



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 13, 2017 – 10:08 pm GMT

PDB ID : 2CBQ  
Title : CRYSTAL STRUCTURE OF THE NEOCARZINOSTATIN 1TES15 MUTANT BOUND TO TESTOSTERONE HEMISUCCINATE.  
Authors : Drevelle, A.; Graille, M.; Heyd, B.; Sorel, I.; Ulryck, N.; Pecorari, F.; Desmadril, M.; Van Tilbeurgh, H.; Minard, P.  
Deposited on : 2006-01-06  
Resolution : 2.60 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

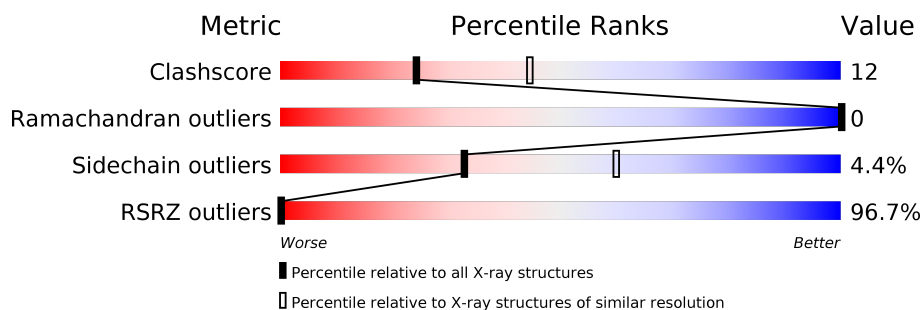
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.60 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))
Clashscore	112137	2895 (2.60-2.60)
Ramachandran outliers	110173	2848 (2.60-2.60)
Sidechain outliers	110143	2848 (2.60-2.60)
RSRZ outliers	101464	2550 (2.60-2.60)

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	114	<div> <div>96%</div> <div> <div></div> <div>75%</div> <div>20%</div> <div>..</div> </div> </div>
1	B	114	<div> <div>95%</div> <div> <div></div> <div>75%</div> <div>22%</div> <div>...</div> </div> </div>
1	C	114	<div> <div>95%</div> <div> <div></div> <div>75%</div> <div>21%</div> <div>..</div> </div> </div>
1	D	114	<div> <div>94%</div> <div> <div></div> <div>74%</div> <div>24%</div> <div>..</div> </div> </div>
1	E	114	<div> <div>96%</div> <div> <div></div> <div>75%</div> <div>20%</div> <div>...</div> </div> </div>
1	F	114	<div> <div>94%</div> <div> <div></div> <div>75%</div> <div>18%</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
2	SO4	C	1114	-	-	-	X
3	TH2	A	1114	-	-	-	X
3	TH2	A	1115	-	-	-	X
3	TH2	B	1116	-	-	-	X
3	TH2	B	1117	-	-	-	X
3	TH2	C	1115	-	-	-	X
3	TH2	D	1114	-	-	-	X
3	TH2	E	1115	-	-	-	X
3	TH2	F	1114	-	-	-	X

## 2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 5016 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 NEOCARZINOSTATIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	111	Total	C	N	O	S	0	0	0
			773	475	134	162	2			
1	B	113	Total	C	N	O	S	0	0	0
			791	485	139	165	2			
1	C	112	Total	C	N	O	S	0	0	0
			781	479	136	164	2			
1	D	112	Total	C	N	O	S	0	0	0
			781	479	136	164	2			
1	E	112	Total	C	N	O	S	0	0	0
			781	479	136	164	2			
1	F	111	Total	C	N	O	S	0	0	0
			773	475	134	162	2			

There are 42 discrepancies between the modelled and reference sequences:

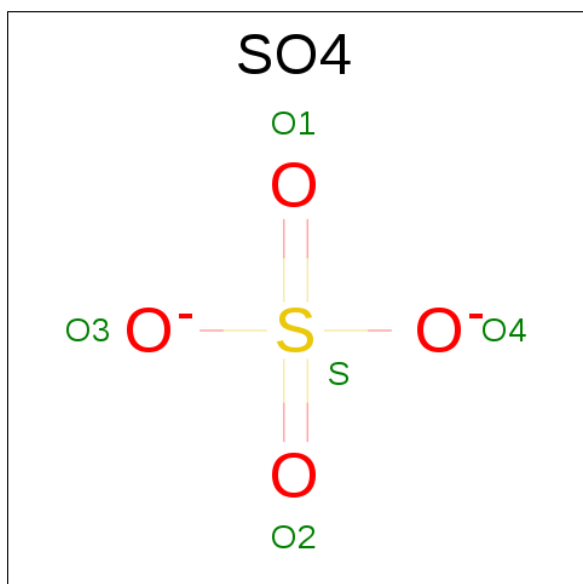
Chain	Residue	Modelled	Actual	Comment	Reference
A	33	TRP	ASP	ENGINEERED MUTATION	UNP P0A3R9
A	35	TYR	GLY	ENGINEERED MUTATION	UNP P0A3R9
A	37	ARG	CYS	ENGINEERED MUTATION	UNP P0A3R9
A	39	ALA	TRP	ENGINEERED MUTATION	UNP P0A3R9
A	45	HIS	LEU	ENGINEERED MUTATION	UNP P0A3R9
A	47	SER	CYS	ENGINEERED MUTATION	UNP P0A3R9
A	52	LEU	PHE	ENGINEERED MUTATION	UNP P0A3R9
B	33	TRP	ASP	ENGINEERED MUTATION	UNP P0A3R9
B	35	TYR	GLY	ENGINEERED MUTATION	UNP P0A3R9
B	37	ARG	CYS	ENGINEERED MUTATION	UNP P0A3R9
B	39	ALA	TRP	ENGINEERED MUTATION	UNP P0A3R9
B	45	HIS	LEU	ENGINEERED MUTATION	UNP P0A3R9
B	47	SER	CYS	ENGINEERED MUTATION	UNP P0A3R9
B	52	LEU	PHE	ENGINEERED MUTATION	UNP P0A3R9
C	33	TRP	ASP	ENGINEERED MUTATION	UNP P0A3R9
C	35	TYR	GLY	ENGINEERED MUTATION	UNP P0A3R9
C	37	ARG	CYS	ENGINEERED MUTATION	UNP P0A3R9

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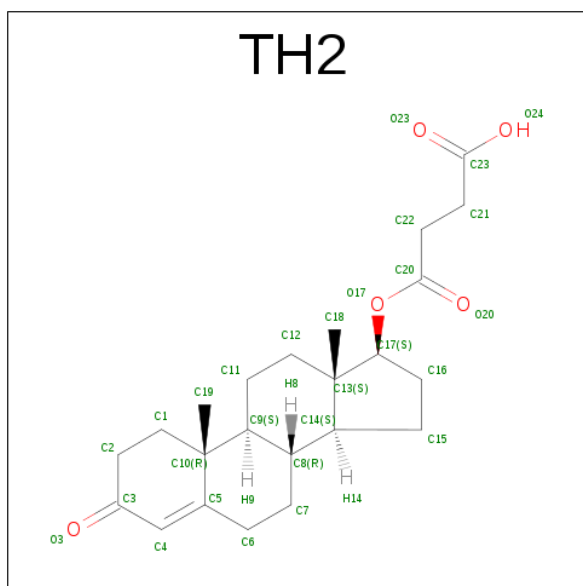
Chain	Residue	Modelled	Actual	Comment	Reference
C	39	ALA	TRP	ENGINEERED MUTATION	UNP P0A3R9
C	45	HIS	LEU	ENGINEERED MUTATION	UNP P0A3R9
C	47	SER	CYS	ENGINEERED MUTATION	UNP P0A3R9
C	52	LEU	PHE	ENGINEERED MUTATION	UNP P0A3R9
D	33	TRP	ASP	ENGINEERED MUTATION	UNP P0A3R9
D	35	TYR	GLY	ENGINEERED MUTATION	UNP P0A3R9
D	37	ARG	CYS	ENGINEERED MUTATION	UNP P0A3R9
D	39	ALA	TRP	ENGINEERED MUTATION	UNP P0A3R9
D	45	HIS	LEU	ENGINEERED MUTATION	UNP P0A3R9
D	47	SER	CYS	ENGINEERED MUTATION	UNP P0A3R9
D	52	LEU	PHE	ENGINEERED MUTATION	UNP P0A3R9
E	33	TRP	ASP	ENGINEERED MUTATION	UNP P0A3R9
E	35	TYR	GLY	ENGINEERED MUTATION	UNP P0A3R9
E	37	ARG	CYS	ENGINEERED MUTATION	UNP P0A3R9
E	39	ALA	TRP	ENGINEERED MUTATION	UNP P0A3R9
E	45	HIS	LEU	ENGINEERED MUTATION	UNP P0A3R9
E	47	SER	CYS	ENGINEERED MUTATION	UNP P0A3R9
E	52	LEU	PHE	ENGINEERED MUTATION	UNP P0A3R9
F	33	TRP	ASP	ENGINEERED MUTATION	UNP P0A3R9
F	35	TYR	GLY	ENGINEERED MUTATION	UNP P0A3R9
F	37	ARG	CYS	ENGINEERED MUTATION	UNP P0A3R9
F	39	ALA	TRP	ENGINEERED MUTATION	UNP P0A3R9
F	45	HIS	LEU	ENGINEERED MUTATION	UNP P0A3R9
F	47	SER	CYS	ENGINEERED MUTATION	UNP P0A3R9
F	52	LEU	PHE	ENGINEERED MUTATION	UNP P0A3R9

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



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

- Molecule 3 is TESTOSTERONE HEMISUCCINATE (three-letter code: TH2) (formula:  $C_{23}H_{32}O_5$ ).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total C O 28 23 5	0	0
3	A	1	Total C O 28 23 5	0	0
3	B	1	Total C O 28 23 5	0	0
3	B	1	Total C O 28 23 5	0	0
3	C	1	Total C O 28 23 5	0	0
3	D	1	Total C O 28 23 5	0	0

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	E	1	Total	C	O	0	0
			28	23	5		
3	F	1	Total	C	O	0	0
			28	23	5		

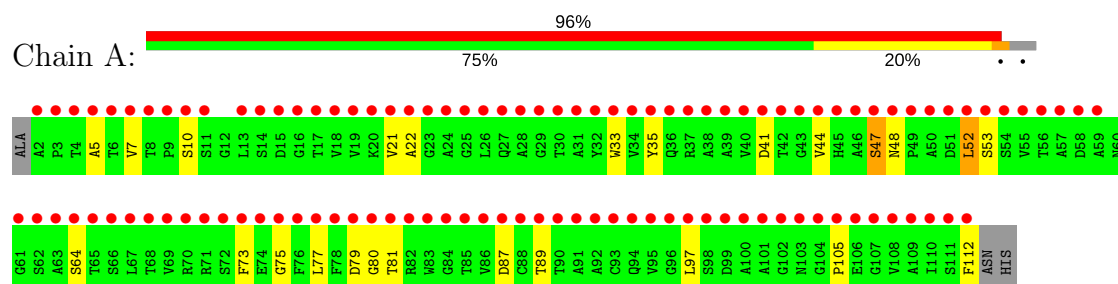
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	15	Total	O	0	0
			15	15		
4	B	17	Total	O	0	0
			17	17		
4	C	17	Total	O	0	0
			17	17		
4	D	17	Total	O	0	0
			17	17		
4	E	14	Total	O	0	0
			14	14		
4	F	7	Total	O	0	0
			7	7		

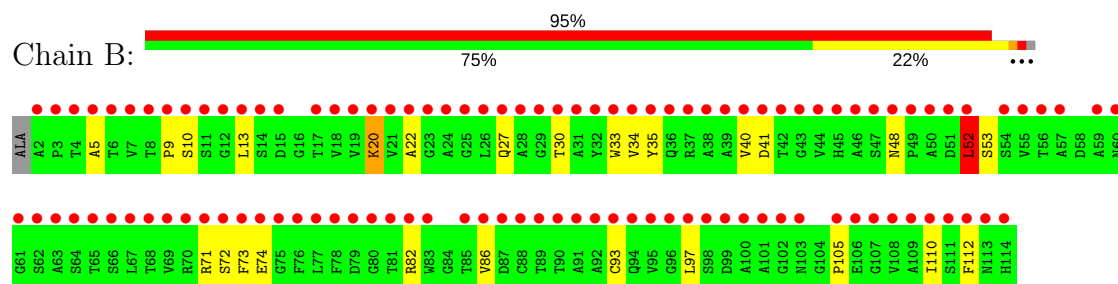
### 3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of 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 ( $\text{RSRZ} > 2$ ). 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.

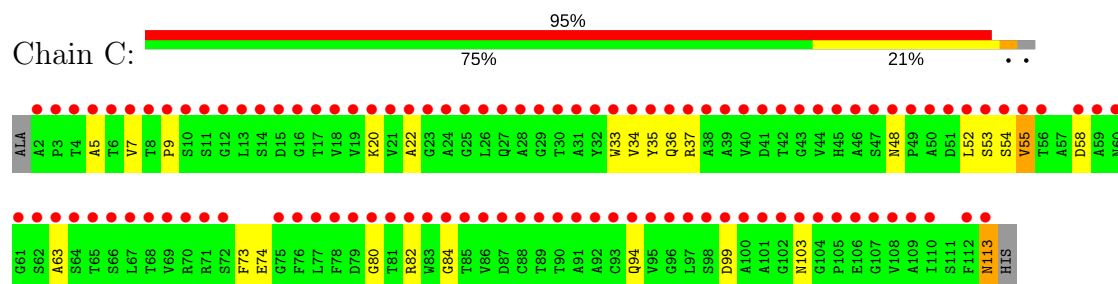
#### • Molecule 1: NEOCARZINOSTATIN



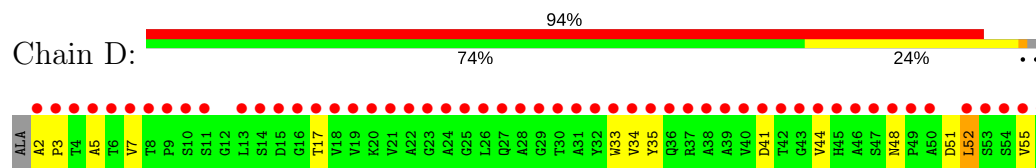
#### • Molecule 1: NEOCARZINOSTATIN



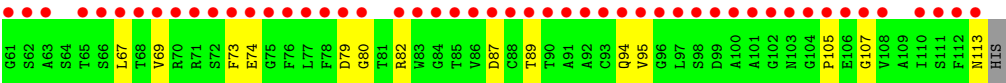
#### • Molecule 1: NEOCARZINOSTATIN



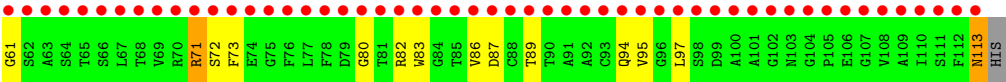
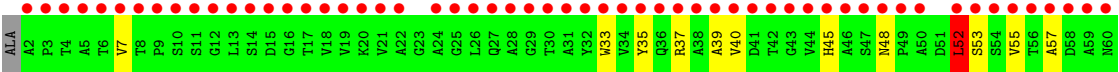
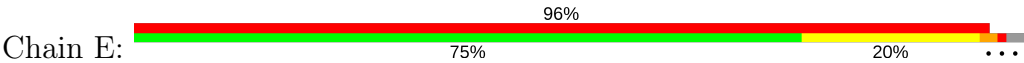
#### • Molecule 1: NEOCARZINOSTATIN



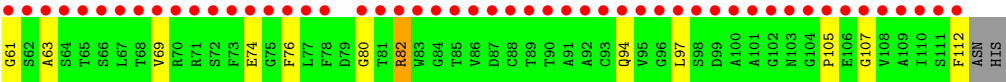
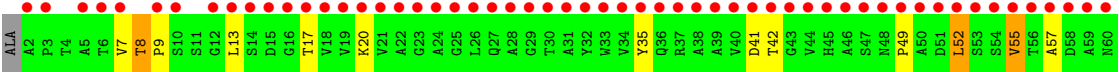
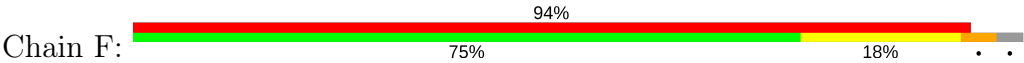




● Molecule 1: NEOCARZINOSTATIN



● Molecule 1: NEOCARZINOSTATIN



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	52.98Å 97.83Å 129.27Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	20.00 – 2.60 25.51 – 1.28	Depositor EDS
% Data completeness (in resolution range)	94.6 (20.00-2.60) 42.5 (25.51-1.28)	Depositor EDS
$R_{merge}$	0.11	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	0.74 (at 1.28Å)	Xtriage
Refinement program	CNS 1.0	Depositor
R, $R_{free}$	0.207 , 0.257 0.785 , (Not available)	Depositor DCC
$R_{free}$ test set	No test flags present.	DCC
Wilson B-factor (Å <sup>2</sup> )	24.4	Xtriage
Anisotropy	0.650	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.43 , 19.3	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.67$ , $\langle L^2 \rangle = 0.55$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.30	EDS
Total number of atoms	5016	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	28.0	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 73.30 % 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 1.8852e-06. 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, TH2

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z  > 5$	RMSZ	$\# Z  > 5$
1	A	0.35	0/787	0.64	0/1078
1	B	0.38	0/806	0.64	1/1104 (0.1%)
1	C	0.43	1/795 (0.1%)	0.68	1/1089 (0.1%)
1	D	0.42	1/795 (0.1%)	0.66	1/1089 (0.1%)
1	E	0.41	1/795 (0.1%)	0.67	2/1089 (0.2%)
1	F	0.36	0/787	0.63	0/1078
All	All	0.39	3/4765 (0.1%)	0.66	5/6527 (0.1%)

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	113	ASN	CG-OD1	5.51	1.36	1.24
1	D	113	ASN	CG-OD1	5.50	1.36	1.24
1	E	113	ASN	CG-OD1	5.47	1.35	1.24

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	113	ASN	OD1-CG-ND2	-6.88	106.08	121.90
1	D	113	ASN	OD1-CG-ND2	-6.88	106.08	121.90
1	C	113	ASN	OD1-CG-ND2	-6.87	106.11	121.90
1	E	52	LEU	CA-CB-CG	5.89	128.84	115.30
1	B	52	LEU	CA-CB-CG	5.47	127.87	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	773	0	731	21	0
1	B	791	0	744	24	0
1	C	781	0	737	23	0
1	D	781	0	737	16	0
1	E	781	0	737	22	0
1	F	773	0	731	19	0
2	A	5	0	0	0	0
2	B	5	0	0	0	0
2	C	5	0	0	0	0
2	E	5	0	0	0	0
2	F	5	0	0	0	0
3	A	56	0	62	3	0
3	B	56	0	62	1	0
3	C	28	0	31	0	0
3	D	28	0	31	0	0
3	E	28	0	31	0	0
3	F	28	0	31	0	0
4	A	15	0	0	0	0
4	B	17	0	0	1	0
4	C	17	0	0	2	0
4	D	17	0	0	0	0
4	E	14	0	0	0	0
4	F	7	0	0	0	0
All	All	5016	0	4665	119	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 12.

All (119) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:37:ARG:HE	1:C:94:GLN:HE21	1.17	0.92
1:D:35:TYR:HB3	1:D:52:LEU:HD23	1.53	0.90
3:A:1115:TH2:H6C2	1:F:20:LYS:HB2	1.53	0.88
3:B:1117:TH2:H6C2	1:C:20:LYS:HB2	1.64	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:37:ARG:NE	1:E:94:GLN:HE21	1.86	0.74
1:E:82:ARG:HG3	1:E:82:ARG:HH11	1.55	0.70
1:B:34:VAL:HG22	1:B:97:LEU:CD1	2.21	0.69
1:A:87:ASP:OD2	1:A:89:THR:HB	1.93	0.69
1:E:39:ALA:HA	1:E:45:HIS:HD2	1.58	0.69
1:A:52:LEU:HD22	1:A:53:SER:H	1.60	0.66
1:C:55:VAL:HG22	1:C:63:ALA:HB1	1.79	0.65
1:C:37:ARG:NE	1:C:94:GLN:HE21	1.92	0.64
1:B:34:VAL:HG22	1:B:97:LEU:HD12	1.79	0.64
1:E:37:ARG:CZ	1:E:94:GLN:HE21	2.12	0.63
1:F:82:ARG:HG2	1:F:82:ARG:NH1	2.14	0.63
1:C:34:VAL:HG23	1:C:54:SER:HA	1.80	0.62
1:E:39:ALA:HA	1:E:45:HIS:CD2	2.34	0.62
1:B:74:GLU:HG3	1:B:82:ARG:NH1	2.15	0.61
1:E:40:VAL:HB	1:E:83:TRP:CZ2	2.34	0.61
1:D:87:ASP:OD2	1:D:89:THR:HB	2.01	0.61
1:B:93:CYS:HB2	4:B:2014:HOH:O	2.00	0.61
1:C:35:TYR:HB3	1:C:52:LEU:HD23	1.84	0.60
1:F:82:ARG:HG2	1:F:82:ARG:HH11	1.69	0.58
1:C:99:ASP:OD2	1:C:103:ASN:HB2	2.04	0.57
1:A:48:ASN:HB2	1:A:73:PHE:CD1	2.39	0.57
1:E:82:ARG:HG3	1:E:82:ARG:NH1	2.20	0.56
1:B:10:SER:O	1:B:110:ILE:HA	2.05	0.56
1:E:52:LEU:HD13	1:E:53:SER:N	2.19	0.56
1:D:7:VAL:HG21	1:D:95:VAL:HB	1.87	0.55
1:C:74:GLU:OE1	1:C:82:ARG:NE	2.40	0.55
1:A:41:ASP:HB3	1:A:44:VAL:HB	1.89	0.54
1:B:34:VAL:HG22	1:B:97:LEU:HD11	1.88	0.54
1:A:52:LEU:HD13	1:A:53:SER:N	2.22	0.54
1:B:48:ASN:HB2	1:B:73:PHE:CD1	2.42	0.54
1:B:20:LYS:NZ	1:B:22:ALA:HB2	2.23	0.54
1:C:58:ASP:HB2	4:C:2010:HOH:O	2.08	0.54
1:C:48:ASN:HB2	1:C:73:PHE:CD1	2.44	0.53
1:D:52:LEU:HD13	1:D:52:LEU:C	2.28	0.53
1:A:33:TRP:CE3	1:A:52:LEU:HD21	2.43	0.53
1:F:82:ARG:HH11	1:F:82:ARG:CG	2.23	0.52
1:F:76:PHE:CE1	1:F:82:ARG:HG3	2.45	0.52
1:F:94:GLN:OE1	1:F:107:GLY:HA3	2.09	0.52
1:C:33:TRP:CE3	1:C:52:LEU:HD11	2.45	0.52
1:C:37:ARG:HH21	1:C:94:GLN:NE2	2.08	0.51
1:A:33:TRP:CZ2	1:C:80:GLY:HA2	2.45	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:37:ARG:CZ	1:E:94:GLN:NE2	2.72	0.51
1:A:52:LEU:C	1:A:52:LEU:HD13	2.31	0.51
1:E:48:ASN:HB2	1:E:73:PHE:CD1	2.45	0.51
1:C:37:ARG:HE	1:C:94:GLN:NE2	1.97	0.50
1:C:52:LEU:HD13	1:C:53:SER:N	2.27	0.50
1:D:80:GLY:HA2	1:E:33:TRP:CZ2	2.47	0.50
1:A:52:LEU:HD22	1:A:53:SER:N	2.26	0.49
1:F:97:LEU:HD23	1:F:105:PRO:HG3	1.94	0.49
1:F:7:VAL:HG12	1:F:9:PRO:O	2.13	0.49
1:E:52:LEU:HD13	1:E:52:LEU:C	2.32	0.49
1:B:35:TYR:CD2	1:B:35:TYR:N	2.80	0.48
1:A:5:ALA:HB2	1:A:105:PRO:HG3	1.94	0.48
1:B:72:SER:HA	1:B:86:VAL:O	2.13	0.48
1:E:87:ASP:OD2	1:E:89:THR:HB	2.14	0.48
1:E:7:VAL:HG21	1:E:95:VAL:HB	1.96	0.48
1:E:35:TYR:CD2	1:E:35:TYR:N	2.82	0.48
1:A:33:TRP:HE3	1:A:52:LEU:HD21	1.78	0.47
1:A:33:TRP:CH2	1:C:80:GLY:HA2	2.50	0.47
1:F:57:ALA:HB1	1:F:61:GLY:HA2	1.97	0.47
1:C:52:LEU:C	1:C:52:LEU:HD13	2.36	0.46
1:A:47:SER:HB2	3:A:1114:TH2:O3	2.15	0.46
1:B:52:LEU:HD22	1:B:53:SER:N	2.31	0.46
1:E:71:ARG:HH21	1:E:71:ARG:HB2	1.80	0.45
1:A:77:LEU:HD12	1:A:81:THR:HB	1.97	0.45
1:B:40:VAL:O	1:B:41:ASP:HB2	2.15	0.45
1:B:27:GLN:O	1:B:30:THR:HB	2.16	0.45
1:C:55:VAL:CG2	1:C:63:ALA:HB1	2.46	0.45
1:D:34:VAL:HG12	1:D:67:LEU:HD22	1.98	0.45
1:A:7:VAL:O	1:A:10:SER:HB3	2.15	0.45
1:B:112:PHE:CD1	1:B:112:PHE:N	2.84	0.45
1:F:41:ASP:OD1	1:F:42:THR:N	2.47	0.45
1:D:74:GLU:OE1	1:D:82:ARG:NE	2.37	0.45
1:D:5:ALA:HB2	1:D:105:PRO:HG3	1.99	0.44
1:A:21:VAL:O	1:A:64:SER:HA	2.17	0.44
1:A:80:GLY:HA2	1:C:33:TRP:CZ2	2.53	0.44
1:E:57:ALA:HB1	1:E:61:GLY:HA2	1.99	0.44
1:B:52:LEU:HD22	1:B:53:SER:H	1.82	0.44
1:B:33:TRP:CE3	1:B:52:LEU:HD21	2.53	0.43
1:C:7:VAL:HG12	1:C:9:PRO:O	2.17	0.43
1:F:8:THR:HA	1:F:9:PRO:C	2.37	0.43
1:D:33:TRP:CZ2	1:E:80:GLY:HA2	2.54	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:48:ASN:HB2	1:E:73:PHE:CG	2.54	0.43
1:B:35:TYR:HB3	1:B:52:LEU:HD23	2.00	0.43
1:D:48:ASN:ND2	1:D:51:ASP:HB2	2.34	0.43
1:B:33:TRP:CZ3	1:B:52:LEU:HD11	2.54	0.43
1:E:37:ARG:NH1	1:E:45:HIS:ND1	2.66	0.43
1:A:112:PHE:N	1:A:112:PHE:CD1	2.86	0.43
1:D:41:ASP:HB3	1:D:44:VAL:CG2	2.49	0.43
1:A:47:SER:O	1:A:75:GLY:HA2	2.19	0.42
1:E:72:SER:HA	1:E:86:VAL:O	2.19	0.42
1:C:36:GLN:HB2	4:C:2005:HOH:O	2.19	0.42
1:B:20:LYS:HZ3	1:B:22:ALA:HB2	1.84	0.42
1:C:82:ARG:HH22	1:C:84:GLY:HA2	1.85	0.42
1:C:5:ALA:HA	1:C:22:ALA:O	2.19	0.42
1:B:9:PRO:HG2	1:B:13:LEU:CD2	2.50	0.41
1:B:97:LEU:HB3	1:B:105:PRO:HD2	2.02	0.41
1:F:49:PRO:HA	1:F:52:LEU:HB2	2.02	0.41
1:E:82:ARG:CG	1:E:82:ARG:NH1	2.83	0.41
1:F:17:THR:O	1:F:69:VAL:HG22	2.20	0.41
1:D:2:ALA:HA	1:D:3:PRO:HD3	1.89	0.41
1:F:9:PRO:HG2	1:F:13:LEU:CD2	2.50	0.41
1:F:74:GLU:CD	1:F:82:ARG:NH1	2.73	0.41
1:B:5:ALA:HB2	1:B:105:PRO:HG3	2.03	0.41
1:F:55:VAL:HG22	1:F:63:ALA:HB1	2.03	0.41
1:A:5:ALA:HA	1:A:22:ALA:O	2.20	0.41
1:D:94:GLN:OE1	1:D:107:GLY:HA3	2.21	0.41
1:D:17:THR:O	1:D:69:VAL:HG22	2.20	0.41
1:D:48:ASN:HB2	1:D:73:PHE:CD1	2.56	0.41
1:D:35:TYR:N	1:D:35:TYR:CD2	2.88	0.41
1:F:112:PHE:N	1:F:112:PHE:CD1	2.89	0.41
1:F:35:TYR:HB3	1:F:52:LEU:HD23	2.02	0.40
1:A:35:TYR:CD2	3:A:1114:TH2:H6C1	2.57	0.40
1:B:33:TRP:O	1:B:97:LEU:HA	2.20	0.40
1:B:33:TRP:CZ2	1:F:80:GLY:HA2	2.57	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles

### 5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	109/114 (96%)	106 (97%)	3 (3%)	0	100	100
1	B	111/114 (97%)	107 (96%)	4 (4%)	0	100	100
1	C	110/114 (96%)	104 (94%)	6 (6%)	0	100	100
1	D	110/114 (96%)	105 (96%)	5 (4%)	0	100	100
1	E	110/114 (96%)	107 (97%)	3 (3%)	0	100	100
1	F	109/114 (96%)	105 (96%)	4 (4%)	0	100	100
All	All	659/684 (96%)	634 (96%)	25 (4%)	0	100	100

There are no Ramachandran outliers to report.

### 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	79/81 (98%)	75 (95%)	4 (5%)	28	52
1	B	81/81 (100%)	78 (96%)	3 (4%)	39	66
1	C	80/81 (99%)	78 (98%)	2 (2%)	53	79
1	D	80/81 (99%)	77 (96%)	3 (4%)	38	66
1	E	80/81 (99%)	75 (94%)	5 (6%)	21	42
1	F	79/81 (98%)	75 (95%)	4 (5%)	28	52
All	All	479/486 (99%)	458 (96%)	21 (4%)	33	60



All (21) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	47	SER
1	A	52	LEU
1	A	79	ASP
1	A	97	LEU
1	B	20	LYS
1	B	52	LEU
1	B	71	ARG
1	C	55	VAL
1	C	113	ASN
1	D	52	LEU
1	D	55	VAL
1	D	79	ASP
1	E	52	LEU
1	E	55	VAL
1	E	71	ARG
1	E	97	LEU
1	E	113	ASN
1	F	8	THR
1	F	52	LEU
1	F	55	VAL
1	F	82	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	45	HIS
1	A	94	GLN
1	C	94	GLN
1	D	45	HIS
1	E	94	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](#)

13 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
2	SO4	A	1113	-	4,4,4	0.35	0	6,6,6	0.06	0
3	TH2	A	1114	-	28,31,31	1.59	6 (21%)	45,48,48	1.98	11 (24%)
3	TH2	A	1115	-	28,31,31	1.63	8 (28%)	45,48,48	1.98	10 (22%)
2	SO4	B	1115	-	4,4,4	0.37	0	6,6,6	0.16	0
3	TH2	B	1116	-	28,31,31	1.61	6 (21%)	45,48,48	1.93	10 (22%)
3	TH2	B	1117	-	28,31,31	1.63	7 (25%)	45,48,48	2.04	11 (24%)
2	SO4	C	1114	-	4,4,4	0.34	0	6,6,6	0.13	0
3	TH2	C	1115	-	28,31,31	1.59	6 (21%)	45,48,48	1.94	10 (22%)
3	TH2	D	1114	-	28,31,31	1.62	7 (25%)	45,48,48	1.99	10 (22%)
2	SO4	E	1114	-	4,4,4	0.34	0	6,6,6	0.09	0
3	TH2	E	1115	-	28,31,31	1.57	8 (28%)	45,48,48	2.01	11 (24%)
2	SO4	F	1113	-	4,4,4	0.32	0	6,6,6	0.11	0
3	TH2	F	1114	-	28,31,31	1.53	9 (32%)	45,48,48	1.96	9 (20%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	SO4	A	1113	-	-	0/0/0/0	0/0/0/0
3	TH2	A	1114	-	-	0/7/67/67	0/4/4/4
3	TH2	A	1115	-	-	0/7/67/67	0/4/4/4
2	SO4	B	1115	-	-	0/0/0/0	0/0/0/0
3	TH2	B	1116	-	-	0/7/67/67	0/4/4/4

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	TH2	B	1117	-	-	0/7/67/67	0/4/4/4
2	SO4	C	1114	-	-	0/0/0/0	0/0/0/0
3	TH2	C	1115	-	-	0/7/67/67	0/4/4/4
3	TH2	D	1114	-	-	1/7/67/67	0/4/4/4
2	SO4	E	1114	-	-	0/0/0/0	0/0/0/0
3	TH2	E	1115	-	-	0/7/67/67	0/4/4/4
2	SO4	F	1113	-	-	0/0/0/0	0/0/0/0
3	TH2	F	1114	-	-	0/7/67/67	0/4/4/4

All (57) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	1116	TH2	O17-C17	-2.70	1.41	1.46
3	A	1114	TH2	O17-C17	-2.56	1.41	1.46
3	E	1115	TH2	O17-C17	-2.46	1.42	1.46
3	F	1114	TH2	O17-C17	-2.37	1.42	1.46
3	B	1116	TH2	O17-C20	-2.31	1.27	1.34
3	C	1115	TH2	O17-C17	-2.29	1.42	1.46
3	E	1115	TH2	O17-C20	-2.27	1.27	1.34
3	A	1114	TH2	O17-C20	-2.19	1.27	1.34
3	D	1114	TH2	O17-C17	-2.14	1.42	1.46
3	F	1114	TH2	O17-C20	-2.02	1.28	1.34
3	C	1115	TH2	O3-C3	-2.01	1.19	1.23
3	B	1117	TH2	O17-C17	-2.00	1.42	1.46
3	F	1114	TH2	C8-C9	2.02	1.57	1.53
3	F	1114	TH2	C1-C10	2.03	1.58	1.54
3	E	1115	TH2	C11-C9	2.04	1.57	1.53
3	C	1115	TH2	C4-C5	2.06	1.37	1.34
3	F	1114	TH2	C4-C5	2.08	1.37	1.34
3	C	1115	TH2	C10-C9	2.08	1.59	1.56
3	B	1116	TH2	C10-C9	2.08	1.59	1.56
3	E	1115	TH2	C1-C10	2.10	1.58	1.54
3	D	1114	TH2	C1-C10	2.14	1.58	1.54
3	A	1114	TH2	C10-C9	2.14	1.59	1.56
3	A	1114	TH2	C8-C9	2.16	1.57	1.53
3	F	1114	TH2	C16-C17	2.16	1.58	1.53
3	A	1115	TH2	C10-C9	2.16	1.59	1.56
3	E	1115	TH2	C4-C5	2.21	1.37	1.34
3	A	1115	TH2	C11-C9	2.22	1.57	1.53
3	A	1115	TH2	C13-C17	2.23	1.57	1.53
3	B	1116	TH2	C16-C17	2.28	1.58	1.53
3	F	1114	TH2	C7-C8	2.28	1.57	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	1117	TH2	C7-C8	2.29	1.57	1.53
3	D	1114	TH2	C8-C9	2.32	1.58	1.53
3	A	1115	TH2	C8-C9	2.32	1.58	1.53
3	B	1116	TH2	C11-C9	2.32	1.57	1.53
3	B	1117	TH2	C16-C17	2.33	1.59	1.53
3	A	1115	TH2	C1-C10	2.35	1.58	1.54
3	D	1114	TH2	C16-C17	2.35	1.59	1.53
3	B	1117	TH2	C4-C5	2.37	1.37	1.34
3	D	1114	TH2	C7-C8	2.38	1.57	1.53
3	F	1114	TH2	C10-C9	2.38	1.60	1.56
3	A	1115	TH2	C16-C17	2.40	1.59	1.53
3	A	1114	TH2	C11-C9	2.42	1.57	1.53
3	C	1115	TH2	C11-C9	2.42	1.58	1.53
3	B	1117	TH2	C8-C9	2.42	1.58	1.53
3	E	1115	TH2	C8-C9	2.45	1.58	1.53
3	B	1117	TH2	C11-C9	2.46	1.58	1.53
3	E	1115	TH2	C10-C5	2.52	1.57	1.52
3	A	1115	TH2	C4-C5	2.54	1.38	1.34
3	E	1115	TH2	C16-C17	2.60	1.59	1.53
3	D	1114	TH2	C11-C9	2.65	1.58	1.53
3	F	1114	TH2	C10-C5	2.66	1.58	1.52
3	A	1115	TH2	C10-C5	2.87	1.58	1.52
3	B	1116	TH2	C10-C5	3.00	1.58	1.52
3	C	1115	TH2	C10-C5	3.14	1.59	1.52
3	B	1117	TH2	C10-C5	3.18	1.59	1.52
3	D	1114	TH2	C10-C5	3.28	1.59	1.52
3	A	1114	TH2	C10-C5	3.37	1.59	1.52

All (82) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	E	1115	TH2	C11-C9-C10	-4.49	106.89	113.10
3	B	1116	TH2	C11-C9-C10	-4.18	107.32	113.10
3	B	1117	TH2	C11-C9-C10	-4.15	107.37	113.10
3	D	1114	TH2	C11-C9-C10	-4.13	107.38	113.10
3	A	1114	TH2	C11-C9-C10	-4.13	107.40	113.10
3	C	1115	TH2	C11-C9-C10	-4.11	107.41	113.10
3	A	1115	TH2	C11-C9-C10	-4.11	107.42	113.10
3	F	1114	TH2	C11-C9-C10	-4.05	107.50	113.10
3	D	1114	TH2	C12-C11-C9	-3.88	106.36	113.12
3	B	1117	TH2	C12-C11-C9	-3.75	106.58	113.12
3	A	1115	TH2	C12-C11-C9	-3.64	106.78	113.12

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	1114	TH2	C12-C11-C9	-3.63	106.79	113.12
3	F	1114	TH2	C12-C11-C9	-3.57	106.89	113.12
3	E	1115	TH2	C12-C11-C9	-3.55	106.93	113.12
3	B	1116	TH2	C12-C11-C9	-3.40	107.19	113.12
3	C	1115	TH2	C12-C11-C9	-3.29	107.39	113.12
3	A	1115	TH2	C16-C17-C13	-2.99	102.00	105.19
3	B	1117	TH2	C16-C17-C13	-2.95	102.03	105.19
3	C	1115	TH2	C16-C17-C13	-2.87	102.12	105.19
3	D	1114	TH2	C16-C17-C13	-2.81	102.19	105.19
3	F	1114	TH2	C16-C17-C13	-2.79	102.21	105.19
3	A	1114	TH2	C16-C17-C13	-2.78	102.22	105.19
3	E	1115	TH2	C16-C17-C13	-2.76	102.24	105.19
3	B	1116	TH2	C16-C17-C13	-2.63	102.38	105.19
3	A	1114	TH2	C9-C10-C5	-2.56	105.64	109.65
3	A	1114	TH2	O20-C20-C22	-2.49	113.85	123.68
3	B	1117	TH2	O20-C20-C22	-2.48	113.90	123.68
3	F	1114	TH2	O20-C20-C22	-2.46	113.96	123.68
3	D	1114	TH2	O20-C20-C22	-2.42	114.11	123.68
3	A	1115	TH2	C9-C10-C5	-2.41	105.88	109.65
3	B	1116	TH2	O20-C20-C22	-2.37	114.33	123.68
3	A	1115	TH2	O20-C20-C22	-2.29	114.62	123.68
3	D	1114	TH2	C9-C10-C5	-2.29	106.06	109.65
3	C	1115	TH2	O20-C20-C22	-2.26	114.74	123.68
3	E	1115	TH2	O20-C20-C22	-2.25	114.77	123.68
3	C	1115	TH2	C9-C10-C5	-2.25	106.13	109.65
3	E	1115	TH2	C9-C10-C5	-2.21	106.19	109.65
3	B	1117	TH2	C9-C10-C5	-2.17	106.25	109.65
3	A	1114	TH2	C22-C21-C23	-2.13	109.02	112.66
3	E	1115	TH2	C19-C10-C9	-2.07	109.12	111.68
3	B	1117	TH2	C19-C10-C9	-2.07	109.12	111.68
3	B	1116	TH2	C15-C16-C17	2.01	108.13	104.75
3	C	1115	TH2	C15-C16-C17	2.11	108.30	104.75
3	B	1116	TH2	C18-C13-C14	2.25	115.98	111.73
3	E	1115	TH2	C18-C13-C14	2.25	115.99	111.73
3	A	1114	TH2	C18-C13-C14	2.30	116.08	111.73
3	A	1115	TH2	C18-C13-C14	2.56	116.57	111.73
3	D	1114	TH2	C18-C13-C14	2.68	116.81	111.73
3	D	1114	TH2	O17-C20-O20	2.70	130.41	123.68
3	F	1114	TH2	C18-C13-C14	2.72	116.88	111.73
3	F	1114	TH2	O17-C20-O20	2.79	130.62	123.68
3	B	1117	TH2	C18-C13-C14	2.80	117.03	111.73
3	A	1115	TH2	O17-C20-O20	2.90	130.91	123.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	1116	TH2	O17-C20-O20	3.02	131.21	123.68
3	B	1117	TH2	O17-C20-O20	3.12	131.45	123.68
3	E	1115	TH2	O17-C20-O20	3.16	131.55	123.68
3	C	1115	TH2	O17-C20-O20	3.21	131.69	123.68
3	A	1114	TH2	O17-C20-O20	3.29	131.89	123.68
3	E	1115	TH2	O17-C17-C13	3.67	120.00	111.14
3	D	1114	TH2	C17-O17-C20	4.14	126.24	117.98
3	F	1114	TH2	C17-O17-C20	4.16	126.27	117.98
3	A	1114	TH2	C17-O17-C20	4.19	126.33	117.98
3	B	1116	TH2	C17-O17-C20	4.30	126.56	117.98
3	B	1116	TH2	O17-C17-C13	4.36	121.67	111.14
3	C	1115	TH2	C17-O17-C20	4.63	127.20	117.98
3	A	1115	TH2	C17-O17-C20	4.69	127.33	117.98
3	C	1115	TH2	O17-C17-C13	4.72	122.54	111.14
3	A	1114	TH2	O17-C17-C16	4.72	122.78	110.99
3	B	1117	TH2	O17-C17-C13	4.75	122.62	111.14
3	A	1115	TH2	O17-C17-C13	4.81	122.76	111.14
3	C	1115	TH2	O17-C17-C16	4.82	123.02	110.99
3	F	1114	TH2	O17-C17-C13	4.91	123.01	111.14
3	E	1115	TH2	C17-O17-C20	5.00	127.95	117.98
3	D	1114	TH2	O17-C17-C13	5.08	123.42	111.14
3	B	1117	TH2	C17-O17-C20	5.09	128.13	117.98
3	D	1114	TH2	O17-C17-C16	5.10	123.71	110.99
3	A	1114	TH2	O17-C17-C13	5.13	123.53	111.14
3	B	1116	TH2	O17-C17-C16	5.23	124.05	110.99
3	F	1114	TH2	O17-C17-C16	5.26	124.12	110.99
3	A	1115	TH2	O17-C17-C16	5.28	124.15	110.99
3	B	1117	TH2	O17-C17-C16	5.52	124.76	110.99
3	E	1115	TH2	O17-C17-C16	5.91	125.74	110.99

There are no chirality outliers.

All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	D	1114	TH2	C20-O17-C17-C16

There are no ring outliers.

3 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	1114	TH2	2	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	1115	TH2	1	0
3	B	1117	TH2	1	0

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

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

There are no chain breaks in this entry.

## 6 Fit of model and data

### 6.1 Protein, DNA and RNA chains

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95<sup>th</sup> percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q < 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å²)	Q<0.9
1	A	111/114 (97%)	12.24	109 (98%)	0	0	17, 27, 36, 45	0
1	B	113/114 (99%)	11.79	108 (95%)	0	0	13, 24, 35, 46	0
1	C	112/114 (98%)	11.61	108 (96%)	0	0	16, 25, 36, 50	0
1	D	112/114 (98%)	11.59	107 (95%)	0	0	16, 24, 40, 49	0
1	E	112/114 (98%)	11.62	110 (98%)	0	0	18, 30, 45, 56	0
1	F	111/114 (97%)	13.36	107 (96%)	0	0	17, 31, 45, 50	0
All	All	671/684 (98%)	12.03	649 (96%)	0	0	13, 27, 42, 56	0

All (649) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	101	ALA	73.0
1	E	2	ALA	49.5
1	B	107	GLY	49.0
1	F	25	GLY	48.3
1	D	10	SER	46.2
1	C	101	ALA	42.9
1	B	9	PRO	42.4
1	F	5	ALA	40.9
1	A	2	ALA	39.8
1	E	15	ASP	39.7
1	F	43	GLY	39.4
1	C	63	ALA	38.6
1	F	60	ASN	37.3
1	E	29	GLY	36.6
1	C	100	ALA	36.5
1	A	91	ALA	36.3
1	F	105	PRO	36.2
1	F	84	GLY	35.3
1	F	9	PRO	35.1

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Mol	Chain	Res	Type	RSRZ
1	A	90	THR	34.3
1	C	44	VAL	33.3
1	E	111	SER	33.3
1	A	96	GLY	33.2
1	C	66	SER	33.0
1	B	44	VAL	32.6
1	C	61	GLY	32.4
1	C	92	ALA	32.1
1	F	101	ALA	31.7
1	D	75	GLY	31.6
1	F	109	ALA	31.5
1	E	44	VAL	31.4
1	A	3	PRO	31.1
1	B	5	ALA	31.0
1	B	89	THR	30.9
1	F	29	GLY	30.8
1	C	94	GLN	30.7
1	A	108	VAL	30.5
1	B	32	TYR	30.0
1	B	39	ALA	30.0
1	E	112	PHE	29.6
1	A	92	ALA	29.6
1	B	4	THR	28.9
1	D	100	ALA	28.8
1	C	72	SER	28.6
1	E	89	THR	28.2
1	B	63	ALA	28.0
1	A	68	THR	27.9
1	F	59	ALA	27.8
1	F	108	VAL	27.8
1	E	59	ALA	27.6
1	D	39	ALA	27.4
1	B	93	CYS	27.3
1	D	103	ASN	26.5
1	C	43	GLY	26.5
1	F	57	ALA	26.5
1	E	21	VAL	26.3
1	A	69	VAL	26.2
1	B	23	GLY	26.2
1	A	61	GLY	26.2
1	D	112	PHE	26.1
1	A	106	GLU	26.0

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Mol	Chain	Res	Type	RSRZ
1	E	18	VAL	26.0
1	D	90	THR	25.8
1	A	43	GLY	25.8
1	E	24	ALA	25.6
1	D	32	TYR	25.4
1	B	106	GLU	25.3
1	F	42	THR	25.1
1	A	9	PRO	24.9
1	F	100	ALA	24.8
1	C	2	ALA	24.8
1	F	90	THR	24.7
1	C	109	ALA	24.3
1	A	110	ILE	24.3
1	B	7	VAL	24.2
1	F	13	LEU	24.0
1	B	14	SER	24.0
1	E	67	LEU	24.0
1	B	109	ALA	23.8
1	B	111	SER	23.8
1	A	45	HIS	23.7
1	B	102	GLY	23.4
1	C	9	PRO	23.3
1	A	29	GLY	23.1
1	D	84	GLY	23.1
1	E	91	ALA	23.0
1	F	36	GLN	22.9
1	E	98	SER	22.8
1	D	95	VAL	22.7
1	A	98	SER	22.6
1	B	73	PHE	22.5
1	A	104	GLY	22.4
1	E	103	ASN	22.2
1	C	10	SER	22.2
1	B	57	ALA	21.8
1	D	98	SER	21.6
1	D	27	GLN	21.6
1	B	28	ALA	21.5
1	F	88	CYS	21.5
1	D	41	ASP	21.3
1	A	67	LEU	21.2
1	E	34	VAL	21.0
1	D	48	ASN	21.0

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Mol	Chain	Res	Type	RSRZ
1	B	51	ASP	20.8
1	D	54	SER	20.8
1	D	2	ALA	20.7
1	C	18	VAL	20.7
1	B	110	ILE	20.5
1	D	52	LEU	20.4
1	E	49	PRO	20.1
1	F	16	GLY	20.1
1	D	77	LEU	20.1
1	A	80	GLY	20.0
1	E	77	LEU	19.9
1	A	63	ALA	19.8
1	F	38	ALA	19.6
1	C	48	ASN	19.3
1	D	24	ALA	19.3
1	A	83	TRP	19.2
1	D	42	THR	19.2
1	A	78	PHE	19.1
1	A	23	GLY	19.1
1	F	70	ARG	19.0
1	E	39	ALA	19.0
1	D	4	THR	19.0
1	E	6	THR	19.0
1	F	83	TRP	18.9
1	A	89	THR	18.9
1	D	74	GLU	18.9
1	E	72	SER	18.6
1	D	72	SER	18.5
1	E	9	PRO	18.5
1	C	108	VAL	18.4
1	F	99	ASP	18.4
1	E	38	ALA	18.2
1	B	92	ALA	18.1
1	D	93	CYS	18.1
1	C	20	LYS	18.0
1	F	107	GLY	17.9
1	D	17	THR	17.8
1	D	47	SER	17.8
1	F	6	THR	17.6
1	E	99	ASP	17.6
1	E	36	GLN	17.5
1	A	44	VAL	17.4

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Mol	Chain	Res	Type	RSRZ
1	D	19	VAL	17.4
1	C	28	ALA	17.2
1	B	20	LYS	17.1
1	D	65	THR	17.1
1	B	90	THR	17.0
1	C	68	THR	17.0
1	F	37	ARG	16.9
1	A	79	ASP	16.9
1	E	19	VAL	16.8
1	D	78	PHE	16.8
1	B	88	CYS	16.7
1	F	102	GLY	16.7
1	B	29	GLY	16.6
1	F	81	THR	16.6
1	C	27	GLN	16.6
1	B	15	ASP	16.5
1	E	65	THR	16.4
1	E	13	LEU	16.4
1	B	34	VAL	16.3
1	B	100	ALA	16.3
1	C	81	THR	16.1
1	C	47	SER	16.1
1	C	84	GLY	16.1
1	C	40	VAL	16.0
1	E	90	THR	16.0
1	C	21	VAL	16.0
1	D	70	ARG	16.0
1	B	114	HIS	15.9
1	B	113	ASN	15.9
1	A	95	VAL	15.9
1	A	62	SER	15.9
1	E	60	ASN	15.8
1	F	34	VAL	15.8
1	E	86	VAL	15.8
1	E	37	ARG	15.8
1	C	112	PHE	15.8
1	D	40	VAL	15.7
1	C	71	ARG	15.7
1	A	72	SER	15.7
1	B	6	THR	15.6
1	F	55	VAL	15.6
1	B	11	SER	15.6

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Mol	Chain	Res	Type	RSRZ
1	C	88	CYS	15.5
1	C	34	VAL	15.4
1	F	82	ARG	15.4
1	A	35	TYR	15.3
1	C	110	ILE	15.2
1	C	65	THR	15.2
1	D	96	GLY	15.2
1	D	14	SER	15.1
1	F	27	GLN	15.1
1	A	66	SER	15.1
1	F	104	GLY	15.1
1	B	43	GLY	15.0
1	D	61	GLY	14.9
1	A	64	SER	14.8
1	B	47	SER	14.8
1	F	46	ALA	14.8
1	C	49	PRO	14.7
1	F	50	ALA	14.7
1	A	46	ALA	14.6
1	F	54	SER	14.6
1	F	19	VAL	14.6
1	E	68	THR	14.5
1	E	26	LEU	14.5
1	F	111	SER	14.5
1	E	43	GLY	14.4
1	C	83	TRP	14.4
1	F	12	GLY	14.4
1	F	110	ILE	14.2
1	F	10	SER	14.2
1	D	25	GLY	14.2
1	A	15	ASP	14.1
1	E	47	SER	14.1
1	C	6	THR	14.0
1	C	86	VAL	14.0
1	D	34	VAL	13.9
1	E	33	TRP	13.9
1	C	85	THR	13.8
1	F	58	ASP	13.8
1	F	85	THR	13.7
1	D	94	GLN	13.7
1	F	112	PHE	13.7
1	A	105	PRO	13.7

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Mol	Chain	Res	Type	RSRZ
1	F	40	VAL	13.6
1	B	59	ALA	13.6
1	E	88	CYS	13.6
1	B	78	PHE	13.6
1	C	17	THR	13.5
1	A	56	THR	13.4
1	C	13	LEU	13.4
1	C	32	TYR	13.2
1	F	73	PHE	13.2
1	F	93	CYS	13.1
1	E	83	TRP	13.1
1	A	36	GLN	13.1
1	B	37	ARG	13.0
1	D	55	VAL	12.9
1	B	103	ASN	12.9
1	A	101	ALA	12.9
1	A	74	GLU	12.8
1	D	35	TYR	12.8
1	C	31	ALA	12.8
1	C	54	SER	12.7
1	A	32	TYR	12.7
1	F	48	ASN	12.6
1	E	97	LEU	12.5
1	F	63	ALA	12.4
1	A	84	GLY	12.4
1	F	89	THR	12.4
1	D	105	PRO	12.3
1	B	112	PHE	12.3
1	E	108	VAL	12.3
1	F	24	ALA	12.2
1	D	68	THR	12.1
1	F	18	VAL	12.1
1	D	87	ASP	12.1
1	A	17	THR	12.0
1	F	2	ALA	11.9
1	B	33	TRP	11.9
1	B	62	SER	11.8
1	C	89	THR	11.8
1	E	110	ILE	11.6
1	F	32	TYR	11.6
1	F	33	TRP	11.5
1	C	106	GLU	11.5

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Mol	Chain	Res	Type	RSRZ
1	B	35	TYR	11.4
1	A	51	ASP	11.4
1	E	16	GLY	11.4
1	F	35	TYR	11.3
1	F	103	ASN	11.3
1	A	28	ALA	11.3
1	F	76	PHE	11.3
1	D	38	ALA	11.2
1	E	28	ALA	11.2
1	C	39	ALA	11.2
1	C	50	ALA	11.1
1	B	18	VAL	11.1
1	C	91	ALA	11.1
1	A	11	SER	11.1
1	A	13	LEU	11.0
1	B	97	LEU	11.0
1	E	10	SER	11.0
1	E	7	VAL	10.9
1	B	56	THR	10.9
1	C	26	LEU	10.9
1	A	39	ALA	10.9
1	C	5	ALA	10.9
1	F	87	ASP	10.8
1	C	60	ASN	10.8
1	D	21	VAL	10.8
1	D	8	THR	10.8
1	B	94	GLN	10.7
1	C	3	PRO	10.7
1	F	49	PRO	10.7
1	F	91	ALA	10.6
1	A	10	SER	10.5
1	A	55	VAL	10.5
1	D	60	ASN	10.4
1	F	71	ARG	10.4
1	A	20	LYS	10.3
1	E	20	LYS	10.3
1	A	6	THR	10.2
1	B	101	ALA	10.2
1	A	71	ARG	10.2
1	E	92	ALA	10.2
1	C	77	LEU	10.2
1	B	36	GLN	10.1

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Mol	Chain	Res	Type	RSRZ
1	F	47	SER	10.1
1	A	7	VAL	10.1
1	A	99	ASP	10.0
1	F	39	ALA	10.0
1	E	70	ARG	10.0
1	D	6	THR	10.0
1	D	67	LEU	9.9
1	A	27	GLN	9.9
1	D	63	ALA	9.8
1	F	15	ASP	9.8
1	A	73	PHE	9.8
1	A	82	ARG	9.8
1	A	111	SER	9.8
1	B	49	PRO	9.8
1	F	23	GLY	9.8
1	C	23	GLY	9.7
1	B	19	VAL	9.7
1	C	12	GLY	9.7
1	A	52	LEU	9.7
1	D	102	GLY	9.6
1	A	88	CYS	9.6
1	D	37	ARG	9.6
1	D	56	THR	9.6
1	D	28	ALA	9.5
1	C	80	GLY	9.4
1	A	59	ALA	9.4
1	A	41	ASP	9.3
1	E	62	SER	9.3
1	E	73	PHE	9.3
1	B	42	THR	9.2
1	E	42	THR	9.2
1	D	3	PRO	9.2
1	B	31	ALA	9.1
1	B	83	TRP	9.1
1	C	82	ARG	9.1
1	E	106	GLU	9.1
1	A	38	ALA	9.1
1	E	5	ALA	9.1
1	D	86	VAL	9.1
1	E	46	ALA	9.0
1	A	77	LEU	9.0
1	E	100	ALA	9.0

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Mol	Chain	Res	Type	RSRZ
1	D	108	VAL	8.9
1	D	58	ASP	8.9
1	A	70	ARG	8.9
1	C	51	ASP	8.9
1	C	103	ASN	8.8
1	C	15	ASP	8.7
1	C	29	GLY	8.7
1	D	33	TRP	8.6
1	D	20	LYS	8.6
1	D	22	ALA	8.6
1	B	74	GLU	8.6
1	D	71	ARG	8.5
1	B	81	THR	8.5
1	E	52	LEU	8.5
1	B	99	ASP	8.4
1	F	52	LEU	8.4
1	E	105	PRO	8.4
1	D	111	SER	8.4
1	B	76	PHE	8.3
1	A	5	ALA	8.3
1	C	59	ALA	8.3
1	C	102	GLY	8.3
1	D	113	ASN	8.3
1	A	109	ALA	8.2
1	B	85	THR	8.2
1	B	60	ASN	8.1
1	A	81	THR	8.1
1	A	54	SER	8.0
1	F	69	VAL	8.0
1	B	91	ALA	8.0
1	E	40	VAL	8.0
1	E	27	GLN	7.9
1	E	54	SER	7.8
1	B	50	ALA	7.8
1	A	42	THR	7.6
1	B	52	LEU	7.6
1	C	8	THR	7.6
1	B	79	ASP	7.6
1	C	75	GLY	7.5
1	D	49	PRO	7.5
1	B	82	ARG	7.5
1	A	100	ALA	7.4

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Mol	Chain	Res	Type	RSRZ
1	C	53	SER	7.4
1	F	41	ASP	7.4
1	A	57	ALA	7.3
1	C	87	ASP	7.3
1	D	89	THR	7.3
1	D	46	ALA	7.3
1	C	104	GLY	7.3
1	E	104	GLY	7.3
1	F	92	ALA	7.3
1	A	53	SER	7.2
1	B	86	VAL	7.2
1	A	8	THR	7.2
1	B	13	LEU	7.2
1	C	52	LEU	7.2
1	B	71	ARG	7.2
1	E	35	TYR	7.2
1	B	80	GLY	7.2
1	E	78	PHE	7.2
1	F	67	LEU	7.1
1	F	31	ALA	7.1
1	E	4	THR	7.1
1	C	70	ARG	7.1
1	F	66	SER	7.1
1	F	98	SER	7.0
1	E	84	GLY	7.0
1	A	50	ALA	6.9
1	E	56	THR	6.9
1	F	65	THR	6.9
1	D	9	PRO	6.8
1	D	80	GLY	6.8
1	A	49	PRO	6.8
1	B	12	GLY	6.8
1	C	76	PHE	6.8
1	D	106	GLU	6.7
1	F	45	HIS	6.7
1	A	48	ASN	6.7
1	F	14	SER	6.6
1	B	66	SER	6.6
1	D	92	ALA	6.5
1	C	99	ASP	6.5
1	E	82	ARG	6.5
1	E	55	VAL	6.4

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Mol	Chain	Res	Type	RSRZ
1	F	17	THR	6.4
1	F	94	GLN	6.4
1	B	69	VAL	6.4
1	C	96	GLY	6.4
1	A	18	VAL	6.4
1	D	15	ASP	6.3
1	F	28	ALA	6.3
1	E	113	ASN	6.3
1	A	112	PHE	6.3
1	A	21	VAL	6.2
1	F	96	GLY	6.2
1	D	83	TRP	6.2
1	A	30	THR	6.2
1	D	97	LEU	6.2
1	E	45	HIS	6.2
1	E	57	ALA	6.2
1	E	32	TYR	6.2
1	E	76	PHE	6.2
1	C	113	ASN	6.1
1	F	95	VAL	6.1
1	C	95	VAL	6.1
1	E	61	GLY	6.1
1	E	71	ARG	6.0
1	A	103	ASN	6.0
1	D	29	GLY	6.0
1	B	64	SER	6.0
1	A	97	LEU	6.0
1	B	46	ALA	5.9
1	B	70	ARG	5.9
1	F	77	LEU	5.9
1	D	23	GLY	5.9
1	A	47	SER	5.9
1	C	4	THR	5.8
1	F	72	SER	5.8
1	A	19	VAL	5.8
1	C	90	THR	5.8
1	C	58	ASP	5.8
1	C	36	GLN	5.8
1	F	3	PRO	5.8
1	A	31	ALA	5.8
1	F	7	VAL	5.7
1	F	51	ASP	5.6

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Mol	Chain	Res	Type	RSRZ
1	F	68	THR	5.6
1	C	11	SER	5.6
1	E	66	SER	5.6
1	C	56	THR	5.6
1	E	14	SER	5.6
1	E	58	ASP	5.5
1	F	62	SER	5.5
1	A	33	TRP	5.5
1	E	74	GLU	5.5
1	B	26	LEU	5.5
1	B	48	ASN	5.4
1	C	7	VAL	5.4
1	E	17	THR	5.4
1	C	62	SER	5.4
1	C	55	VAL	5.4
1	A	37	ARG	5.3
1	B	22	ALA	5.3
1	C	45	HIS	5.3
1	E	69	VAL	5.2
1	B	25	GLY	5.2
1	D	36	GLN	5.2
1	D	73	PHE	5.2
1	D	76	PHE	5.2
1	B	67	LEU	5.2
1	E	8	THR	5.1
1	F	74	GLU	5.1
1	E	25	GLY	5.1
1	F	86	VAL	5.0
1	A	107	GLY	5.0
1	F	26	LEU	5.0
1	B	3	PRO	5.0
1	F	78	PHE	4.9
1	E	109	ALA	4.9
1	F	21	VAL	4.9
1	E	48	ASN	4.9
1	D	13	LEU	4.8
1	E	63	ALA	4.8
1	D	30	THR	4.8
1	E	85	THR	4.8
1	B	65	THR	4.8
1	C	69	VAL	4.8
1	C	107	GLY	4.8

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Mol	Chain	Res	Type	RSRZ
1	E	80	GLY	4.8
1	B	17	THR	4.7
1	B	61	GLY	4.7
1	F	20	LYS	4.7
1	C	33	TRP	4.7
1	D	16	GLY	4.7
1	E	96	GLY	4.7
1	E	50	ALA	4.6
1	B	87	ASP	4.6
1	E	12	GLY	4.6
1	C	78	PHE	4.6
1	F	80	GLY	4.6
1	B	72	SER	4.6
1	C	64	SER	4.6
1	C	38	ALA	4.5
1	B	55	VAL	4.5
1	A	14	SER	4.4
1	C	97	LEU	4.4
1	C	46	ALA	4.4
1	E	95	VAL	4.4
1	B	75	GLY	4.4
1	B	95	VAL	4.4
1	A	93	CYS	4.3
1	C	35	TYR	4.3
1	D	107	GLY	4.3
1	B	105	PRO	4.2
1	F	97	LEU	4.2
1	B	45	HIS	4.2
1	C	37	ARG	4.2
1	A	86	VAL	4.2
1	C	42	THR	4.1
1	C	30	THR	4.1
1	D	62	SER	4.1
1	F	64	SER	4.0
1	B	108	VAL	4.0
1	B	96	GLY	4.0
1	C	19	VAL	4.0
1	D	53	SER	3.9
1	F	30	THR	3.9
1	A	24	ALA	3.8
1	E	102	GLY	3.8
1	A	22	ALA	3.8

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Mol	Chain	Res	Type	RSRZ
1	A	94	GLN	3.8
1	D	50	ALA	3.8
1	D	5	ALA	3.8
1	D	59	ALA	3.7
1	A	40	VAL	3.7
1	D	88	CYS	3.7
1	E	101	ALA	3.7
1	B	38	ALA	3.7
1	A	58	ASP	3.6
1	E	31	ALA	3.6
1	B	77	LEU	3.6
1	D	91	ALA	3.6
1	C	24	ALA	3.5
1	D	69	VAL	3.5
1	C	98	SER	3.5
1	E	94	GLN	3.5
1	B	68	THR	3.4
1	A	65	THR	3.4
1	A	85	THR	3.4
1	C	14	SER	3.4
1	E	22	ALA	3.3
1	C	25	GLY	3.3
1	E	87	ASP	3.3
1	F	44	VAL	3.2
1	B	21	VAL	3.2
1	C	105	PRO	3.2
1	F	106	GLU	3.2
1	E	41	ASP	3.2
1	E	79	ASP	3.2
1	F	61	GLY	3.2
1	D	79	ASP	3.1
1	B	8	THR	3.1
1	D	31	ALA	3.0
1	D	18	VAL	3.0
1	E	3	PRO	3.0
1	C	22	ALA	2.9
1	E	93	CYS	2.9
1	B	41	ASP	2.9
1	D	104	GLY	2.9
1	D	57	ALA	2.9
1	F	53	SER	2.9
1	D	44	VAL	2.9

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Mol	Chain	Res	Type	RSRZ
1	C	93	CYS	2.9
1	E	30	THR	2.9
1	E	81	THR	2.8
1	D	43	GLY	2.8
1	D	99	ASP	2.8
1	A	4	THR	2.8
1	E	53	SER	2.8
1	C	67	LEU	2.8
1	C	16	GLY	2.8
1	F	22	ALA	2.7
1	D	66	SER	2.7
1	D	7	VAL	2.7
1	B	10	SER	2.7
1	B	40	VAL	2.6
1	D	26	LEU	2.6
1	A	26	LEU	2.6
1	A	76	PHE	2.6
1	B	24	ALA	2.5
1	B	2	ALA	2.5
1	A	34	VAL	2.5
1	B	98	SER	2.5
1	A	16	GLY	2.5
1	D	45	HIS	2.5
1	E	75	GLY	2.5
1	B	30	THR	2.5
1	E	11	SER	2.4
1	B	54	SER	2.4
1	A	75	GLY	2.4
1	D	85	THR	2.4
1	A	87	ASP	2.3
1	D	82	ARG	2.3
1	E	107	GLY	2.3
1	A	25	GLY	2.2
1	B	27	GLN	2.2
1	E	64	SER	2.2
1	C	41	ASP	2.2
1	D	11	SER	2.2
1	C	79	ASP	2.1
1	A	102	GLY	2.1
1	D	110	ILE	2.1
1	F	56	THR	2.1
1	F	75	GLY	2.0

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

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

## 6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
2	SO4	C	1114	5/5	-0.44	2.38	3.86	53,53,53,54	0
3	TH2	A	1115	28/28	-0.32	1.25	0.12	58,62,84,85	0
3	TH2	F	1114	28/28	0.03	1.10	0.05	24,31,53,54	0
3	TH2	C	1115	28/28	0.01	0.95	-0.08	24,29,53,53	0
3	TH2	A	1114	28/28	0.04	0.78	-0.13	27,32,58,61	0
3	TH2	B	1116	28/28	0.09	0.86	-0.14	12,16,45,46	0
3	TH2	E	1115	28/28	-0.00	0.76	-0.48	29,34,51,52	0
3	TH2	B	1117	28/28	-0.14	0.75	-0.55	28,36,53,54	0
3	TH2	D	1114	28/28	0.34	0.45	-0.89	22,34,57,59	0
2	SO4	B	1115	5/5	0.21	0.28	-	41,41,42,44	0
2	SO4	A	1113	5/5	0.41	0.77	-	77,77,78,78	0
2	SO4	E	1114	5/5	-0.09	1.33	-	76,76,77,77	0
2	SO4	F	1113	5/5	-0.32	3.10	-	65,65,65,66	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.