



Full wwPDB X-ray Structure Validation Report ⓘ

Jan 31, 2016 – 10:43 PM GMT

PDB ID : 1UPC
Title : CARBOXYETHYLARGININE SYNTHASE FROM STREPTOMYCES CLAVULIGERUS
Authors : Caines, M.E.C.; Elkins, J.M.; Hewitson, K.S.; Schofield, C.J.
Deposited on : 2003-09-29
Resolution : 2.45 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
A user guide is available at
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix) : 1.9-1692
EDS : rb-20026688
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac : 5.8.0135
CCP4 : 6.5.0
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : trunk26865

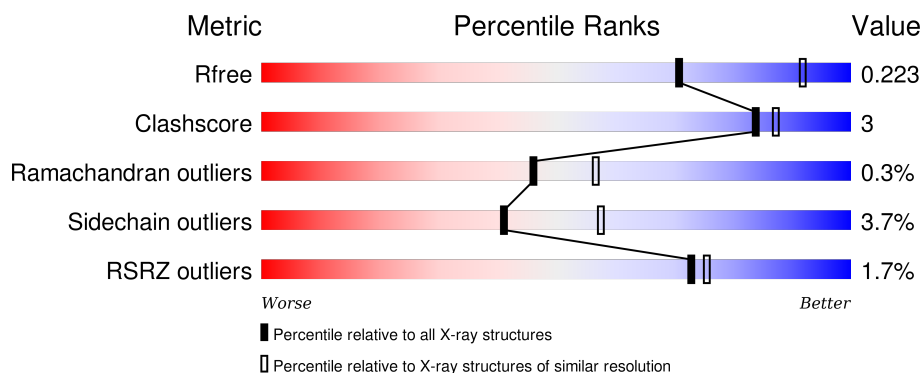
1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.45 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	91344	4776 (2.50-2.42)
Clashscore	102246	1030 (2.48-2.44)
Ramachandran outliers	100387	1024 (2.48-2.44)
Sidechain outliers	100360	1024 (2.48-2.44)
RSRZ outliers	91569	4787 (2.50-2.42)

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 ≥ 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	573	<div> <div>%</div> <div>87% 9% ..</div> </div>
1	B	573	<div> <div>2%</div> <div>89% 7% ..</div> </div>
1	C	573	<div> <div>%</div> <div>88% 8% ..</div> </div>
1	D	573	<div> <div>%</div> <div>89% 8% ..</div> </div>
1	E	573	<div> <div>3%</div> <div>88% 8% ..</div> </div>

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Mol	Chain	Length	Quality of chain
1	F	573	<div> <div></div> <div>88%</div> <div>8% ..</div> </div>

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
4	SO4	B	603	-	-	-	X
4	SO4	D	603	-	-	-	X

2 Entry composition [i](#)

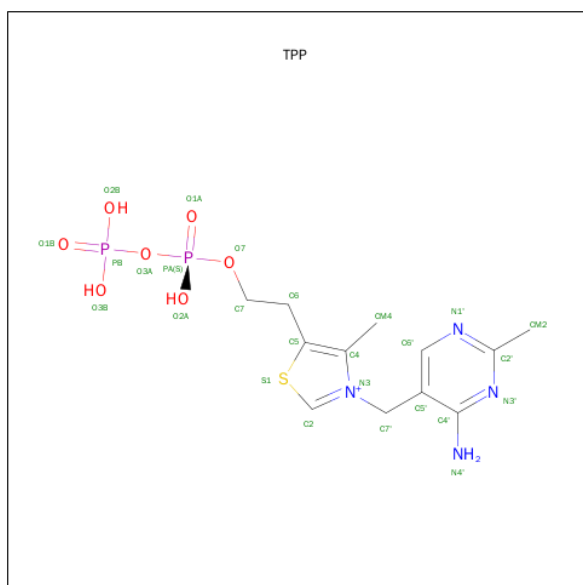
There are 5 unique types of molecules in this entry. The entry contains 26083 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 CARBOXYETHYLARGININE SYNTHASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	559	Total	C	N	O	S	0	0	0
			4172	2649	721	789	13			
1	B	559	Total	C	N	O	S	0	0	0
			4182	2653	723	793	13			
1	C	557	Total	C	N	O	S	0	0	0
			4149	2635	718	783	13			
1	D	559	Total	C	N	O	S	0	0	0
			4174	2649	722	790	13			
1	E	558	Total	C	N	O	S	0	0	0
			4169	2646	721	789	13			
1	F	558	Total	C	N	O	S	0	0	0
			4163	2643	718	789	13			

- Molecule 2 is THIAMINE DIPHOSPHATE (three-letter code: TPP) (formula: $C_{12}H_{19}N_4O_7P_2S$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	S	
			26	12	4	7	2	1	0
2	B	1	Total	C	N	O	P	S	
			26	12	4	7	2	1	0
2	C	1	Total	C	N	O	P	S	
			26	12	4	7	2	1	0
2	D	1	Total	C	N	O	P	S	
			26	12	4	7	2	1	0
2	E	1	Total	C	N	O	P	S	
			26	12	4	7	2	1	0
2	F	1	Total	C	N	O	P	S	
			26	12	4	7	2	1	0

- Molecule 3 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	D	1	Total	Mg		
			1	1	0	0
3	E	1	Total	Mg		
			1	1	0	0
3	B	1	Total	Mg		
			1	1	0	0
3	C	1	Total	Mg		
			1	1	0	0
3	A	1	Total	Mg		
			1	1	0	0
3	F	1	Total	Mg		
			1	1	0	0

- Molecule 4 is SULFATE ION (three-letter code: SO4) (formula: O₄S).



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

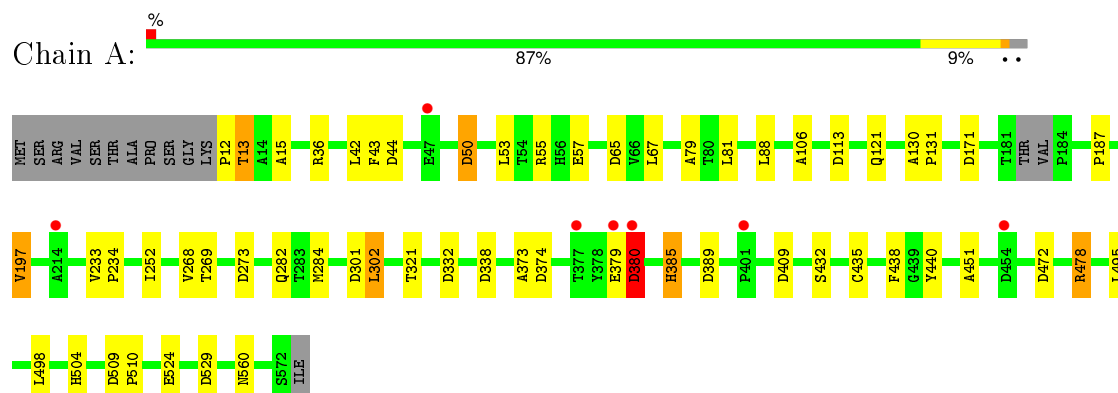
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	139	Total 139	O 139	0	0
5	B	185	Total 185	O 185	0	0
5	C	118	Total 118	O 118	0	0
5	D	157	Total 157	O 157	0	0
5	E	117	Total 117	O 117	0	0
5	F	136	Total 136	O 136	0	0

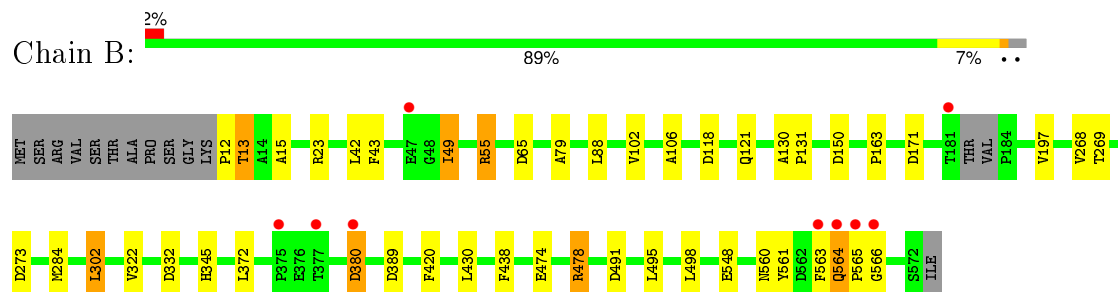
3 Residue-property plots [i](#)

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

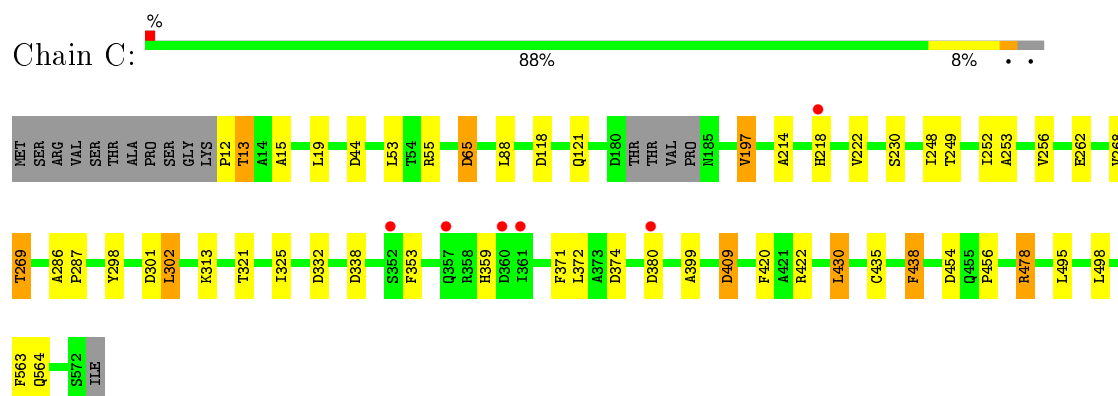
- Molecule 1: CARBOXYETHYLARGININE SYNTHASE



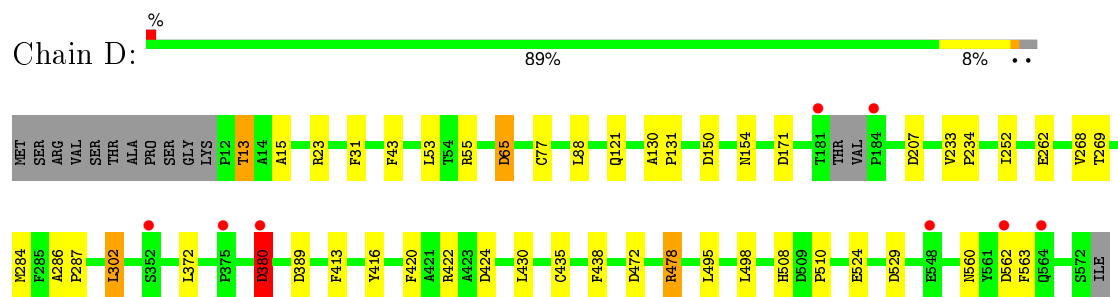
- Molecule 1: CARBOXYETHYLARGININE SYNTHASE



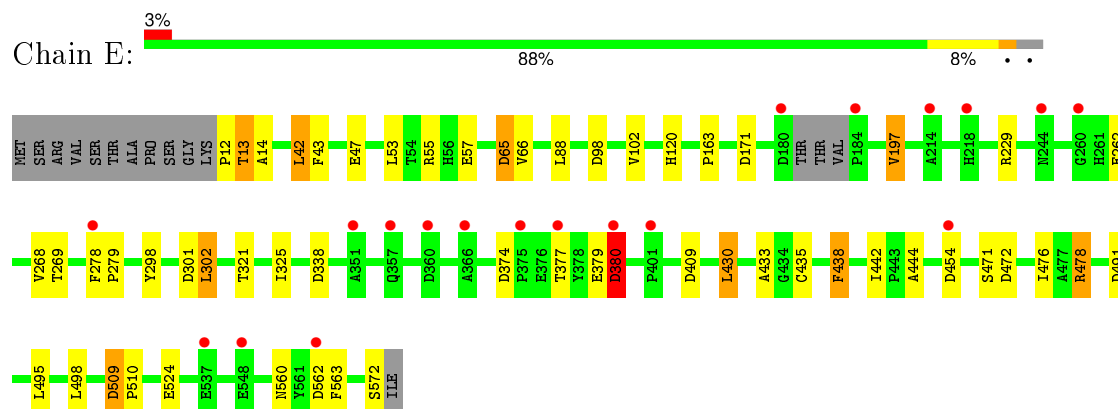
- Molecule 1: CARBOXYETHYLARGININE SYNTHASE



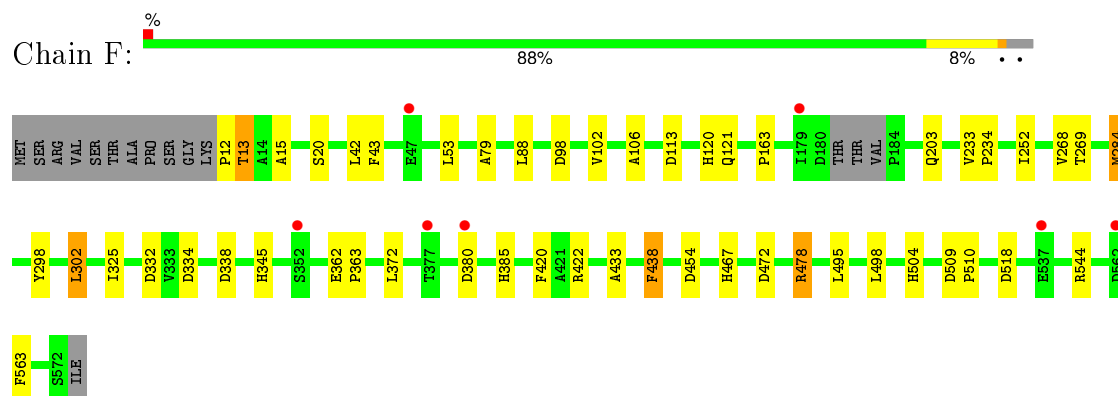
- Molecule 1: CARBOXYETHYLARGININE SYNTHASE



• Molecule 1: CARBOXYETHYLARGININE SYNTHASE



• Molecule 1: CARBOXYETHYLARGININE SYNTHASE



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, α , β , γ	123.07Å 187.20Å 198.62Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	38.00 – 2.45 35.05 – 2.45	Depositor EDS
% Data completeness (in resolution range)	99.8 (38.00-2.45) 99.8 (35.05-2.45)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.35 (at 2.45Å)	Xtriage
Refinement program	REFMAC 5.1.24	Depositor
R, R_{free}	0.176 , 0.216 0.185 , 0.223	Depositor DCC
R_{free} test set	8434 reflections (5.29%)	DCC
Wilson B-factor (Å ²)	27.8	Xtriage
Anisotropy	0.400	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 34.0	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.34$	Xtriage
Outliers	0 of 167962 reflections	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	26083	wwPDB-VP
Average B, all atoms (Å ²)	31.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.68% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: MG, SO4, TPP

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	0.66	0/4267	0.86	14/5827 (0.2%)
1	B	0.67	0/4277	0.87	12/5840 (0.2%)
1	C	0.68	0/4243	0.83	9/5796 (0.2%)
1	D	0.65	0/4269	0.85	12/5830 (0.2%)
1	E	0.68	0/4264	0.85	15/5823 (0.3%)
1	F	0.66	0/4258	0.83	11/5816 (0.2%)
All	All	0.67	0/25578	0.85	73/34932 (0.2%)

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
1	A	0	1
1	B	0	1
1	C	0	1
1	E	0	1
1	F	0	1
All	All	0	5

There are no bond length outliers.

All (73) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	478	ARG	NE-CZ-NH1	-10.61	115.00	120.30
1	B	478	ARG	NE-CZ-NH2	9.60	125.10	120.30
1	E	301	ASP	CB-CG-OD2	8.97	126.37	118.30
1	D	55	ARG	NE-CZ-NH2	-8.71	115.94	120.30
1	D	55	ARG	NE-CZ-NH1	8.20	124.40	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	478	ARG	NE-CZ-NH1	-8.09	116.25	120.30
1	D	478	ARG	NE-CZ-NH2	7.99	124.30	120.30
1	E	478	ARG	NE-CZ-NH2	7.95	124.28	120.30
1	B	55	ARG	NE-CZ-NH2	-7.93	116.33	120.30
1	F	478	ARG	NE-CZ-NH1	-7.55	116.52	120.30
1	F	478	ARG	NE-CZ-NH2	7.25	123.93	120.30
1	A	478	ARG	NE-CZ-NH1	-7.09	116.75	120.30
1	E	478	ARG	NE-CZ-NH1	-7.06	116.77	120.30
1	A	478	ARG	NE-CZ-NH2	6.73	123.67	120.30
1	E	338	ASP	CB-CG-OD2	6.67	124.30	118.30
1	C	65	ASP	CB-CG-OD2	6.46	124.11	118.30
1	A	113	ASP	CB-CG-OD2	6.41	124.07	118.30
1	B	65	ASP	CB-CG-OD2	6.40	124.06	118.30
1	C	118	ASP	CB-CG-OD2	6.22	123.90	118.30
1	E	98	ASP	CB-CG-OD2	6.21	123.89	118.30
1	E	562	ASP	CB-CG-OD2	6.17	123.86	118.30
1	C	301	ASP	CB-CG-OD2	6.16	123.84	118.30
1	F	332	ASP	CB-CG-OD2	6.13	123.82	118.30
1	F	98	ASP	CB-CG-OD2	6.09	123.78	118.30
1	A	50	ASP	CB-CG-OD2	6.04	123.74	118.30
1	E	472	ASP	CB-CG-OD2	6.04	123.73	118.30
1	E	171	ASP	CB-CG-OD2	6.03	123.73	118.30
1	A	338	ASP	CB-CG-OD2	6.02	123.72	118.30
1	E	55	ARG	NE-CZ-NH2	-6.00	117.30	120.30
1	B	171	ASP	CB-CG-OD2	5.99	123.69	118.30
1	D	171	ASP	CB-CG-OD2	5.99	123.69	118.30
1	B	118	ASP	CB-CG-OD2	5.98	123.68	118.30
1	C	454	ASP	CB-CG-OD2	5.97	123.67	118.30
1	F	454	ASP	CB-CG-OD2	5.89	123.60	118.30
1	C	332	ASP	CB-CG-OD2	5.88	123.60	118.30
1	C	55	ARG	NE-CZ-NH2	-5.86	117.37	120.30
1	E	65	ASP	CB-CG-OD2	5.80	123.52	118.30
1	D	472	ASP	CB-CG-OD2	5.78	123.50	118.30
1	D	65	ASP	CB-CG-OD2	5.78	123.50	118.30
1	A	332	ASP	CB-CG-OD2	5.69	123.42	118.30
1	F	472	ASP	CB-CG-OD2	5.68	123.42	118.30
1	A	273	ASP	CB-CG-OD2	5.67	123.40	118.30
1	D	529	ASP	CB-CG-OD2	5.62	123.36	118.30
1	A	389	ASP	CB-CG-OD2	5.61	123.35	118.30
1	E	229	ARG	NE-CZ-NH1	5.55	123.08	120.30
1	F	338	ASP	CB-CG-OD2	5.55	123.30	118.30
1	B	332	ASP	CB-CG-OD2	5.52	123.27	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	454	ASP	CB-CG-OD2	5.51	123.26	118.30
1	C	338	ASP	CB-CG-OD2	5.50	123.25	118.30
1	E	374	ASP	CB-CG-OD2	5.50	123.25	118.30
1	A	529	ASP	CB-CG-OD2	5.47	123.22	118.30
1	B	491	ASP	CB-CG-OD2	5.45	123.20	118.30
1	F	518	ASP	CB-CG-OD1	5.43	123.19	118.30
1	C	409	ASP	CB-CG-OD2	5.42	123.18	118.30
1	A	301	ASP	CB-CG-OD2	5.41	123.17	118.30
1	F	544	ARG	NE-CZ-NH1	5.38	122.99	120.30
1	B	273	ASP	CB-CG-OD2	5.29	123.06	118.30
1	D	207	ASP	CB-CG-OD2	5.23	123.00	118.30
1	A	409	ASP	CB-CG-OD2	5.20	122.98	118.30
1	E	491	ASP	CB-CG-OD1	5.19	122.97	118.30
1	B	389	ASP	CB-CG-OD2	5.16	122.94	118.30
1	A	36	ARG	NE-CZ-NH1	5.14	122.87	120.30
1	A	171	ASP	CB-CG-OD2	5.13	122.92	118.30
1	D	389	ASP	CB-CG-OD2	5.12	122.91	118.30
1	B	55	ARG	NE-CZ-NH1	5.12	122.86	120.30
1	D	150	ASP	CB-CG-OD2	5.12	122.91	118.30
1	B	150	ASP	CB-CG-OD2	5.07	122.86	118.30
1	C	478	ARG	NE-CZ-NH2	5.07	122.83	120.30
1	F	334	ASP	CB-CG-OD2	5.06	122.86	118.30
1	E	509	ASP	CB-CG-OD1	5.05	122.84	118.30
1	D	424	ASP	CB-CG-OD2	5.02	122.82	118.30
1	A	472	ASP	CB-CG-OD2	5.02	122.82	118.30
1	F	113	ASP	CB-CG-OD2	5.00	122.80	118.30

There are no chirality outliers.

All (5) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	12	PRO	Peptide
1	B	12	PRO	Peptide
1	C	12	PRO	Peptide
1	E	12	PRO	Peptide
1	F	12	PRO	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	4172	0	4110	23	0
1	B	4182	0	4118	20	0
1	C	4149	0	4083	24	0
1	D	4174	0	4108	17	0
1	E	4169	0	4106	22	0
1	F	4163	0	4095	27	0
2	A	26	0	16	5	0
2	B	26	0	16	7	0
2	C	26	0	16	5	0
2	D	26	0	16	4	0
2	E	26	0	16	6	0
2	F	26	0	16	6	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
3	C	1	0	0	0	0
3	D	1	0	0	0	0
3	E	1	0	0	0	0
3	F	1	0	0	0	0
4	A	10	0	0	1	0
4	B	10	0	0	0	0
4	C	10	0	0	0	0
4	D	10	0	0	0	0
4	E	10	0	0	0	0
4	F	10	0	0	0	0
5	A	139	0	0	1	0
5	B	185	0	0	4	0
5	C	118	0	0	3	0
5	D	157	0	0	1	0
5	E	117	0	0	1	0
5	F	136	0	0	2	0
All	All	26083	0	24716	148	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 3.

All (148) 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)
2:F:600:TPP:C2	2:F:600:TPP:HN42	1.44	1.31

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:600:TPP:HN42	2:A:600:TPP:C2	1.41	1.31
2:B:600:TPP:C2	2:B:600:TPP:HN42	1.45	1.27
2:C:600:TPP:HN42	2:C:600:TPP:C2	1.50	1.24
2:E:600:TPP:C2	2:E:600:TPP:HN42	1.54	1.21
2:D:600:TPP:HN42	2:D:600:TPP:C2	1.52	1.20
2:A:600:TPP:N4'	2:A:600:TPP:C2	2.11	1.14
2:C:600:TPP:H2	2:C:600:TPP:HN42	1.04	1.13
2:E:600:TPP:HN42	2:E:600:TPP:H2	1.03	1.11
2:F:600:TPP:H2	2:F:600:TPP:HN42	1.02	1.10
2:A:600:TPP:H2	2:A:600:TPP:HN42	0.99	1.09
2:B:600:TPP:HN42	2:B:600:TPP:H2	1.12	1.08
2:F:600:TPP:C2	2:F:600:TPP:N4'	2.16	1.08
2:D:600:TPP:HN42	2:D:600:TPP:H2	1.12	1.05
2:C:600:TPP:C2	2:C:600:TPP:N4'	2.17	1.05
2:B:600:TPP:C2	2:B:600:TPP:N4'	2.18	1.04
2:E:600:TPP:N4'	2:E:600:TPP:C2	2.20	1.03
2:D:600:TPP:C2	2:D:600:TPP:N4'	2.22	1.01
1:B:13:THR:HG21	5:B:2007:HOH:O	1.74	0.88
2:C:600:TPP:H2	2:C:600:TPP:N4'	1.87	0.84
2:E:600:TPP:N4'	2:E:600:TPP:H2	1.88	0.84
1:C:13:THR:HG21	5:C:2008:HOH:O	1.83	0.78
2:A:600:TPP:N4'	2:A:600:TPP:H2	1.84	0.78
2:F:600:TPP:H2	2:F:600:TPP:N4'	1.86	0.78
1:F:13:THR:HG21	5:F:2006:HOH:O	1.85	0.77
1:E:13:THR:HG21	5:E:2008:HOH:O	1.87	0.74
2:D:600:TPP:H2	2:D:600:TPP:N4'	1.94	0.71
1:A:385:HIS:H	1:A:385:HIS:CD2	2.09	0.68
2:B:600:TPP:H2	2:B:600:TPP:N4'	1.95	0.67
1:C:252:ILE:HG12	5:C:2076:HOH:O	1.99	0.62
1:F:268:VAL:HB	1:F:302:LEU:HD22	1.82	0.61
1:E:53:LEU:O	1:E:478:ARG:NH1	2.34	0.60
1:F:53:LEU:O	1:F:478:ARG:NH1	2.35	0.59
1:D:380:ASP:HB2	1:D:560:ASN:OD1	2.03	0.58
1:A:79:ALA:O	1:A:106:ALA:HA	2.03	0.57
1:A:268:VAL:HB	1:A:302:LEU:HD22	1.87	0.57
2:E:600:TPP:C4'	2:E:600:TPP:C2	2.82	0.57
1:C:268:VAL:HB	1:C:302:LEU:HD22	1.86	0.57
1:E:438:PHE:CE1	2:E:600:TPP:HM23	2.41	0.56
1:A:560:ASN:ND2	4:A:603:SO4:O2	2.35	0.56
1:B:268:VAL:HB	1:B:302:LEU:HD22	1.88	0.56
1:C:44:ASP:HB3	1:D:508:HIS:CE1	2.40	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:474:GLU:OE2	1:B:478:ARG:HD3	2.06	0.55
1:A:233:VAL:HB	1:A:234:PRO:HD3	1.88	0.55
1:F:268:VAL:HG22	1:F:284:MET:CE	2.36	0.54
1:C:218:HIS:ND1	1:C:359:HIS:HB3	2.21	0.54
1:B:345:HIS:CE1	5:B:2128:HOH:O	2.60	0.54
1:E:471:SER:HB3	1:F:467:HIS:CD2	2.42	0.54
1:E:442:ILE:HG23	1:E:476:ILE:HD11	1.90	0.54
1:C:298:TYR:CG	1:C:325:ILE:HD13	2.43	0.54
1:B:561:TYR:OH	2:B:600:TPP:O1B	2.20	0.53
1:D:372:LEU:HD21	1:D:420:PHE:HB3	1.89	0.53
1:E:435:CYS:O	1:F:121:GLN:HG2	2.08	0.53
1:B:564:GLN:O	1:B:566:GLY:N	2.42	0.52
1:A:53:LEU:O	1:A:478:ARG:NH1	2.35	0.51
1:B:322:VAL:HG11	1:D:154:ASN:HB3	1.92	0.51
1:B:102:VAL:O	1:B:163:PRO:HA	2.11	0.50
1:D:508:HIS:CD2	1:D:510:PRO:HD2	2.47	0.50
1:F:372:LEU:HD21	1:F:420:PHE:HB3	1.93	0.50
1:C:222:VAL:HA	1:C:248:ILE:O	2.12	0.50
1:A:385:HIS:H	1:A:385:HIS:HD2	1.57	0.50
1:E:42:LEU:HG	1:F:504:HIS:ND1	2.26	0.50
1:A:435:CYS:O	1:B:121:GLN:HG2	2.12	0.49
1:C:372:LEU:HD21	1:C:420:PHE:HB3	1.95	0.49
1:F:509:ASP:N	1:F:510:PRO:CD	2.75	0.49
1:D:252:ILE:HG12	5:D:2079:HOH:O	2.12	0.49
1:C:399:ALA:HB2	1:C:456:PRO:HG2	1.95	0.49
1:B:372:LEU:HD21	1:B:420:PHE:HB3	1.94	0.48
1:D:268:VAL:HB	1:D:302:LEU:HD22	1.95	0.48
1:C:53:LEU:O	1:C:478:ARG:NH1	2.44	0.48
1:D:53:LEU:O	1:D:478:ARG:NH1	2.37	0.48
1:E:197:VAL:CG2	1:E:321:THR:HA	2.43	0.48
1:C:13:THR:HG22	1:C:15:ALA:HB3	1.96	0.48
1:E:120:HIS:ND1	1:F:433:ALA:O	2.47	0.47
1:E:102:VAL:O	1:E:163:PRO:HA	2.14	0.47
1:D:233:VAL:HB	1:D:234:PRO:HD3	1.96	0.47
1:A:55:ARG:HD2	5:B:2155:HOH:O	2.14	0.47
1:D:13:THR:HG22	1:D:15:ALA:HB3	1.96	0.47
1:A:432:SER:HB2	1:A:440:TYR:CE1	2.50	0.46
1:C:121:GLN:HG2	1:D:435:CYS:O	2.15	0.46
1:E:509:ASP:N	1:E:510:PRO:CD	2.78	0.46
1:F:252:ILE:HG12	5:F:2078:HOH:O	2.15	0.46
1:E:42:LEU:O	1:E:43:PHE:HB2	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:79:ALA:O	1:B:106:ALA:HA	2.15	0.46
1:C:214:ALA:HB2	1:C:353:PHE:CZ	2.51	0.45
2:B:600:TPP:N4'	2:B:600:TPP:N3	2.59	0.45
1:C:286:ALA:HB3	1:C:287:PRO:HD3	1.98	0.45
1:F:385:HIS:CD2	1:F:385:HIS:H	2.34	0.45
1:D:130:ALA:N	1:D:131:PRO:CD	2.79	0.45
1:D:13:THR:HG23	1:D:15:ALA:H	1.80	0.45
1:B:380:ASP:N	1:B:380:ASP:OD1	2.49	0.45
1:E:433:ALA:O	1:F:120:HIS:ND1	2.49	0.45
1:F:13:THR:HG23	1:F:15:ALA:H	1.82	0.45
1:C:268:VAL:HG12	1:C:269:THR:N	2.30	0.45
1:E:13:THR:HG23	1:E:14:ALA:N	2.32	0.44
1:F:102:VAL:O	1:F:163:PRO:HA	2.17	0.44
1:E:66:VAL:HG21	1:E:444:ALA:HA	1.99	0.44
1:B:49:ILE:HG22	5:B:2009:HOH:O	2.17	0.44
1:A:67:LEU:HD12	1:A:451:ALA:HB2	2.00	0.44
1:C:253:ALA:O	1:C:256:VAL:HG13	2.17	0.43
1:D:413:PHE:O	1:D:416:TYR:HB2	2.18	0.43
1:A:57:GLU:OE2	2:B:600:TPP:N1'	2.52	0.43
1:E:298:TYR:CG	1:E:325:ILE:HD13	2.54	0.43
1:E:268:VAL:HB	1:E:302:LEU:HD22	2.01	0.43
1:C:13:THR:CG2	1:C:15:ALA:H	2.31	0.43
1:A:42:LEU:O	1:A:43:PHE:HB2	2.18	0.43
1:A:81:LEU:HG	1:A:121:GLN:HB3	2.00	0.43
1:F:362:GLU:N	1:F:363:PRO:CD	2.81	0.43
1:F:42:LEU:O	1:F:43:PHE:HB2	2.19	0.43
1:E:120:HIS:CE1	1:F:433:ALA:O	2.72	0.42
1:C:438:PHE:CE1	2:C:600:TPP:HM23	2.54	0.42
1:F:268:VAL:HG22	1:F:284:MET:HE2	1.99	0.42
1:B:13:THR:HG22	1:B:15:ALA:HB3	2.00	0.42
1:F:298:TYR:CG	1:F:325:ILE:HD13	2.54	0.42
1:E:57:GLU:OE2	2:F:600:TPP:N1'	2.52	0.42
1:D:31:PHE:O	1:D:77:CYS:HA	2.20	0.42
1:F:345:HIS:HD2	1:F:345:HIS:O	2.01	0.42
5:A:2114:HOH:O	1:B:55:ARG:HD2	2.19	0.42
1:F:233:VAL:HB	1:F:234:PRO:HD3	2.01	0.42
1:A:282:GLN:HE21	1:A:282:GLN:HB3	1.70	0.42
1:C:197:VAL:HG22	5:C:2059:HOH:O	2.19	0.42
1:F:438:PHE:CE1	2:F:600:TPP:HM23	2.55	0.42
2:A:600:TPP:C4'	2:A:600:TPP:C2	2.82	0.42
1:A:197:VAL:CG2	1:A:321:THR:HA	2.50	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:13:THR:CG2	1:F:15:ALA:HB3	2.50	0.41
1:C:249:THR:HB	1:C:253:ALA:HB3	2.01	0.41
1:B:130:ALA:N	1:B:131:PRO:CD	2.83	0.41
1:A:379:GLU:O	1:A:380:ASP:O	2.38	0.41
1:F:345:HIS:CD2	1:F:345:HIS:O	2.73	0.41
1:E:380:ASP:HB2	1:E:560:ASN:OD1	2.20	0.41
1:C:430:LEU:HA	1:C:430:LEU:HD12	1.93	0.41
1:C:19:LEU:HD23	1:C:19:LEU:HA	1.90	0.41
1:E:278:PHE:CG	1:E:279:PRO:HD2	2.55	0.41
1:A:13:THR:HG22	1:A:15:ALA:HB3	2.01	0.41
1:C:197:VAL:CG2	1:C:321:THR:HA	2.50	0.41
1:A:509:ASP:N	1:A:510:PRO:CD	2.83	0.41
1:A:44:ASP:OD1	1:A:44:ASP:C	2.59	0.41
1:A:373:ALA:O	1:A:374:ASP:C	2.59	0.41
1:E:430:LEU:HD12	1:E:430:LEU:HA	1.97	0.41
1:D:286:ALA:N	1:D:287:PRO:CD	2.83	0.41
1:A:504:HIS:CG	1:B:42:LEU:HG	2.56	0.41
1:A:130:ALA:N	1:A:131:PRO:CD	2.83	0.40
1:B:380:ASP:HB2	1:B:560:ASN:OD1	2.21	0.40
1:B:42:LEU:O	1:B:43:PHE:HB2	2.21	0.40
1:C:435:CYS:O	1:D:121:GLN:HG2	2.21	0.40
1:F:79:ALA:O	1:F:106:ALA:HA	2.21	0.40
1:F:203:GLN:HB3	1:F:345:HIS:HE1	1.86	0.40
1:B:13:THR:HG23	1:B:15:ALA:H	1.86	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	555/573 (97%)	533 (96%)	21 (4%)	1 (0%)	52 64

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	B	555/573 (97%)	539 (97%)	15 (3%)	1 (0%)	52	64
1	C	553/573 (96%)	532 (96%)	19 (3%)	2 (0%)	39	49
1	D	555/573 (97%)	539 (97%)	14 (2%)	2 (0%)	39	49
1	E	554/573 (97%)	532 (96%)	19 (3%)	3 (0%)	34	41
1	F	554/573 (97%)	539 (97%)	15 (3%)	0	100	100
All	All	3326/3438 (97%)	3214 (97%)	103 (3%)	9 (0%)	46	57

All (9) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	380	ASP
1	B	565	PRO
1	D	380	ASP
1	E	409	ASP
1	E	379	GLU
1	C	409	ASP
1	D	43	PHE
1	E	380	ASP
1	C	374	ASP

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	434/452 (96%)	418 (96%)	16 (4%)	41	57
1	B	436/452 (96%)	420 (96%)	16 (4%)	41	57
1	C	430/452 (95%)	412 (96%)	18 (4%)	36	51
1	D	434/452 (96%)	417 (96%)	17 (4%)	39	54
1	E	434/452 (96%)	416 (96%)	18 (4%)	37	52
1	F	433/452 (96%)	421 (97%)	12 (3%)	51	68
All	All	2601/2712 (96%)	2504 (96%)	97 (4%)	41	57

All (97) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	13	THR
1	A	50	ASP
1	A	65	ASP
1	A	88	LEU
1	A	187	PRO
1	A	197	VAL
1	A	252	ILE
1	A	269	THR
1	A	284	MET
1	A	302	LEU
1	A	380	ASP
1	A	385	HIS
1	A	438	PHE
1	A	495	LEU
1	A	498	LEU
1	A	524	GLU
1	B	13	THR
1	B	23	ARG
1	B	49	ILE
1	B	88	LEU
1	B	197	VAL
1	B	269	THR
1	B	284	MET
1	B	302	LEU
1	B	380	ASP
1	B	430	LEU
1	B	438	PHE
1	B	495	LEU
1	B	498	LEU
1	B	548	GLU
1	B	563	PHE
1	B	564	GLN
1	C	13	THR
1	C	65	ASP
1	C	88	LEU
1	C	197	VAL
1	C	230	SER
1	C	262	GLU
1	C	269	THR
1	C	302	LEU
1	C	313	LYS
1	C	371	PHE

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Mol	Chain	Res	Type
1	C	380	ASP
1	C	422	ARG
1	C	430	LEU
1	C	438	PHE
1	C	495	LEU
1	C	498	LEU
1	C	563	PHE
1	C	564	GLN
1	D	13	THR
1	D	23	ARG
1	D	65	ASP
1	D	88	LEU
1	D	262	GLU
1	D	269	THR
1	D	284	MET
1	D	302	LEU
1	D	380	ASP
1	D	422	ARG
1	D	430	LEU
1	D	438	PHE
1	D	495	LEU
1	D	498	LEU
1	D	524	GLU
1	D	562	ASP
1	D	563	PHE
1	E	13	THR
1	E	42	LEU
1	E	47	GLU
1	E	65	ASP
1	E	88	LEU
1	E	197	VAL
1	E	262	GLU
1	E	269	THR
1	E	302	LEU
1	E	377	THR
1	E	380	ASP
1	E	430	LEU
1	E	438	PHE
1	E	495	LEU
1	E	498	LEU
1	E	524	GLU
1	E	563	PHE

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Mol	Chain	Res	Type
1	E	572	SER
1	F	13	THR
1	F	20	SER
1	F	88	LEU
1	F	269	THR
1	F	284	MET
1	F	302	LEU
1	F	380	ASP
1	F	422	ARG
1	F	438	PHE
1	F	495	LEU
1	F	498	LEU
1	F	563	PHE

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (24) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	277	ASN
1	A	282	GLN
1	A	308	GLN
1	A	359	HIS
1	A	385	HIS
1	A	504	HIS
1	B	140	GLN
1	B	282	GLN
1	B	308	GLN
1	C	308	GLN
1	C	385	HIS
1	C	504	HIS
1	D	16	HIS
1	D	112	HIS
1	D	282	GLN
1	D	308	GLN
1	D	504	HIS
1	E	282	GLN
1	E	308	GLN
1	E	385	HIS
1	F	282	GLN
1	F	308	GLN
1	F	345	HIS
1	F	385	HIS

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 ⓘ

Of 24 ligands modelled in this entry, 6 are monoatomic - leaving 18 for Mogul analysis.

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	TPP	A	600	3	20,27,27	2.15	6 (30%)	31,40,40	2.35	9 (29%)
4	SO4	A	602	-	4,4,4	0.67	0	6,6,6	0.39	0
4	SO4	A	603	-	4,4,4	0.27	0	6,6,6	0.22	0
2	TPP	B	600	3	20,27,27	1.77	4 (20%)	31,40,40	2.10	8 (25%)
4	SO4	B	602	-	4,4,4	0.42	0	6,6,6	0.34	0
4	SO4	B	603	-	4,4,4	0.10	0	6,6,6	0.16	0
2	TPP	C	600	3	20,27,27	1.90	5 (25%)	31,40,40	2.20	8 (25%)
4	SO4	C	602	-	4,4,4	0.54	0	6,6,6	0.29	0
4	SO4	C	603	-	4,4,4	0.25	0	6,6,6	0.14	0
2	TPP	D	600	3	20,27,27	1.93	6 (30%)	31,40,40	2.12	7 (22%)
4	SO4	D	602	-	4,4,4	0.49	0	6,6,6	0.43	0
4	SO4	D	603	-	4,4,4	0.19	0	6,6,6	0.29	0
2	TPP	E	600	3	20,27,27	2.15	6 (30%)	31,40,40	2.35	10 (32%)
4	SO4	E	602	-	4,4,4	0.54	0	6,6,6	0.82	0
4	SO4	E	603	-	4,4,4	0.24	0	6,6,6	0.11	0
2	TPP	F	600	3	20,27,27	1.85	5 (25%)	31,40,40	2.20	8 (25%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	SO4	F	602	-	4,4,4	0.74	0	6,6,6	0.56	0
4	SO4	F	603	-	4,4,4	0.15	0	6,6,6	0.17	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
2	TPP	A	600	3	-	0/16/17/17	0/2/2/2
4	SO4	A	602	-	-	0/0/0/0	0/0/0/0
4	SO4	A	603	-	-	0/0/0/0	0/0/0/0
2	TPP	B	600	3	-	0/16/17/17	0/2/2/2
4	SO4	B	602	-	-	0/0/0/0	0/0/0/0
4	SO4	B	603	-	-	0/0/0/0	0/0/0/0
2	TPP	C	600	3	-	0/16/17/17	0/2/2/2
4	SO4	C	602	-	-	0/0/0/0	0/0/0/0
4	SO4	C	603	-	-	0/0/0/0	0/0/0/0
2	TPP	D	600	3	-	0/16/17/17	0/2/2/2
4	SO4	D	602	-	-	0/0/0/0	0/0/0/0
4	SO4	D	603	-	-	0/0/0/0	0/0/0/0
2	TPP	E	600	3	-	0/16/17/17	0/2/2/2
4	SO4	E	602	-	-	0/0/0/0	0/0/0/0
4	SO4	E	603	-	-	0/0/0/0	0/0/0/0
2	TPP	F	600	3	-	0/16/17/17	0/2/2/2
4	SO4	F	602	-	-	0/0/0/0	0/0/0/0
4	SO4	F	603	-	-	0/0/0/0	0/0/0/0

All (32) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	E	600	TPP	C4-N3	-6.24	1.34	1.39
2	A	600	TPP	C4-N3	-5.96	1.34	1.39
2	F	600	TPP	C4-N3	-5.27	1.35	1.39
2	C	600	TPP	C4-N3	-4.93	1.35	1.39
2	B	600	TPP	C4-N3	-4.90	1.35	1.39
2	D	600	TPP	C4-N3	-4.79	1.35	1.39
2	E	600	TPP	C7'-N3	-4.32	1.40	1.48
2	A	600	TPP	C7'-N3	-4.08	1.41	1.48
2	C	600	TPP	C7'-N3	-3.79	1.41	1.48
2	F	600	TPP	C7'-N3	-3.27	1.42	1.48
2	D	600	TPP	C7'-N3	-3.15	1.42	1.48

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	600	TPP	C7'-N3	-2.19	1.44	1.48
2	C	600	TPP	C2'-N3'	2.02	1.37	1.34
2	C	600	TPP	C6'-N1'	2.04	1.38	1.34
2	E	600	TPP	C2'-N1'	2.07	1.37	1.34
2	D	600	TPP	C7'-C5'	2.09	1.55	1.51
2	A	600	TPP	C2'-N3'	2.10	1.38	1.34
2	E	600	TPP	C6'-N1'	2.14	1.39	1.34
2	F	600	TPP	C4'-N3'	2.18	1.38	1.35
2	D	600	TPP	C2'-N1'	2.25	1.38	1.34
2	A	600	TPP	C6'-N1'	2.32	1.39	1.34
2	F	600	TPP	C6'-N1'	2.37	1.39	1.34
2	E	600	TPP	C2'-N3'	2.48	1.38	1.34
2	D	600	TPP	C6'-N1'	2.50	1.39	1.34
2	B	600	TPP	C2'-N1'	2.53	1.38	1.34
2	F	600	TPP	C2'-N1'	2.63	1.38	1.34
2	B	600	TPP	C6'-N1'	2.69	1.40	1.34
2	E	600	TPP	C4'-N3'	2.83	1.39	1.35
2	C	600	TPP	C2'-N1'	2.87	1.39	1.34
2	A	600	TPP	C4'-N3'	2.90	1.39	1.35
2	A	600	TPP	C2'-N1'	2.96	1.39	1.34
2	D	600	TPP	C4'-N3'	3.12	1.39	1.35

All (50) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	E	600	TPP	C5'-C7'-N3	-9.90	96.78	113.33
2	A	600	TPP	C5'-C7'-N3	-9.28	97.81	113.33
2	C	600	TPP	C5'-C7'-N3	-8.58	98.98	113.33
2	F	600	TPP	C5'-C7'-N3	-7.30	101.13	113.33
2	D	600	TPP	C5'-C7'-N3	-7.17	101.34	113.33
2	B	600	TPP	C5'-C7'-N3	-6.24	102.91	113.33
2	F	600	TPP	C6-C5-S1	-3.95	114.71	120.24
2	D	600	TPP	N1'-C2'-N3'	-3.61	118.92	125.60
2	A	600	TPP	PA-O3A-PB	-3.54	120.78	132.67
2	A	600	TPP	N1'-C2'-N3'	-3.31	119.48	125.60
2	D	600	TPP	PA-O3A-PB	-3.28	121.65	132.67
2	B	600	TPP	PA-O3A-PB	-3.27	121.70	132.67
2	B	600	TPP	N1'-C2'-N3'	-3.14	119.79	125.60
2	E	600	TPP	PA-O3A-PB	-3.09	122.30	132.67
2	F	600	TPP	N1'-C2'-N3'	-2.91	120.21	125.60
2	C	600	TPP	N1'-C2'-N3'	-2.81	120.40	125.60
2	C	600	TPP	PA-O3A-PB	-2.52	124.22	132.67

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	600	TPP	C5'-C4'-N4'	-2.41	118.72	122.25
2	B	600	TPP	C6-C5-S1	-2.38	116.91	120.24
2	E	600	TPP	N1'-C2'-N3'	-2.36	121.24	125.60
2	E	600	TPP	C5'-C6'-N1'	-2.34	119.80	123.86
2	F	600	TPP	PA-O3A-PB	-2.31	124.91	132.67
2	E	600	TPP	C6-C5-S1	-2.28	117.05	120.24
2	A	600	TPP	C6-C5-S1	-2.20	117.16	120.24
2	A	600	TPP	O2B-PB-O1B	-2.12	103.76	110.58
2	B	600	TPP	CM4-C4-C5	-2.10	124.17	128.90
2	C	600	TPP	C6-C5-S1	-2.08	117.33	120.24
2	E	600	TPP	C6'-C5'-C4'	2.00	118.59	115.72
2	E	600	TPP	CM2-C2'-N1'	2.14	119.59	117.03
2	A	600	TPP	O3B-PB-O2B	2.26	115.99	107.38
2	C	600	TPP	O3B-PB-O2B	2.36	116.36	107.38
2	E	600	TPP	O3A-PA-O7	2.40	109.32	102.94
2	C	600	TPP	C6'-N1'-C2'	2.42	120.00	115.77
2	A	600	TPP	CM4-C4-N3	2.47	125.88	122.59
2	B	600	TPP	C6'-N1'-C2'	2.55	120.22	115.77
2	F	600	TPP	C6'-N1'-C2'	2.60	120.32	115.77
2	F	600	TPP	CM4-C4-N3	2.68	126.16	122.59
2	A	600	TPP	C6'-N1'-C2'	2.80	120.66	115.77
2	E	600	TPP	C6'-N1'-C2'	2.91	120.86	115.77
2	D	600	TPP	C6'-N1'-C2'	2.93	120.90	115.77
2	C	600	TPP	CM4-C4-N3	2.94	126.51	122.59
2	E	600	TPP	CM4-C4-N3	2.94	126.51	122.59
2	F	600	TPP	C6-C5-C4	3.01	130.26	127.56
2	D	600	TPP	CM4-C4-N3	3.13	126.76	122.59
2	B	600	TPP	CM4-C4-N3	3.19	126.83	122.59
2	D	600	TPP	CM2-C2'-N1'	4.05	121.89	117.03
2	A	600	TPP	CM2-C2'-N1'	4.34	122.24	117.03
2	C	600	TPP	CM2-C2'-N1'	4.72	122.69	117.03
2	F	600	TPP	CM2-C2'-N1'	4.90	122.91	117.03
2	B	600	TPP	CM2-C2'-N1'	5.28	123.37	117.03

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

7 monomers are involved in 34 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	600	TPP	5	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	603	SO4	1	0
2	B	600	TPP	7	0
2	C	600	TPP	5	0
2	D	600	TPP	4	0
2	E	600	TPP	6	0
2	F	600	TPP	6	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, 95th 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 ²)	Q<0.9
1	A	559/573 (97%)	-0.36	7 (1%) 79 81	20, 31, 46, 59	0
1	B	559/573 (97%)	-0.35	9 (1%) 74 77	19, 30, 45, 62	0
1	C	557/573 (97%)	-0.28	6 (1%) 82 84	19, 31, 45, 58	0
1	D	559/573 (97%)	-0.34	8 (1%) 78 80	18, 30, 45, 58	0
1	E	558/573 (97%)	-0.22	19 (3%) 49 52	19, 31, 45, 57	0
1	F	558/573 (97%)	-0.33	7 (1%) 79 81	19, 30, 45, 57	0
All	All	3350/3438 (97%)	-0.31	56 (1%) 73 75	18, 30, 45, 62	0

All (56) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	E	380	ASP	5.0
1	B	565	PRO	4.8
1	B	564	GLN	4.1
1	D	380	ASP	3.6
1	F	380	ASP	3.5
1	C	380	ASP	3.4
1	B	563	PHE	3.3
1	E	357	GLN	3.3
1	B	181	THR	3.1
1	D	184	PRO	3.1
1	E	562	ASP	3.0
1	C	352	SER	3.0
1	B	380	ASP	3.0
1	F	352	SER	3.0
1	D	181	THR	2.8
1	C	218	HIS	2.8
1	E	537	GLU	2.8
1	E	260	GLY	2.8
1	E	375	PRO	2.7

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Mol	Chain	Res	Type	RSRZ
1	E	351	ALA	2.7
1	A	379	GLU	2.7
1	A	380	ASP	2.7
1	A	47	GLU	2.6
1	C	361	ILE	2.6
1	A	401	PRO	2.5
1	F	47	GLU	2.5
1	E	454	ASP	2.5
1	E	377	THR	2.5
1	F	377	THR	2.4
1	D	564	GLN	2.3
1	E	180	ASP	2.3
1	A	377	THR	2.3
1	F	179	ILE	2.3
1	B	47	GLU	2.3
1	E	214	ALA	2.3
1	E	401	PRO	2.3
1	B	375	PRO	2.3
1	E	278	PHE	2.2
1	D	548	GLU	2.2
1	D	562	ASP	2.2
1	E	366	ALA	2.2
1	E	244	ASN	2.2
1	E	218	HIS	2.2
1	D	375	PRO	2.2
1	A	454	ASP	2.2
1	E	360	ASP	2.2
1	E	548	GLU	2.1
1	C	360	ASP	2.1
1	B	566	GLY	2.1
1	D	352	SER	2.1
1	C	357	GLN	2.1
1	E	184	PRO	2.1
1	A	214	ALA	2.0
1	F	562	ASP	2.0
1	F	537	GLU	2.0
1	B	377	THR	2.0

6.2 Non-standard residues in protein, DNA, RNA chains ⓘ

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

6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

6.4 Ligands ⓘ

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, 95th 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 ²)	Q<0.9
4	SO4	D	603	5/5	0.82	0.39	3.40	89,91,92,92	0
4	SO4	B	603	5/5	0.85	0.37	2.58	91,91,92,92	0
4	SO4	F	603	5/5	0.86	0.28	1.98	90,91,91,91	0
4	SO4	C	603	5/5	0.90	0.22	1.74	89,89,91,91	0
4	SO4	E	603	5/5	0.94	0.29	1.46	90,90,91,91	0
4	SO4	A	603	5/5	0.86	0.20	0.77	89,90,91,91	0
4	SO4	C	602	5/5	0.99	0.13	-0.03	30,33,34,35	0
3	MG	A	601	1/1	0.97	0.13	-0.23	14,14,14,14	0
2	TPP	E	600	26/26	0.97	0.13	-0.47	22,28,31,33	0
4	SO4	F	602	5/5	0.99	0.12	-0.52	30,31,33,33	0
2	TPP	D	600	26/26	0.98	0.12	-0.54	22,26,29,30	0
3	MG	B	601	1/1	0.98	0.11	-0.55	13,13,13,13	0
2	TPP	C	600	26/26	0.98	0.12	-0.57	22,27,30,31	0
2	TPP	A	600	26/26	0.97	0.13	-0.70	22,26,30,31	0
4	SO4	E	602	5/5	0.98	0.13	-0.73	32,32,34,35	0
2	TPP	B	600	26/26	0.98	0.11	-0.74	22,27,29,32	0
4	SO4	B	602	5/5	0.99	0.12	-0.78	33,34,35,35	0
3	MG	F	601	1/1	0.97	0.09	-1.05	15,15,15,15	0
4	SO4	A	602	5/5	0.99	0.11	-1.06	27,29,30,30	0
2	TPP	F	600	26/26	0.97	0.10	-1.10	21,26,29,31	0
3	MG	D	601	1/1	0.98	0.09	-1.17	15,15,15,15	0
3	MG	E	601	1/1	0.98	0.09	-1.35	17,17,17,17	0
4	SO4	D	602	5/5	0.99	0.10	-1.39	29,30,31,32	0
3	MG	C	601	1/1	0.99	0.09	-1.53	12,12,12,12	0

6.5 Other polymers ⓘ

There are no such residues in this entry.