



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 14, 2017 – 04:01 pm GMT

PDB ID : 4ALL  
Title : Crystal structure of S. aureus FabI in complex with NADP and triclosan (P212121)  
Authors : Schiebel, J.; Chang, A.; Tonge, P.J.; Kisker, C.  
Deposited on : 2012-03-04  
Resolution : 2.80 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

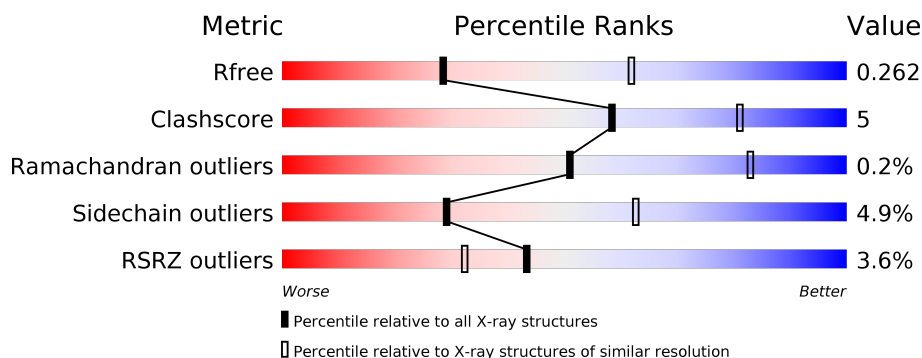
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.80 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	2583 (2.80-2.80)
Clashscore	112137	3033 (2.80-2.80)
Ramachandran outliers	110173	2983 (2.80-2.80)
Sidechain outliers	110143	2985 (2.80-2.80)
RSRZ outliers	101464	2610 (2.80-2.80)

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	277	<div> <div>4%</div> <div> <div></div> <div>76%</div> <div>15%</div> <div>8%</div> </div> </div>
1	B	277	<div> <div>2%</div> <div> <div></div> <div>77%</div> <div>14%</div> <div>8%</div> </div> </div>
1	C	277	<div> <div>4%</div> <div> <div></div> <div>79%</div> <div>12%</div> <div>8%</div> </div> </div>
1	D	277	<div> <div>4%</div> <div> <div></div> <div>77%</div> <div>14%</div> <div>8%</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 crite-

ria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	TCL	A	1257	-	-	X	-

## 2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 8101 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 ENOYL-[ACYL-CARRIER-PROTEIN] REDUCTASE [NADPH].

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	256	Total	C	N	O	S	0	0	0
			1970	1243	340	382	5			
1	B	254	Total	C	N	O	S	0	0	0
			1954	1232	338	380	4			
1	C	254	Total	C	N	O	S	0	0	0
			1954	1232	338	380	4			
1	D	254	Total	C	N	O	S	0	0	0
			1954	1232	338	380	4			

There are 84 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-20	MET	-	EXPRESSION TAG	UNP Q7A6D8
A	-19	GLY	-	EXPRESSION TAG	UNP Q7A6D8
A	-18	HIS	-	EXPRESSION TAG	UNP Q7A6D8
A	-17	HIS	-	EXPRESSION TAG	UNP Q7A6D8
A	-16	HIS	-	EXPRESSION TAG	UNP Q7A6D8
A	-15	HIS	-	EXPRESSION TAG	UNP Q7A6D8
A	-14	HIS	-	EXPRESSION TAG	UNP Q7A6D8
A	-13	HIS	-	EXPRESSION TAG	UNP Q7A6D8
A	-12	HIS	-	EXPRESSION TAG	UNP Q7A6D8
A	-11	HIS	-	EXPRESSION TAG	UNP Q7A6D8
A	-10	HIS	-	EXPRESSION TAG	UNP Q7A6D8
A	-9	HIS	-	EXPRESSION TAG	UNP Q7A6D8
A	-8	SER	-	EXPRESSION TAG	UNP Q7A6D8
A	-7	SER	-	EXPRESSION TAG	UNP Q7A6D8
A	-6	GLY	-	EXPRESSION TAG	UNP Q7A6D8
A	-5	HIS	-	EXPRESSION TAG	UNP Q7A6D8
A	-4	ILE	-	EXPRESSION TAG	UNP Q7A6D8
A	-3	GLU	-	EXPRESSION TAG	UNP Q7A6D8
A	-2	GLY	-	EXPRESSION TAG	UNP Q7A6D8
A	-1	ARG	-	EXPRESSION TAG	UNP Q7A6D8

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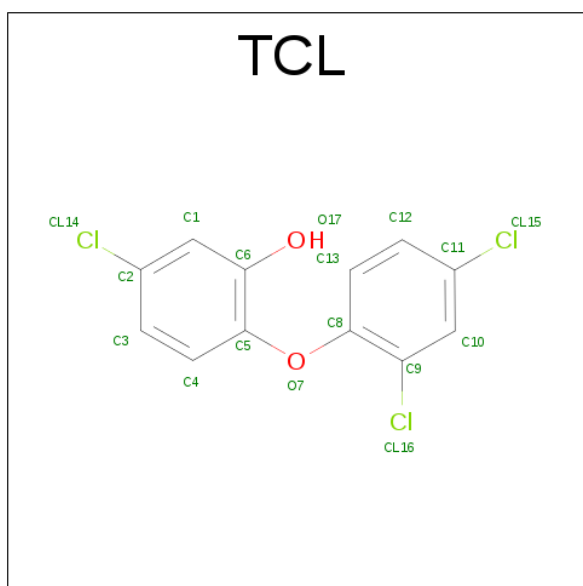
Chain	Residue	Modelled	Actual	Comment	Reference
A	0	HIS	-	EXPRESSION TAG	UNP Q7A6D8
B	-20	MET	-	EXPRESSION TAG	UNP Q7A6D8
B	-19	GLY	-	EXPRESSION TAG	UNP Q7A6D8
B	-18	HIS	-	EXPRESSION TAG	UNP Q7A6D8
B	-17	HIS	-	EXPRESSION TAG	UNP Q7A6D8
B	-16	HIS	-	EXPRESSION TAG	UNP Q7A6D8
B	-15	HIS	-	EXPRESSION TAG	UNP Q7A6D8
B	-14	HIS	-	EXPRESSION TAG	UNP Q7A6D8
B	-13	HIS	-	EXPRESSION TAG	UNP Q7A6D8
B	-12	HIS	-	EXPRESSION TAG	UNP Q7A6D8
B	-11	HIS	-	EXPRESSION TAG	UNP Q7A6D8
B	-10	HIS	-	EXPRESSION TAG	UNP Q7A6D8
B	-9	HIS	-	EXPRESSION TAG	UNP Q7A6D8
B	-8	SER	-	EXPRESSION TAG	UNP Q7A6D8
B	-7	SER	-	EXPRESSION TAG	UNP Q7A6D8
B	-6	GLY	-	EXPRESSION TAG	UNP Q7A6D8
B	-5	HIS	-	EXPRESSION TAG	UNP Q7A6D8
B	-4	ILE	-	EXPRESSION TAG	UNP Q7A6D8
B	-3	GLU	-	EXPRESSION TAG	UNP Q7A6D8
B	-2	GLY	-	EXPRESSION TAG	UNP Q7A6D8
B	-1	ARG	-	EXPRESSION TAG	UNP Q7A6D8
B	0	HIS	-	EXPRESSION TAG	UNP Q7A6D8
C	-20	MET	-	EXPRESSION TAG	UNP Q7A6D8
C	-19	GLY	-	EXPRESSION TAG	UNP Q7A6D8
C	-18	HIS	-	EXPRESSION TAG	UNP Q7A6D8
C	-17	HIS	-	EXPRESSION TAG	UNP Q7A6D8
C	-16	HIS	-	EXPRESSION TAG	UNP Q7A6D8
C	-15	HIS	-	EXPRESSION TAG	UNP Q7A6D8
C	-14	HIS	-	EXPRESSION TAG	UNP Q7A6D8
C	-13	HIS	-	EXPRESSION TAG	UNP Q7A6D8
C	-12	HIS	-	EXPRESSION TAG	UNP Q7A6D8
C	-11	HIS	-	EXPRESSION TAG	UNP Q7A6D8
C	-10	HIS	-	EXPRESSION TAG	UNP Q7A6D8
C	-9	HIS	-	EXPRESSION TAG	UNP Q7A6D8
C	-8	SER	-	EXPRESSION TAG	UNP Q7A6D8
C	-7	SER	-	EXPRESSION TAG	UNP Q7A6D8
C	-6	GLY	-	EXPRESSION TAG	UNP Q7A6D8
C	-5	HIS	-	EXPRESSION TAG	UNP Q7A6D8
C	-4	ILE	-	EXPRESSION TAG	UNP Q7A6D8
C	-3	GLU	-	EXPRESSION TAG	UNP Q7A6D8
C	-2	GLY	-	EXPRESSION TAG	UNP Q7A6D8
C	-1	ARG	-	EXPRESSION TAG	UNP Q7A6D8

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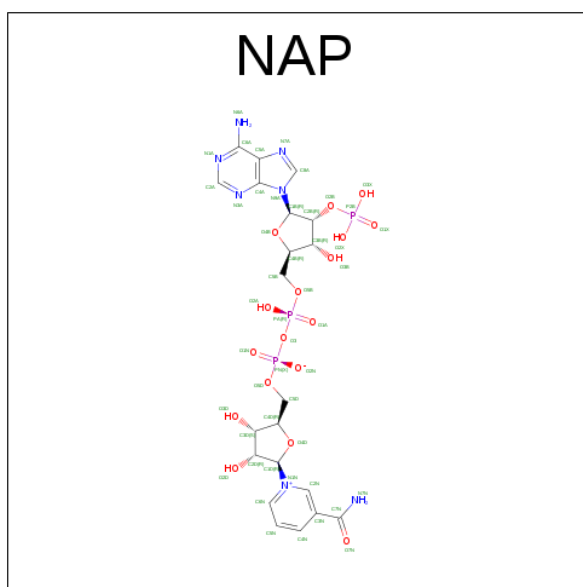
Chain	Residue	Modelled	Actual	Comment	Reference
C	0	HIS	-	EXPRESSION TAG	UNP Q7A6D8
D	-20	MET	-	EXPRESSION TAG	UNP Q7A6D8
D	-19	GLY	-	EXPRESSION TAG	UNP Q7A6D8
D	-18	HIS	-	EXPRESSION TAG	UNP Q7A6D8
D	-17	HIS	-	EXPRESSION TAG	UNP Q7A6D8
D	-16	HIS	-	EXPRESSION TAG	UNP Q7A6D8
D	-15	HIS	-	EXPRESSION TAG	UNP Q7A6D8
D	-14	HIS	-	EXPRESSION TAG	UNP Q7A6D8
D	-13	HIS	-	EXPRESSION TAG	UNP Q7A6D8
D	-12	HIS	-	EXPRESSION TAG	UNP Q7A6D8
D	-11	HIS	-	EXPRESSION TAG	UNP Q7A6D8
D	-10	HIS	-	EXPRESSION TAG	UNP Q7A6D8
D	-9	HIS	-	EXPRESSION TAG	UNP Q7A6D8
D	-8	SER	-	EXPRESSION TAG	UNP Q7A6D8
D	-7	SER	-	EXPRESSION TAG	UNP Q7A6D8
D	-6	GLY	-	EXPRESSION TAG	UNP Q7A6D8
D	-5	HIS	-	EXPRESSION TAG	UNP Q7A6D8
D	-4	ILE	-	EXPRESSION TAG	UNP Q7A6D8
D	-3	GLU	-	EXPRESSION TAG	UNP Q7A6D8
D	-2	GLY	-	EXPRESSION TAG	UNP Q7A6D8
D	-1	ARG	-	EXPRESSION TAG	UNP Q7A6D8
D	0	HIS	-	EXPRESSION TAG	UNP Q7A6D8

- Molecule 2 is TRICLOSAN (three-letter code: TCL) (formula:  $C_{12}H_7Cl_3O_2$ ).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	Cl	O	0	0
			17	12	3	2		
2	B	1	Total	C	Cl	O	0	0
			17	12	3	2		
2	C	1	Total	C	Cl	O	0	0
			17	12	3	2		
2	D	1	Total	C	Cl	O	0	0
			17	12	3	2		

- Molecule 3 is NADP NICOTINAMIDE-ADENINE-DINUCLEOTIDE PHOSPHATE (three-letter code: NAP) (formula:  $C_{21}H_{28}N_7O_{17}P_3$ ).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	N	O	P	0
			48	21	7	17	3	0
3	B	1	Total	C	N	O	P	0
			48	21	7	17	3	0
3	C	1	Total	C	N	O	P	0
			48	21	7	17	3	0
3	D	1	Total	C	N	O	P	0
			48	21	7	17	3	0

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	4	Total	O	0	0
			4	4		

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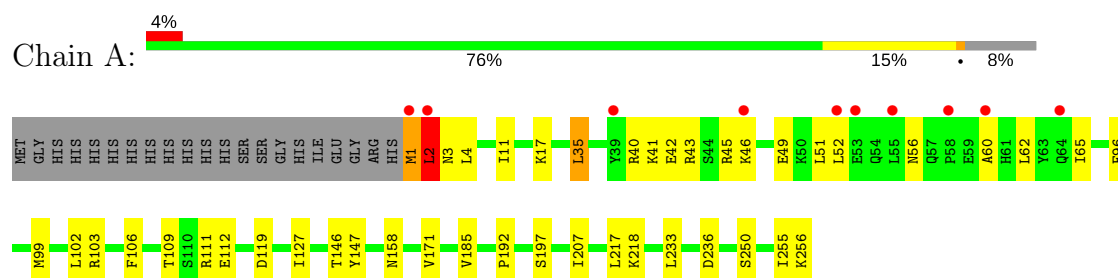
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	B	3	Total 3	O 3	0	0
4	C	1	Total 1	O 1	0	0
4	D	1	Total 1	O 1	0	0



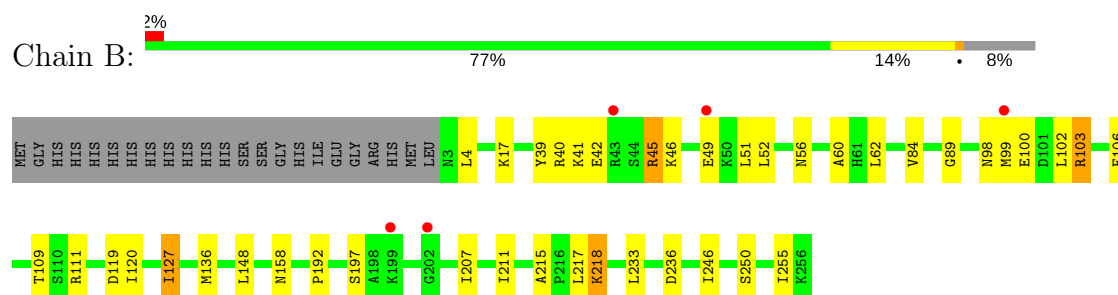
### 3 Residue-property plots [i](#)

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.

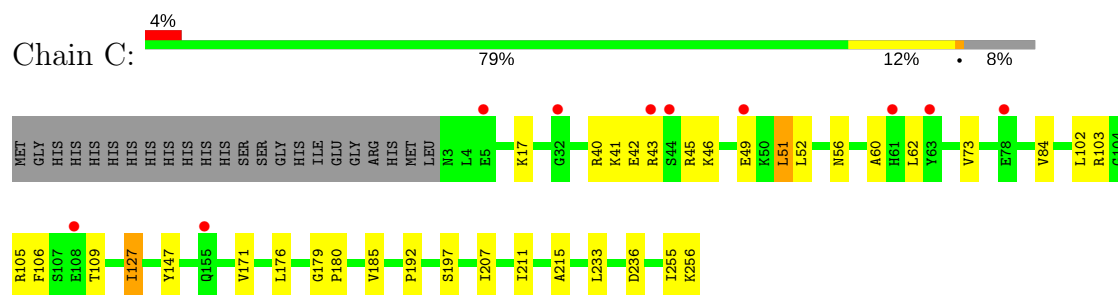
#### • Molecule 1: ENOYL-[ACYL-CARRIER-PROTEIN] REDUCTASE [NADPH]



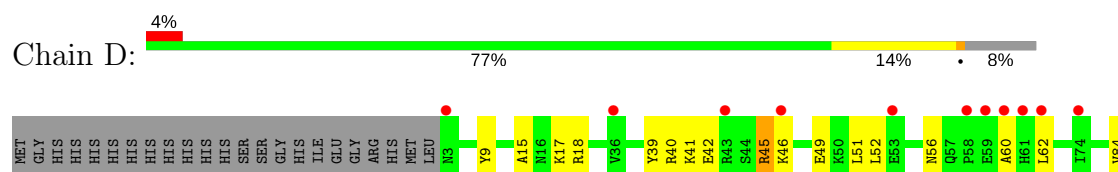
#### • Molecule 1: ENOYL-[ACYL-CARRIER-PROTEIN] REDUCTASE [NADPH]

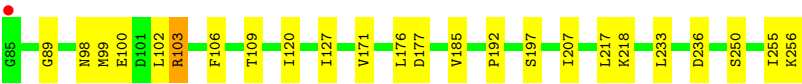


#### • Molecule 1: ENOYL-[ACYL-CARRIER-PROTEIN] REDUCTASE [NADPH]



#### • Molecule 1: ENOYL-[ACYL-CARRIER-PROTEIN] REDUCTASE [NADPH]





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	83.52Å 111.91Å 111.64Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	79.04 – 2.80 42.91 – 2.80	Depositor EDS
% Data completeness (in resolution range)	85.9 (79.04-2.80) 85.9 (42.91-2.80)	Depositor EDS
$R_{merge}$	0.15	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.37 (at 2.81Å)	Xtriage
Refinement program	REFMAC 5.5.0109	Depositor
R, $R_{free}$	0.214 , 0.262 0.213 , 0.262	Depositor DCC
$R_{free}$ test set	1146 reflections (5.32%)	DCC
Wilson B-factor (Å <sup>2</sup> )	54.4	Xtriage
Anisotropy	1.032	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.31 , 54.8	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.47$ , $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	0.028 for -h,l,k	Xtriage
$F_o, F_c$ correlation	0.93	EDS
Total number of atoms	8101	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	66.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.38% 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: NAP, TCL

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	0.64	0/1997	0.96	10/2692 (0.4%)
1	B	0.62	0/1981	0.85	7/2671 (0.3%)
1	C	0.61	0/1981	0.83	8/2671 (0.3%)
1	D	0.60	0/1981	0.84	6/2671 (0.2%)
All	All	0.62	0/7940	0.87	31/10705 (0.3%)

There are no bond length outliers.

All (31) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	43	ARG	NE-CZ-NH2	-15.30	112.65	120.30
1	A	43	ARG	NE-CZ-NH1	13.49	127.05	120.30
1	D	45	ARG	NE-CZ-NH1	11.22	125.91	120.30
1	D	45	ARG	NE-CZ-NH2	-11.05	114.78	120.30
1	C	45	ARG	NE-CZ-NH1	10.96	125.78	120.30
1	B	45	ARG	NE-CZ-NH1	10.84	125.72	120.30
1	B	45	ARG	NE-CZ-NH2	-10.45	115.08	120.30
1	D	103	ARG	NE-CZ-NH1	10.39	125.50	120.30
1	B	103	ARG	NE-CZ-NH2	-10.16	115.22	120.30
1	B	103	ARG	NE-CZ-NH1	10.15	125.38	120.30
1	D	103	ARG	NE-CZ-NH2	-10.09	115.25	120.30
1	C	103	ARG	NE-CZ-NH2	-9.85	115.38	120.30
1	C	45	ARG	NE-CZ-NH2	-9.82	115.39	120.30
1	A	45	ARG	NE-CZ-NH2	-9.71	115.44	120.30
1	A	45	ARG	NE-CZ-NH1	9.62	125.11	120.30
1	C	103	ARG	NE-CZ-NH1	9.31	124.95	120.30
1	A	103	ARG	NE-CZ-NH1	8.52	124.56	120.30
1	A	103	ARG	NE-CZ-NH2	-8.16	116.22	120.30
1	A	43	ARG	CD-NE-CZ	7.14	133.59	123.60
1	A	2	LEU	CA-CB-CG	6.73	130.77	115.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	45	ARG	CD-NE-CZ	6.05	132.07	123.60
1	C	43	ARG	NE-CZ-NH1	5.95	123.27	120.30
1	C	45	ARG	CD-NE-CZ	5.90	131.86	123.60
1	D	45	ARG	CD-NE-CZ	5.88	131.84	123.60
1	B	45	ARG	CD-NE-CZ	5.80	131.72	123.60
1	C	43	ARG	NE-CZ-NH2	-5.51	117.55	120.30
1	B	103	ARG	CD-NE-CZ	5.30	131.01	123.60
1	B	148	LEU	CA-CB-CG	5.28	127.43	115.30
1	C	103	ARG	CD-NE-CZ	5.12	130.77	123.60
1	A	103	ARG	CD-NE-CZ	5.12	130.77	123.60
1	D	103	ARG	CD-NE-CZ	5.08	130.72	123.60

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	1970	0	1991	27	1
1	B	1954	0	1968	24	0
1	C	1954	0	1968	21	0
1	D	1954	0	1968	19	1
2	A	17	0	7	6	0
2	B	17	0	7	4	0
2	C	17	0	6	2	0
2	D	17	0	7	3	0
3	A	48	0	25	8	0
3	B	48	0	25	1	0
3	C	48	0	25	5	0
3	D	48	0	25	2	0
4	A	4	0	0	1	0
4	B	3	0	0	0	0
4	C	1	0	0	0	0
4	D	1	0	0	0	0
All	All	8101	0	8022	88	1

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 5.

All (88) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:106:PHE:O	1:A:109:THR:HG23	1.81	0.81
1:A:40:ARG:HB3	3:A:1258:NAP:O2X	1.84	0.78
1:D:106:PHE:O	1:D:109:THR:HG23	1.86	0.76
1:C:17:LYS:HB3	1:C:51:LEU:HD11	1.72	0.70
1:A:17:LYS:HB3	1:A:51:LEU:HD21	1.74	0.68
1:B:106:PHE:O	1:B:109:THR:HG23	1.95	0.67
1:A:102:LEU:O	4:A:2001:HOH:O	2.15	0.63
1:C:171:VAL:HG13	1:C:185:VAL:HG12	1.79	0.63
1:C:106:PHE:O	1:C:109:THR:HG23	1.99	0.63
1:A:60:ALA:HB1	1:A:62:LEU:CD2	2.29	0.61
1:B:39:TYR:OH	1:B:45:ARG:HD2	2.01	0.61
1:D:217:LEU:HD12	1:D:250:SER:HA	1.81	0.61
1:D:39:TYR:OH	1:D:45:ARG:HD2	2.00	0.61
1:D:40:ARG:HG2	1:D:41:LYS:HG2	1.82	0.61
1:B:255:ILE:O	1:D:256:LYS:HE3	2.01	0.60
1:B:17:LYS:HB3	1:B:51:LEU:HD21	1.83	0.60
1:B:120:ILE:HD13	3:B:1257:NAP:H61A	1.66	0.60
1:A:2:LEU:HD12	1:A:3:ASN:H	1.68	0.58
1:C:60:ALA:HB1	1:C:62:LEU:CD2	2.33	0.58
2:A:1257:TCL:O7	3:A:1258:NAP:H2D	2.04	0.58
1:A:1:MET:N	1:A:2:LEU:O	2.28	0.58
1:B:197:SER:CB	2:B:1258:TCL:CL16	2.90	0.57
1:D:17:LYS:HB3	1:D:51:LEU:HD21	1.87	0.57
1:B:197:SER:HB3	2:B:1258:TCL:C9	2.35	0.57
1:D:15:ALA:HB2	3:D:1258:NAP:H3B	1.88	0.55
1:C:197:SER:HB3	2:C:1258:TCL:C9	2.36	0.55
1:A:217:LEU:HD12	1:A:250:SER:HA	1.89	0.55
1:A:192:PRO:HG3	1:A:207:ILE:HG22	1.89	0.55
1:A:65:ILE:O	3:A:1258:NAP:H2A	2.08	0.54
1:B:60:ALA:HB1	1:B:62:LEU:CD2	2.38	0.54
1:D:120:ILE:HD13	3:D:1258:NAP:H61A	1.72	0.54
1:A:256:LYS:HE3	1:C:255:ILE:O	2.08	0.53
1:C:192:PRO:HG3	1:C:207:ILE:HG22	1.91	0.53
1:C:40:ARG:HG2	1:C:41:LYS:HG2	1.90	0.53
1:D:60:ALA:HB1	1:D:62:LEU:CD2	2.38	0.53
1:A:197:SER:HB3	2:A:1257:TCL:C9	2.39	0.53
1:A:11:ILE:HD12	1:A:35:LEU:HG	1.91	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:111:ARG:NH1	1:B:119:ASP:OD1	2.43	0.52
1:B:192:PRO:HG3	1:B:207:ILE:HG22	1.92	0.52
1:B:211:ILE:O	1:B:215:ALA:HB3	2.11	0.51
1:C:147:TYR:HB2	3:C:1257:NAP:C5N	2.41	0.51
1:D:192:PRO:HG3	1:D:207:ILE:HG22	1.91	0.51
1:C:46:LYS:HA	1:C:49:GLU:HG3	1.93	0.50
2:A:1257:TCL:CL16	3:A:1258:NAP:H3D	2.47	0.50
1:A:46:LYS:HA	1:A:49:GLU:HG3	1.94	0.50
1:B:217:LEU:HD12	1:B:250:SER:HA	1.93	0.50
1:A:255:ILE:O	1:C:256:LYS:HE3	2.12	0.49
1:B:46:LYS:HA	1:B:49:GLU:HG3	1.94	0.49
1:A:60:ALA:HB1	1:A:62:LEU:HD21	1.93	0.49
1:D:98:ASN:HB3	1:D:100:GLU:OE1	2.13	0.49
2:A:1257:TCL:C3	3:A:1258:NAP:C7N	2.91	0.49
1:B:40:ARG:HG2	1:B:41:LYS:HG2	1.94	0.48
1:A:171:VAL:HG13	1:A:185:VAL:HG12	1.96	0.48
1:C:211:ILE:O	1:C:215:ALA:HB3	2.13	0.48
1:A:40:ARG:HG2	1:A:41:LYS:HG2	1.95	0.47
1:D:102:LEU:HD11	2:D:1257:TCL:CL15	2.51	0.47
1:C:105:ARG:HD2	1:D:177:ASP:OD1	2.13	0.47
1:D:197:SER:HB3	2:D:1257:TCL:C9	2.44	0.47
1:A:146:THR:OG1	1:A:147:TYR:N	2.45	0.47
1:C:60:ALA:HB1	1:C:62:LEU:HD21	1.96	0.47
1:A:2:LEU:HD12	1:A:3:ASN:N	2.30	0.47
1:C:179:GLY:N	1:C:180:PRO:CD	2.78	0.46
1:D:46:LYS:HA	1:D:49:GLU:HG3	1.97	0.46
2:A:1257:TCL:C6	2:A:1257:TCL:H131	2.45	0.46
1:B:197:SER:HB3	2:B:1258:TCL:CL16	2.53	0.46
1:C:192:PRO:HA	3:C:1257:NAP:O7N	2.16	0.46
1:B:255:ILE:HG21	1:C:176:LEU:HD13	1.98	0.45
1:B:89:GLY:HA2	1:B:136:MET:HE1	1.98	0.45
1:C:147:TYR:HB2	3:C:1257:NAP:H5N	1.97	0.45
1:A:119:ASP:OD1	1:B:111:ARG:NH1	2.45	0.45
1:A:147:TYR:HB2	3:A:1258:NAP:C5N	2.47	0.45
1:B:233:LEU:HD21	1:B:246:ILE:HD12	1.99	0.45
1:A:192:PRO:HA	3:A:1258:NAP:O7N	2.18	0.44
1:B:127:ILE:HG13	1:B:127:ILE:H	1.63	0.44
1:A:1:MET:CE	1:A:1:MET:H1	2.30	0.44
3:C:1257:NAP:C7N	2:C:1258:TCL:C3	2.96	0.44
1:C:40:ARG:HD3	3:C:1257:NAP:C6A	2.49	0.43
1:D:255:ILE:C	1:D:255:ILE:HD12	2.39	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:171:VAL:HG13	1:D:185:VAL:HG12	2.00	0.42
1:B:218:LYS:HD3	1:C:180:PRO:HG3	2.01	0.42
1:B:98:ASN:HB3	1:B:100:GLU:OE1	2.20	0.42
1:C:73:VAL:HG21	1:C:127:ILE:HD13	2.02	0.42
1:D:102:LEU:CD1	2:D:1257:TCL:CL15	3.06	0.41
1:A:147:TYR:HB2	3:A:1258:NAP:H5N	2.02	0.41
1:B:102:LEU:HD11	2:B:1258:TCL:CL15	2.58	0.41
1:A:96:PHE:HA	2:A:1257:TCL:CL15	2.58	0.40
1:B:106:PHE:HD1	1:B:158:ASN:HB3	1.86	0.40
1:D:9:TYR:HD1	1:D:89:GLY:HA3	1.87	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:112:GLU:OE2	1:D:18:ARG:NH2[3_554]	2.00	0.20

## 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	254/277 (92%)	238 (94%)	14 (6%)	2 (1%)	22	55
1	B	252/277 (91%)	240 (95%)	12 (5%)	0	100	100
1	C	252/277 (91%)	238 (94%)	14 (6%)	0	100	100
1	D	252/277 (91%)	239 (95%)	13 (5%)	0	100	100
All	All	1010/1108 (91%)	955 (95%)	53 (5%)	2 (0%)	51	83

All (2) Ramachandran outliers are listed below:



Mol	Chain	Res	Type
1	A	2	LEU
1	A	158	ASN

### 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	210/228 (92%)	199 (95%)	11 (5%)	27	60
1	B	208/228 (91%)	198 (95%)	10 (5%)	30	63
1	C	208/228 (91%)	199 (96%)	9 (4%)	33	67
1	D	208/228 (91%)	197 (95%)	11 (5%)	26	59
All	All	834/912 (91%)	793 (95%)	41 (5%)	29	62

All (41) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1	MET
1	A	4	LEU
1	A	35	LEU
1	A	42	GLU
1	A	52	LEU
1	A	56	ASN
1	A	99	MET
1	A	127	ILE
1	A	218	LYS
1	A	233	LEU
1	A	236	ASP
1	B	4	LEU
1	B	42	GLU
1	B	52	LEU
1	B	56	ASN
1	B	84	VAL
1	B	99	MET
1	B	103	ARG
1	B	127	ILE
1	B	218	LYS

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Mol	Chain	Res	Type
1	B	236	ASP
1	C	42	GLU
1	C	51	LEU
1	C	52	LEU
1	C	56	ASN
1	C	84	VAL
1	C	102	LEU
1	C	127	ILE
1	C	233	LEU
1	C	236	ASP
1	D	42	GLU
1	D	52	LEU
1	D	56	ASN
1	D	84	VAL
1	D	99	MET
1	D	103	ARG
1	D	127	ILE
1	D	176	LEU
1	D	218	LYS
1	D	233	LEU
1	D	236	ASP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	155	GLN
1	C	155	GLN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

## 5.6 Ligand geometry

8 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	TCL	A	1257	-	18,18,18	1.95	4 (22%)	25,25,25	0.75	0
3	NAP	A	1258	-	44,52,52	1.79	4 (9%)	51,80,80	2.09	6 (11%)
3	NAP	B	1257	-	44,52,52	1.55	3 (6%)	51,80,80	1.93	6 (11%)
2	TCL	B	1258	-	18,18,18	2.00	7 (38%)	25,25,25	0.73	0
3	NAP	C	1257	-	44,52,52	1.60	3 (6%)	51,80,80	2.11	5 (9%)
2	TCL	C	1258	-	18,18,18	1.81	7 (38%)	25,25,25	0.74	0
2	TCL	D	1257	-	18,18,18	2.08	5 (27%)	25,25,25	0.75	0
3	NAP	D	1258	-	44,52,52	1.75	5 (11%)	51,80,80	2.18	11 (21%)

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	TCL	A	1257	-	-	0/4/4/4	0/2/2/2
3	NAP	A	1258	-	-	0/27/67/67	0/5/5/5
3	NAP	B	1257	-	-	0/27/67/67	0/5/5/5
2	TCL	B	1258	-	-	0/4/4/4	0/2/2/2
3	NAP	C	1257	-	-	0/27/67/67	0/5/5/5
2	TCL	C	1258	-	-	0/4/4/4	0/2/2/2
2	TCL	D	1257	-	-	0/4/4/4	0/2/2/2
3	NAP	D	1258	-	-	0/27/67/67	0/5/5/5

All (38) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	D	1258	NAP	C3N-C7N	-2.61	1.46	1.50
2	C	1258	TCL	O7-C5	-2.46	1.34	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	1258	TCL	C10-C11	2.02	1.41	1.38
2	C	1258	TCL	C2-CL14	2.02	1.78	1.74
2	A	1257	TCL	C9-CL16	2.11	1.78	1.73
3	D	1258	NAP	P2B-O2B	2.25	1.63	1.59
2	B	1258	TCL	C3-C2	2.31	1.42	1.38
2	A	1257	TCL	C12-C11	2.33	1.42	1.38
2	C	1258	TCL	C12-C11	2.37	1.42	1.38
2	B	1258	TCL	C11-CL15	2.38	1.79	1.74
2	D	1257	TCL	C12-C11	2.38	1.42	1.38
2	C	1258	TCL	C9-CL16	2.41	1.79	1.73
3	B	1257	NAP	C2A-N1A	2.44	1.38	1.33
2	D	1257	TCL	C3-C2	2.45	1.42	1.38
2	B	1258	TCL	C12-C11	2.46	1.42	1.38
3	A	1258	NAP	P2B-O2B	2.60	1.64	1.59
2	C	1258	TCL	C11-CL15	2.68	1.80	1.74
2	D	1257	TCL	C9-CL16	2.80	1.80	1.73
3	C	1257	NAP	C2A-N1A	2.82	1.39	1.33
3	B	1257	NAP	C2A-N3A	2.88	1.37	1.32
2	C	1258	TCL	C6-C5	2.92	1.44	1.40
3	A	1258	NAP	C2A-N1A	2.97	1.39	1.33
3	D	1258	NAP	C2A-N1A	3.04	1.39	1.33
2	C	1258	TCL	C8-C9	3.06	1.45	1.39
2	B	1258	TCL	C9-CL16	3.17	1.81	1.73
2	B	1258	TCL	C8-C9	3.24	1.45	1.39
3	C	1257	NAP	C2A-N3A	3.46	1.37	1.32
3	D	1258	NAP	C2A-N3A	3.48	1.38	1.32
2	A	1257	TCL	C8-C9	3.90	1.46	1.39
2	D	1257	TCL	C8-C9	3.90	1.46	1.39
2	B	1258	TCL	C6-C5	4.05	1.46	1.40
3	A	1258	NAP	C2A-N3A	4.25	1.39	1.32
2	A	1257	TCL	C6-C5	4.26	1.46	1.40
2	D	1257	TCL	C6-C5	4.44	1.47	1.40
3	B	1257	NAP	O7N-C7N	7.85	1.40	1.24
3	A	1258	NAP	O7N-C7N	8.17	1.41	1.24
3	C	1257	NAP	O7N-C7N	8.34	1.41	1.24
3	D	1258	NAP	O7N-C7N	8.84	1.42	1.24

All (28) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	1258	NAP	N3A-C2A-N1A	-11.78	118.60	128.86
3	B	1257	NAP	N3A-C2A-N1A	-10.86	119.40	128.86

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	1257	NAP	N3A-C2A-N1A	-10.80	119.45	128.86
3	D	1258	NAP	N3A-C2A-N1A	-10.35	119.85	128.86
3	C	1257	NAP	C4B-O4B-C1B	-6.56	102.79	109.77
3	D	1258	NAP	O7N-C7N-C3N	-4.65	114.19	119.62
3	A	1258	NAP	O4B-C1B-C2B	-4.51	98.69	106.59
3	B	1257	NAP	C1B-N9A-C4A	-4.43	118.98	126.64
3	B	1257	NAP	C4B-O4B-C1B	-3.61	105.93	109.77
3	D	1258	NAP	O4B-C1B-C2B	-3.45	100.55	106.59
3	C	1257	NAP	C3B-C2B-C1B	-3.44	96.03	102.75
3	C	1257	NAP	C1B-N9A-C4A	-3.34	120.86	126.64
3	D	1258	NAP	C1B-N9A-C4A	-3.06	121.35	126.64
3	D	1258	NAP	C4B-O4B-C1B	-2.93	106.66	109.77
3	A	1258	NAP	C5B-C4B-C3B	-2.84	104.46	115.29
3	D	1258	NAP	C3N-C2N-N1N	-2.71	117.70	120.43
3	B	1257	NAP	O7N-C7N-N7N	-2.47	119.07	122.58
3	D	1258	NAP	C4N-C3N-C7N	-2.35	114.82	121.07
3	A	1258	NAP	O2B-P2B-O1X	-2.21	100.59	109.26
3	D	1258	NAP	C5N-C4N-C3N	-2.14	117.83	120.35
3	D	1258	NAP	O2N-PN-O1N	2.03	122.81	112.28
3	A	1258	NAP	C3N-C7N-N7N	2.09	120.16	117.77
3	B	1257	NAP	C2A-N1A-C6A	2.11	122.46	118.77
3	B	1257	NAP	C3N-C7N-N7N	2.40	120.52	117.77
3	A	1258	NAP	O5D-C5D-C4D	2.82	119.01	109.00
3	C	1257	NAP	C3N-C7N-N7N	3.03	121.23	117.77
3	D	1258	NAP	O7N-C7N-N7N	3.98	128.25	122.58
3	D	1258	NAP	C2N-C3N-C4N	4.36	123.23	118.26

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

8 monomers are involved in 27 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	1257	TCL	6	0
3	A	1258	NAP	8	0
3	B	1257	NAP	1	0
2	B	1258	TCL	4	0
3	C	1257	NAP	5	0
2	C	1258	TCL	2	0
2	D	1257	TCL	3	0
3	D	1258	NAP	2	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	256/277 (92%)	0.10	10 (3%) 40 29	41, 64, 100, 121	0
1	B	254/277 (91%)	-0.02	5 (1%) 65 56	39, 62, 96, 120	0
1	C	254/277 (91%)	0.09	10 (3%) 40 29	40, 62, 95, 114	0
1	D	254/277 (91%)	0.23	12 (4%) 32 22	40, 62, 102, 113	0
All	All	1018/1108 (91%)	0.10	37 (3%) 43 32	39, 63, 99, 121	0

All (37) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	58	PRO	5.2
1	A	46	LYS	3.5
1	C	63	TYR	3.5
1	C	43	ARG	3.5
1	C	44	SER	3.5
1	B	202	GLY	3.3
1	D	43	ARG	3.2
1	A	60	ALA	3.2
1	D	60	ALA	3.1
1	D	74	ILE	3.0
1	A	55	LEU	2.9
1	A	58	PRO	2.8
1	C	5	GLU	2.8
1	D	36	VAL	2.8
1	D	3	ASN	2.7
1	D	85	GLY	2.7
1	C	108	GLU	2.6
1	B	43	ARG	2.5
1	D	61	HIS	2.5
1	A	53	GLU	2.5
1	D	59	GLU	2.5

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Mol	Chain	Res	Type	RSRZ
1	B	199	LYS	2.4
1	B	99	MET	2.4
1	D	46	LYS	2.4
1	B	49	GLU	2.3
1	D	53	GLU	2.3
1	C	61	HIS	2.2
1	D	62	LEU	2.2
1	A	64	GLN	2.2
1	A	1	MET	2.2
1	A	52	LEU	2.2
1	A	39	TYR	2.2
1	C	155	GLN	2.1
1	A	2	LEU	2.1
1	C	49	GLU	2.1
1	C	32	GLY	2.1
1	C	78	GLU	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	TCL	A	1257	17/17	0.90	0.23	0.60	49,54,72,72	0
2	TCL	B	1258	17/17	0.90	0.17	-0.30	80,81,85,87	0
2	TCL	C	1258	17/17	0.92	0.17	-0.36	60,66,71,78	0
2	TCL	D	1257	17/17	0.95	0.17	-0.62	42,45,60,63	0
3	NAP	C	1257	48/48	0.93	0.16	-0.66	57,64,81,83	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
3	NAP	B	1257	48/48	0.95	0.14	-0.87	51,56,72,74	0
3	NAP	A	1258	48/48	0.93	0.14	-0.95	33,46,56,60	0
3	NAP	D	1258	48/48	0.96	0.14	-1.12	30,49,58,60	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.