EDO:H22	6:B:508:HOH:O	2.13	0.49
2:E:198:HIS:CD2	2:E:200:GLY:H	2.26	0.49
1:B:185:LEU:N	4:B:4:EDO:H11	2.28	0.48
2:C:143:GLU:CD	2:C:143:GLU:H	2.12	0.48
2:E:115:VAL:HG22	2:E:136:LEU:HD22	1.95	0.48
1:B:239:LYS:HE2	1:B:244:VAL:C	2.34	0.48
1:A:38:GLN:NE2	6:A:353:HOH:O	2.45	0.48
3:D:100(C):ARG:NH1	3:D:100(C):ARG:HB2	2.29	0.48
2:E:151:ASP:CG	2:E:189:HIS:HD2	2.11	0.48
3:D:61:ASP:C	3:D:63:VAL:H	2.17	0.48
3:F:156:SER:H	3:F:197:ASN:ND2	2.12	0.48
2:E:94:LEU:CD2	2:E:96:TYR:CZ	2.97	0.48
3:F:192:GLN:HG2	3:F:194:TYR:CZ	2.48	0.48
1:B:29:TRP:CH2	4:B:7:EDO:H21	2.46	0.48
3:D:165:THR:HG23	3:D:180:SER:HB2	1.95	0.48
2:E:116:PHE:CZ	3:F:137:ALA:HB2	2.45	0.47
2:C:163:VAL:HG22	2:C:175:LEU:HD12	1.96	0.47
2:E:105:GLU:HG2	2:E:106:ILE:N	2.28	0.47
2:E:124:GLN:HE22	2:E:131:SER:CB	2.27	0.47
2:C:175:LEU:HD23	2:C:176:SER:N	2.29	0.47
1:B:230:ARG:HH11	4:B:6:EDO:H12	1.79	0.47
3:D:6:GLN:NE2	3:D:106:GLY:H	2.12	0.47
1:B:185:LEU:H	4:B:4:EDO:H11	1.80	0.47
2:E:55:GLN:HE21	2:E:55:GLN:HA	1.79	0.47
1:A:213:VAL:HG22	1:A:228:TYR:HE2	1.79	0.47
2:C:69:THR:OG1	6:C:369:HOH:O	2.18	0.47
1:A:165:GLN:CA	1:A:165:GLN:HE21	2.27	0.47
3:D:138:LEU:HD12	3:D:138:LEU:C	2.34	0.47
2:E:150:VAL:H	2:E:155:GLN:HE21	1.61	0.47
3:F:96:TYR:HA	6:F:311:HOH:O	2.13	0.47
3:D:182:VAL:CG2	3:D:183:THR:N	2.78	0.47
2:C:175:LEU:CD1	6:C:439:HOH:O	2.62	0.46
2:E:125:LEU:HD21	2:E:186:TYR:CD2	2.50	0.46
3:F:195:ILE:HA	3:F:210:LYS:HA	1.97	0.46
2:E:149:LYS:HG3	2:E:154:LEU:HD23	1.97	0.46
3:F:33:ALA:N	3:F:100(F):GLN:HE22	2.04	0.46
1:A:128:HIS:CE1	6:A:269:HOH:O	2.58	0.46
2:E:49:TYR:CZ	2:E:53:SER:HB3	2.51	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:60(C):ARG:HG2	3:D:28:THR:HG23	1.97	0.46
3:D:139:GLY:O	3:D:154:TRP:HH2	1.98	0.46
1:A:184(A):PHE:HB3	4:A:2:EDO:H21	1.98	0.46
3:D:159:LEU:HD13	3:D:182:VAL:HG11	1.96	0.46
3:D:139:GLY:O	3:D:154:TRP:CH2	2.69	0.46
3:D:22:CYS:HB3	3:D:78:LEU:HB3	1.98	0.46
2:C:159:SER:HA	2:C:178:THR:O	2.16	0.46
3:D:207:VAL:HG12	3:D:208:ASP:H	1.80	0.46
2:C:192:TYR:O	2:C:208:SER:HB2	2.16	0.45
2:C:89:GLN:HG3	2:C:98:PHE:CE1	2.52	0.45
3:F:150:VAL:HG13	3:F:150:VAL:O	2.16	0.45
3:F:160:THR:CG2	6:F:364:HOH:O	2.63	0.45
3:D:64:LYS:CD	3:D:65:GLY:N	2.79	0.45
2:E:161:GLU:HA	2:E:176:SER:O	2.16	0.45
1:B:234:PHE:CD1	4:B:1:EDO:C1	3.00	0.45
3:F:12:VAL:HG21	3:F:82(C):LEU:HD13	1.98	0.45
2:C:66:GLY:N	4:C:216:EDO:H11	2.31	0.45
2:C:95:PRO:HG2	2:C:95:PRO:O	2.17	0.45
1:B:236:ASP:O	1:B:240:GLU:HB2	2.17	0.45
2:C:146:VAL:CG2	2:C:196:VAL:HG13	2.46	0.45
3:D:150:VAL:CG1	3:D:178:LEU:HD21	2.46	0.45
1:A:50:ASN:HD21	1:A:111:PRO:HG3	1.82	0.45
1:B:60(C):ARG:HG2	3:D:28:THR:CG2	2.46	0.45
1:A:84:ARG:NH1	1:A:84:ARG:CG	2.74	0.45
3:D:207:VAL:HG12	3:D:208:ASP:N	2.32	0.45
2:C:27:GLN:NE2	6:C:411:HOH:O	2.42	0.44
1:B:207:ILE:HD11	4:B:7:EDO:H22	1.96	0.44
3:F:100(C):ARG:NH2	6:F:352:HOH:O	2.50	0.44
3:F:185:PRO:O	3:F:188:SER:CB	2.65	0.44
3:F:156:SER:H	3:F:197:ASN:HD21	1.64	0.44
2:C:146:VAL:HG22	2:C:196:VAL:CG2	2.44	0.44
3:D:100(H):VAL:HG13	3:D:100(H):VAL:O	2.18	0.44
3:D:12:VAL:HG23	3:D:111:VAL:HG22	1.99	0.44
2:C:110:VAL:HG21	2:C:199:GLN:NE2	2.33	0.44
2:C:117:ILE:HG22	2:C:207:LYS:HD3	1.99	0.44
3:D:153:SER:OG	3:D:197:ASN:HB2	2.18	0.44
3:D:39:GLN:HG3	3:D:44:GLY:O	2.18	0.44
3:F:123:PRO:HA	3:F:140:CYS:HA	1.99	0.44
3:D:18:LEU:HB3	3:D:82:MET:CE	2.47	0.44
2:E:175:LEU:HD23	2:E:176:SER:N	2.33	0.44
1:A:171:LEU:HD22	1:A:223:ASN:HB3	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:27:TRP:C	4:B:3:EDO:H21	2.37	0.44
1:A:128:HIS:CD2	6:A:284:HOH:O	2.47	0.44
1:B:204(A):ASP:OD2	1:B:206:ARG:CZ	2.65	0.43
3:D:150:VAL:HG13	3:D:178:LEU:HD21	2.00	0.43
2:E:137:ASN:O	2:E:138:ASN:C	2.55	0.43
1:B:117:MET:CE	6:B:357:HOH:O	2.65	0.43
1:B:203:GLU:HA	1:B:203:GLU:OE1	2.18	0.43
2:C:112:ALA:CB	4:C:217:EDO:H22	2.48	0.43
2:C:195:GLU:CB	2:C:206:THR:HB	2.48	0.43
3:D:184:VAL:H	3:D:185:PRO:CD	2.31	0.43
2:E:151:ASP:CB	2:E:189:HIS:HD2	2.31	0.43
2:E:23:CYS:HB2	2:E:35:TRP:CH2	2.54	0.43
3:F:5:VAL:O	3:F:5:VAL:HG12	2.16	0.43
2:C:118:PHE:HE1	3:D:138:LEU:HA	1.83	0.43
3:F:11:LEU:HD12	3:F:110:THR:O	2.19	0.43
2:E:94:LEU:HD22	2:E:96:TYR:CE1	2.53	0.43
2:E:201:LEU:HA	2:E:201:LEU:HD12	1.60	0.43
3:D:148:GLU:HB3	3:D:149:PRO:HA	2.01	0.43
2:E:89:GLN:HG3	2:E:98:PHE:CE1	2.54	0.43
1:A:60(C):ARG:NH2	6:A:343:HOH:O	2.52	0.43
2:E:118:PHE:HB2	2:E:133:VAL:HB	2.01	0.43
3:F:146:PHE:HA	3:F:147:PRO:HA	1.77	0.43
2:C:158:ASN:N	2:C:158:ASN:OD1	2.51	0.43
2:E:140:TYR:CD1	2:E:141:PRO:HA	2.54	0.43
3:F:82:MET:HB3	3:F:82(C):LEU:HD21	2.00	0.42
1:B:96:ASP:OD2	3:D:53:SER:OG	2.33	0.42
1:A:204(A):ASP:OD2	1:A:206:ARG:NE	2.40	0.42
1:B:207:ILE:HD13	4:B:7:EDO:H22	1.96	0.42
3:F:122:PHE:N	3:F:122:PHE:CD1	2.85	0.42
1:A:235:ARG:HD2	1:A:235:ARG:HA	1.88	0.42
3:D:138:LEU:HD12	3:D:139:GLY:N	2.35	0.42
2:C:142:ARG:HD2	6:C:409:HOH:O	2.19	0.42
2:E:35:TRP:CE2	2:E:73:LEU:HB2	2.54	0.42
2:C:58:VAL:HA	2:C:59:PRO:HD3	1.89	0.42
3:D:117:LYS:HD3	3:D:175:LEU:HD21	1.96	0.42
2:E:124:GLN:HG2	2:E:129:THR:O	2.19	0.42
1:B:114:TYR:HA	1:B:118:VAL:O	2.19	0.42
2:C:195:GLU:HB2	2:C:206:THR:HB	2.02	0.42
3:D:201:LYS:N	3:D:202:PRO:HD3	2.35	0.42
2:C:4:MET:HE2	2:C:23:CYS:SG	2.60	0.42
2:C:78:LEU:HD21	2:C:106:ILE:CD1	2.50	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:6:GLN:N	3:D:105:GLN:HE22	2.18	0.41
2:E:118:PHE:CE1	3:F:124:LEU:HB3	2.52	0.41
3:F:185:PRO:O	3:F:188:SER:OG	2.38	0.41
3:D:211:VAL:HG23	3:D:211:VAL:O	2.20	0.41
2:C:78:LEU:HD21	2:C:106:ILE:HD12	2.01	0.41
3:D:12:VAL:HG21	3:D:82(C):LEU:CD1	2.50	0.41
2:E:58:VAL:HA	2:E:59:PRO:HD3	1.90	0.41
1:B:97:PHE:HB2	3:D:52:SER:HB3	2.02	0.41
3:D:182:VAL:HG22	3:D:183:THR:H	1.86	0.41
1:A:177:THR:HB	1:A:178:PRO:HD2	2.02	0.41
1:A:95:ASN:OD1	1:A:98:THR:N	2.45	0.41
2:C:94:LEU:HD23	2:C:96:TYR:CZ	2.54	0.41
2:E:194:CYS:O	2:E:206:THR:HA	2.21	0.41
1:A:171:LEU:C	1:A:173:PRO:HD3	2.40	0.41
3:D:11:LEU:HA	3:D:110:THR:O	2.20	0.41
3:D:154:TRP:HB2	3:D:159:LEU:HB2	2.03	0.41
1:A:231:LEU:HA	1:A:231:LEU:HD23	1.92	0.41
2:C:114:SER:HB2	2:C:137:ASN:HB3	2.03	0.41
2:C:194:CYS:O	2:C:206:THR:HA	2.20	0.41
3:D:123:PRO:HA	3:D:140:CYS:CB	2.50	0.41
3:D:182:VAL:CG2	3:D:183:THR:H	2.33	0.41
6:A:260:HOH:O	3:F:99:TYR:HB2	2.20	0.41
1:A:234:PHE:O	1:A:238:ILE:HG13	2.20	0.41
3:F:173:SER:N	6:F:385:HOH:O	2.53	0.41
1:A:165:GLN:NE2	1:A:230:ARG:NH2	2.68	0.41
2:E:14:SER:O	2:E:17:ASP:HB2	2.21	0.41
3:F:64:LYS:HE2	3:F:64:LYS:HB3	1.86	0.41
2:C:58:VAL:HG13	2:C:59:PRO:HD2	2.02	0.41
3:D:1:GLN:HG2	3:D:2:VAL:N	2.36	0.41
1:A:110:LYS:HB2	1:A:110:LYS:HE3	1.68	0.41
2:C:71:PHE:HA	4:C:216:EDO:O2	2.20	0.41
3:F:186:SER:C	3:F:188:SER:N	2.75	0.41
1:A:61:PRO:HG3	1:A:88:ILE:HG13	2.03	0.40
2:C:146:VAL:HG22	2:C:196:VAL:CB	2.51	0.40
3:D:12:VAL:HG21	3:D:82(C):LEU:HD13	2.03	0.40
3:D:183:THR:CA	3:D:184:VAL:CG2	2.70	0.40
3:D:18:LEU:HA	3:D:18:LEU:HD12	1.89	0.40
3:F:185:PRO:CB	3:F:188:SER:OG	2.68	0.40
1:A:114:TYR:HA	1:A:118:VAL:O	2.21	0.40
1:B:52:LEU:HD11	1:B:108:LEU:HD21	2.03	0.40
3:F:123:PRO:HG3	3:F:209:LYS:HE2	0.51	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:150:VAL:CG2	2:C:155:GLN:NE2	2.84	0.40
2:E:116:PHE:N	2:E:116:PHE:HD2	2.20	0.40
2:E:55:GLN:CA	2:E:55:GLN:HE21	2.33	0.40
3:D:213:PRO:CD	6:D:319:HOH:O	2.69	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	243/241 (101%)	235 (97%)	8 (3%)	0	100	100
1	B	242/241 (100%)	237 (98%)	5 (2%)	0	100	100
2	C	208/214 (97%)	198 (95%)	9 (4%)	1 (0%)	32	32
2	E	210/214 (98%)	203 (97%)	5 (2%)	2 (1%)	18	14
3	D	206/257 (80%)	190 (92%)	14 (7%)	2 (1%)	18	14
3	F	221/257 (86%)	210 (95%)	10 (4%)	1 (0%)	32	32
All	All	1330/1424 (93%)	1273 (96%)	51 (4%)	6 (0%)	32	32

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	D	184	VAL
3	D	62	SER
2	E	138	ASN
2	C	127	SER
3	F	123	PRO
2	E	29	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	201/197 (102%)	192 (96%)	9 (4%)	32	36
1	B	200/197 (102%)	192 (96%)	8 (4%)	36	42
2	C	181/186 (97%)	169 (93%)	12 (7%)	19	19
2	E	182/186 (98%)	165 (91%)	17 (9%)	10	9
3	D	174/210 (83%)	166 (95%)	8 (5%)	31	36
3	F	185/210 (88%)	170 (92%)	15 (8%)	14	12
All	All	1123/1186 (95%)	1054 (94%)	69 (6%)	22	22

All (69) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	48	SER
1	B	60(C)	ARG
1	B	60(F)	ARG
1	B	86	LYS
1	B	110	LYS
1	B	179	ARG
1	B	195	SER
1	B	239	LYS
2	C	7	SER
2	C	12	SER
2	C	24	ARG
2	C	30	SER
2	C	56	SER
2	C	67	SER
2	C	94	LEU
2	C	145	LYS
2	C	170	ASP
2	C	188	LYS
2	C	205	VAL
2	C	206	THR
3	D	21	SER
3	D	63	VAL

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Mol	Chain	Res	Type
3	D	64	LYS
3	D	100(B)	ARG
3	D	100(C)	ARG
3	D	100(H)	VAL
3	D	183	THR
3	D	197	ASN
1	A	33	LEU
1	A	36	LEU
1	A	60(C)	ARG
1	A	60(F)	ARG
1	A	119[A]	ARG
1	A	119[B]	ARG
1	A	165	GLN
1	A	191	CYS
1	A	207	ILE
2	E	22	THR
2	E	24	ARG
2	E	30	SER
2	E	33	LEU
2	E	48	ILE
2	E	55	GLN
2	E	56	SER
2	E	93	ASN
2	E	108	ARG
2	E	110	VAL
2	E	116	PHE
2	E	138	ASN
2	E	170	ASP
2	E	176	SER
2	E	185	ASP
2	E	201	LEU
2	E	207	LYS
3	F	1	GLN
3	F	63	VAL
3	F	71	ARG
3	F	100(C)	ARG
3	F	100(H)	VAL
3	F	113	SER
3	F	122	PHE
3	F	138	LEU
3	F	143	LYS
3	F	161	SER

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Mol	Chain	Res	Type
3	F	170	LEU
3	F	186	SER
3	F	187	SER
3	F	188	SER
3	F	201	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (23) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	128	HIS
1	B	192	GLN
2	C	55	GLN
2	C	93	ASN
2	C	198	HIS
2	C	199	GLN
3	D	6	GLN
3	D	76	ASN
3	D	171	GLN
1	A	38	GLN
1	A	50	ASN
1	A	128	HIS
1	A	165	GLN
2	E	55	GLN
2	E	124	GLN
2	E	189	HIS
2	E	198	HIS
3	F	1	GLN
3	F	81	GLN
3	F	100(F)	GLN
3	F	171	GLN
3	F	197	ASN
3	F	199	ASN

### 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 [i](#)

There are no carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

15 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	$\# Z  > 2$
4	EDO	A	12	-	3,3,3	0.30	0	2,2,2	0.53	0
4	EDO	A	13	-	3,3,3	0.44	0	2,2,2	0.36	0
4	EDO	A	2	-	3,3,3	0.38	0	2,2,2	0.99	0
4	EDO	B	1	-	3,3,3	0.48	0	2,2,2	0.12	0
4	EDO	B	3	-	3,3,3	0.59	0	2,2,2	0.59	0
4	EDO	B	4	-	3,3,3	0.32	0	2,2,2	0.46	0
4	EDO	B	6	-	3,3,3	0.41	0	2,2,2	0.56	0
4	EDO	B	7	-	3,3,3	0.29	0	2,2,2	0.30	0
4	EDO	B	8	-	3,3,3	0.32	0	2,2,2	0.15	0
5	SO4	C	215	-	4,4,4	0.15	0	6,6,6	0.09	0
4	EDO	C	216	-	3,3,3	0.49	0	2,2,2	0.22	0
4	EDO	C	217	-	3,3,3	0.40	0	2,2,2	0.43	0
4	EDO	D	243	-	3,3,3	0.19	0	2,2,2	1.04	0
5	SO4	E	215	-	4,4,4	0.16	0	6,6,6	0.14	0
4	EDO	E	216	-	3,3,3	0.19	0	2,2,2	1.16	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	EDO	A	12	-	-	0/1/1/1	0/0/0/0
4	EDO	A	13	-	-	0/1/1/1	0/0/0/0
4	EDO	A	2	-	-	0/1/1/1	0/0/0/0
4	EDO	B	1	-	-	0/1/1/1	0/0/0/0
4	EDO	B	3	-	-	0/1/1/1	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	EDO	B	4	-	-	0/1/1/1	0/0/0/0
4	EDO	B	6	-	-	0/1/1/1	0/0/0/0
4	EDO	B	7	-	-	0/1/1/1	0/0/0/0
4	EDO	B	8	-	-	0/1/1/1	0/0/0/0
5	SO4	C	215	-	-	0/0/0/0	0/0/0/0
4	EDO	C	216	-	-	0/1/1/1	0/0/0/0
4	EDO	C	217	-	-	0/1/1/1	0/0/0/0
4	EDO	D	243	-	-	0/1/1/1	0/0/0/0
5	SO4	E	215	-	-	0/0/0/0	0/0/0/0
4	EDO	E	216	-	-	0/1/1/1	0/0/0/0

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

12 monomers are involved in 42 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	12	EDO	1	0
4	A	13	EDO	4	0
4	A	2	EDO	5	0
4	B	1	EDO	3	0
4	B	3	EDO	3	0
4	B	4	EDO	3	0
4	B	6	EDO	6	0
4	B	7	EDO	5	0
4	B	8	EDO	1	0
4	C	216	EDO	6	0
4	C	217	EDO	2	0
4	D	243	EDO	3	0

## 5.7 Other polymers

There are no such residues in this entry.

## 5.8 Polymer linkage issues

The following chains have linkage breaks:

Mol	Chain	Number of breaks
3	D	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	D	43:LYS	C	44:GLY	N	1.20

## 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	241/241 (100%)	-0.16	0	100	100	19, 30, 47, 74	1 (0%)
1	B	241/241 (100%)	-0.23	0	100	100	17, 26, 44, 63	1 (0%)
2	C	210/214 (98%)	0.89	40 (19%)	1	1	16, 37, 122, 138	0
2	E	211/214 (98%)	0.42	25 (11%)	5	5	20, 37, 90, 110	0
3	D	211/257 (82%)	0.46	19 (9%)	10	10	17, 42, 95, 111	0
3	F	224/257 (87%)	0.32	17 (7%)	15	15	19, 44, 83, 108	0
All	All	1338/1424 (93%)	0.26	101 (7%)	15	15	16, 34, 95, 138	2 (0%)

All (101) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	F	189	LEU	14.5
3	D	195	ILE	8.6
2	C	180	THR	7.9
2	C	192	TYR	7.9
2	C	153	ALA	7.8
2	C	184	ALA	7.0
2	C	209	PHE	6.9
2	C	191	VAL	6.4
3	D	211	VAL	6.2
2	E	154	LEU	6.1
3	D	158	ALA	5.9
2	C	154	LEU	5.7
3	D	125	ALA	5.6
3	D	138	LEU	5.3
2	C	132	VAL	5.3
2	C	125	LEU	5.1
2	C	193	ALA	4.8
3	D	124	LEU	4.8
2	C	149	LYS	4.8

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Mol	Chain	Res	Type	RSRZ
2	C	150	VAL	4.7
2	C	122	ASP	4.6
3	D	157	GLY	4.6
3	D	214	LYS	4.4
2	C	119	PRO	4.4
2	C	117	ILE	4.4
2	C	146	VAL	4.4
2	E	125	LEU	4.3
3	F	193	THR	4.3
2	C	118	PHE	4.2
2	E	193	ALA	4.0
3	D	210	LYS	3.9
2	C	210	ASN	3.9
2	E	153	ALA	3.9
3	F	209	LYS	3.8
2	E	185	ASP	3.7
2	C	121	SER	3.7
2	C	179	LEU	3.7
2	C	205	VAL	3.6
2	C	159	SER	3.5
2	C	196	VAL	3.5
2	C	187	GLU	3.4
2	C	181	LEU	3.4
3	F	191	THR	3.3
2	C	134	CYS	3.3
3	D	193	THR	3.3
3	F	195	ILE	3.2
3	D	156	SER	3.2
2	E	119	PRO	3.2
2	E	191	VAL	3.2
2	C	151	ASP	3.2
2	E	192	TYR	3.2
2	E	148	TRP	3.1
2	C	194	CYS	3.1
2	E	122	ASP	3.1
2	C	128	GLY	3.0
2	C	208	SER	3.0
2	C	186	TYR	2.9
2	C	131	SER	2.8
3	D	194	TYR	2.8
3	F	136	ALA	2.8
2	E	130	ALA	2.8

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Mol	Chain	Res	Type	RSRZ
3	F	207	VAL	2.8
2	E	151	ASP	2.8
2	E	121	SER	2.8
2	E	118	PHE	2.7
3	D	184	VAL	2.7
3	F	210	LYS	2.7
2	E	150	VAL	2.6
3	F	212	GLU	2.6
3	D	199	ASN	2.6
2	E	202	SER	2.5
2	E	186	TYR	2.5
2	C	155	GLN	2.5
2	C	133	VAL	2.5
2	E	209	PHE	2.5
3	F	198	VAL	2.5
2	C	148	TRP	2.5
2	E	126	LYS	2.5
2	E	152	ASN	2.4
2	E	159	SER	2.4
3	F	185	PRO	2.4
2	C	197	THR	2.4
3	D	122	PHE	2.4
2	E	115	VAL	2.4
3	F	132	SER	2.4
3	F	188	SER	2.3
2	C	129	THR	2.3
3	F	194	TYR	2.3
2	E	146	VAL	2.3
2	E	117	ILE	2.3
2	C	152	ASN	2.3
3	F	135	THR	2.2
2	E	189	HIS	2.2
2	C	126	LYS	2.2
3	D	185	PRO	2.1
2	C	185	ASP	2.1
3	D	212	GLU	2.1
3	D	182	VAL	2.0
3	F	133	GLY	2.0
3	F	213	PRO	2.0
3	D	208	ASP	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
4	EDO	A	13	4/4	0.93	0.24	22.22	33,39,45,54	0
4	EDO	B	1	4/4	0.94	0.27	18.99	55,60,61,63	0
4	EDO	B	7	4/4	0.79	0.21	9.60	47,53,61,63	0
4	EDO	D	243	4/4	0.89	0.29	9.06	58,61,64,64	0
4	EDO	E	216	4/4	0.93	0.15	2.30	48,51,51,55	0
4	EDO	B	3	4/4	0.88	0.18	1.90	21,38,41,47	0
4	EDO	B	6	4/4	0.92	0.11	0.79	23,27,31,32	0
4	EDO	C	217	4/4	0.94	0.13	-0.05	42,43,44,48	0
4	EDO	A	12	4/4	0.80	0.13	-	59,60,61,65	0
4	EDO	B	8	4/4	0.92	0.12	-	42,42,53,61	0
5	SO4	E	215	5/5	0.97	0.11	-	51,57,63,65	0
4	EDO	A	2	4/4	0.94	0.18	-	40,42,42,54	0
5	SO4	C	215	5/5	0.97	0.14	-	60,64,70,77	0
4	EDO	B	4	4/4	0.92	0.15	-	40,45,48,52	0
4	EDO	C	216	4/4	0.77	0.33	-	44,46,53,53	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.