



wwPDB X-ray Structure Validation Summary Report ⓘ

Feb 28, 2026 – 11:55 PM UTC

PDB ID : 2EYQ / pdb_00002eyq
Title : Crystal structure of Escherichia coli transcription-repair coupling factor
Authors : Deaconescu, A.M.; Darst, S.A.
Deposited on : 2005-11-09
Resolution : 3.20 Å(reported)

This is a wwPDB X-ray Structure Validation Summary Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

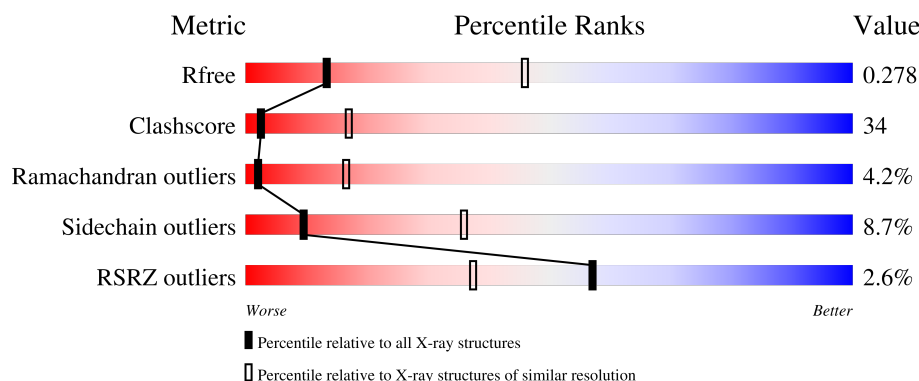
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

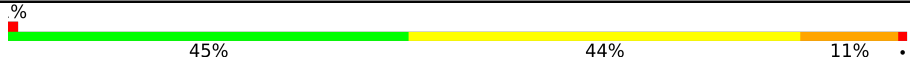
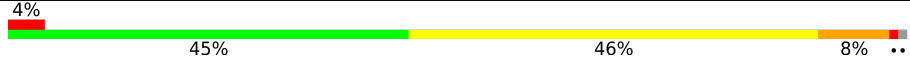
The reported resolution of this entry is 3.20 Å.

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}	180053	1466 (3.20-3.20)
Clashscore	190562	1573 (3.20-3.20)
Ramachandran outliers	187476	1548 (3.20-3.20)
Sidechain outliers	187428	1547 (3.20-3.20)
RSRZ outliers	180081	1466 (3.20-3.20)

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 of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. 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	1151	
1	B	1151	

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
3	EPE	A	1151	-	-	X	-
3	EPE	B	1150	-	-	X	-
3	EPE	B	1151	-	-	X	-

2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 18063 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.

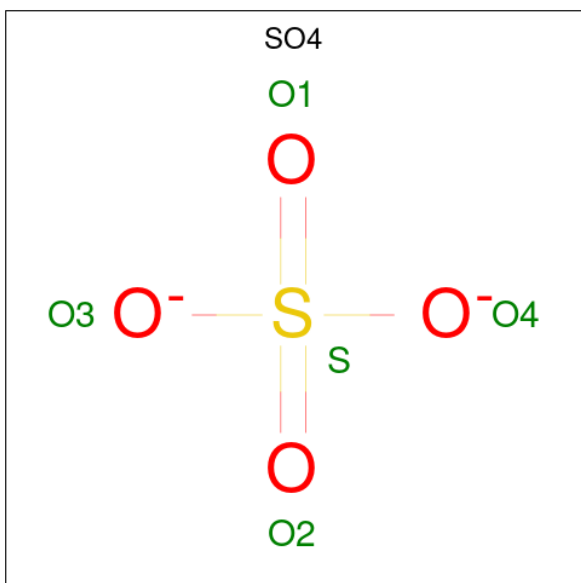
- Molecule 1 is a protein called Transcription-repair coupling factor.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	1146	Total	C	N	O	S	0	0	0
			8980	5683	1605	1656	36			
1	B	1143	Total	C	N	O	S	0	0	0
			8873	5611	1584	1642	36			

There are 6 discrepancies between the modelled and reference sequences:

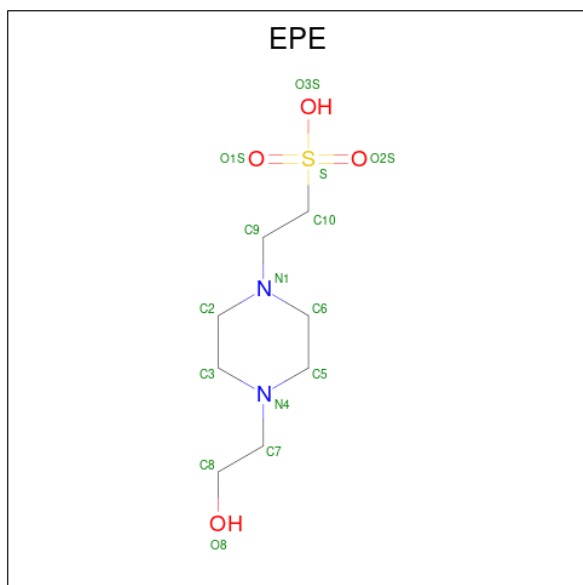
Chain	Residue	Modelled	Actual	Comment	Reference
A	-2	GLY	-	cloning artifact	UNP P30958
A	-1	PRO	-	cloning artifact	UNP P30958
A	0	HIS	-	cloning artifact	UNP P30958
B	-2	GLY	-	cloning artifact	UNP P30958
B	-1	PRO	-	cloning artifact	UNP P30958
B	0	HIS	-	cloning artifact	UNP P30958

- Molecule 2 is SULFATE ION (CCD ID: SO4) (formula: O₄S).



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

- Molecule 3 is 4-(2-HYDROXYETHYL)-1-PIPERAZINE ETHANESULFONIC ACID (CCD ID: EPE) (formula: $C_8H_{18}N_2O_4S$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total C N O S 15 8 2 4 1	0	0
3	A	1	Total C N O S 15 8 2 4 1	0	0
3	B	1	Total C N O S 15 8 2 4 1	0	0
3	B	1	Total C N O S 15 8 2 4 1	0	0
3	B	1	Total C N O S 15 8 2 4 1	0	0

- Molecule 4 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	68	Total O 68 68	0	0

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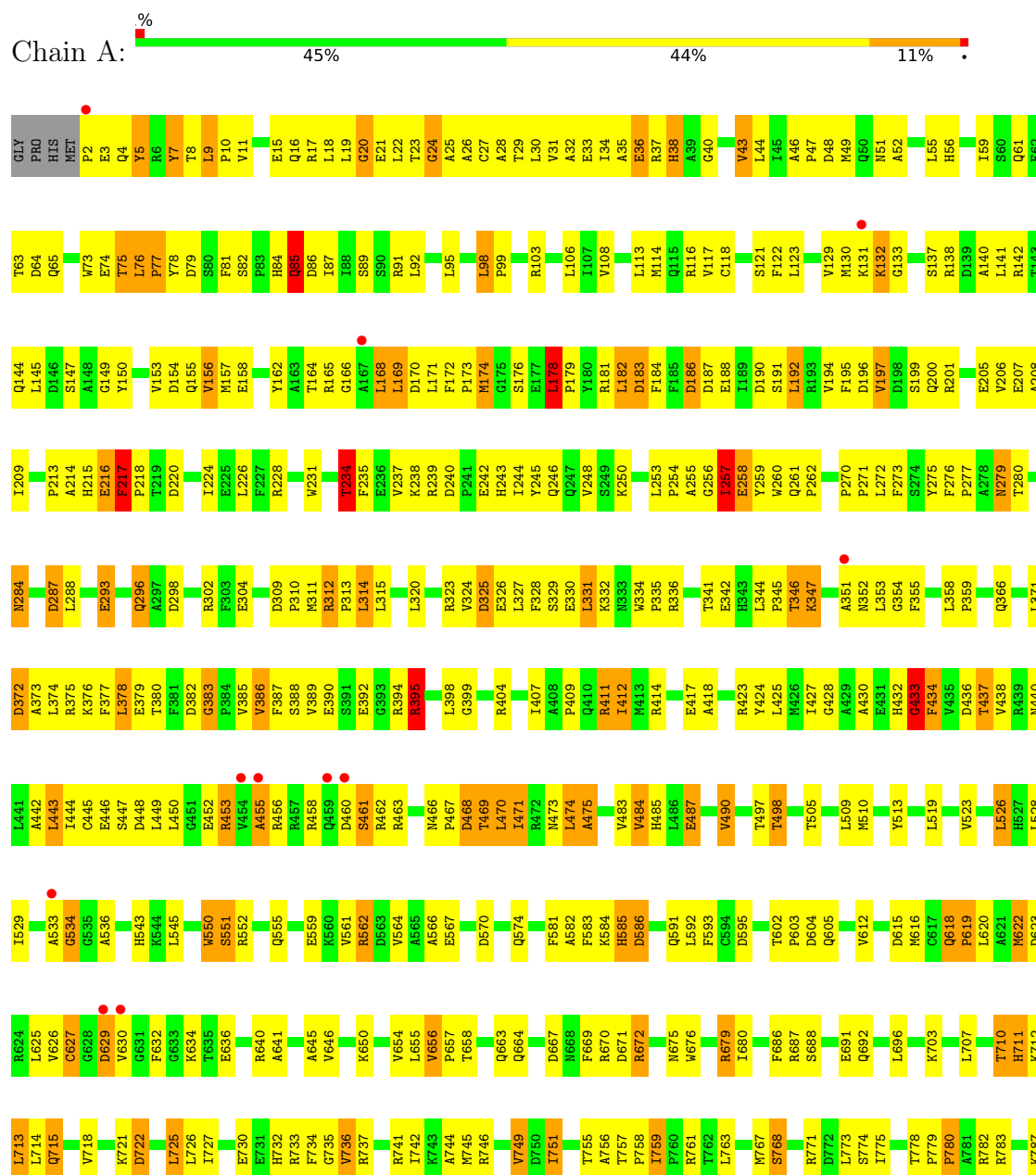
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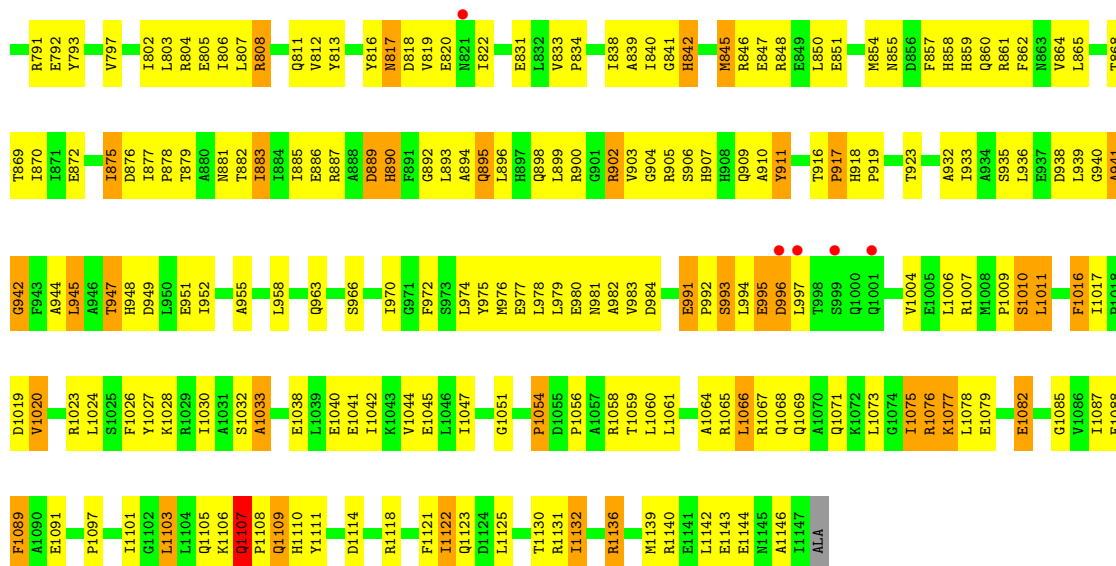
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	B	52	Total	O	0	0
			52	52		

3 Residue-property plots

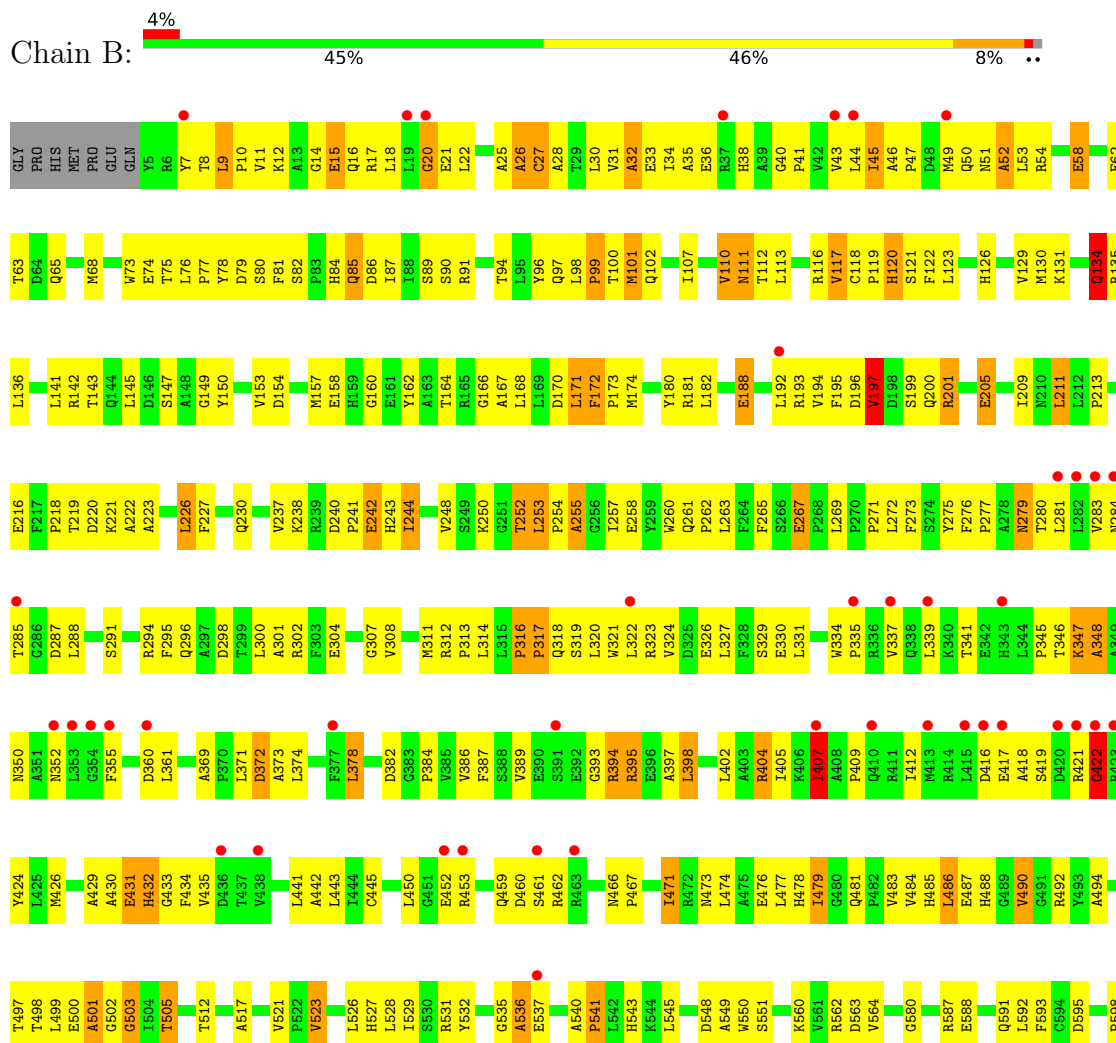
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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: Transcription-repair coupling factor





• Molecule 1: Transcription-repair coupling factor



L1073	L986	H907	G841	I759	B681	F599
G1074	E991	H908	H842	P760	M682	T602
I1075	P992	Q909	Q843	L763	S683	P603
R1076	S993	A910	Q844	L773	S684	D604
K1077	L994	Y911	M845	L776	R685	D605
L1078	E995	L915	B846	L777	F686	I609
G1085	D996	T916	E847	A777	R687	V612
F1089	Q1000	P917	R848	T778	S688	L613
A1090	Q1001	H918	L850	P779	K690	S614
E1091	L1006	P919	M854	R783	E691	D615
K1092	R1007	K920	N855	V796	Q692	M616
V1095	R1008	A921	D856	F796	I695	C617
N1096	P1009	H922	F857	R791	V699	Q618
L1100	P1010	T923	H858	F792	L707	M622
L1104	S1010	T924	H859	Y793	W708	D623
Q1105	L1011	A926	Q860	D794	G709	M624
K1106	I1012	Q927	R861	S795	H710	L625
Q1107	P1013	L930	F862	M796	K712	V626
K1108	F1016	I933	N863	V797	L713	C627
P1109	V1020	L936	C867	W798	L714	G628
H1110	N1021	E937	T868	R799	Q715	D629
L1113	F1026	G940	T869	E800	S716	V630
L1119	Y1027	A941	E872	A801	G631	K634
K1120	K1028	Q942	T873	L803	W718	T635
F1121	T1035	L945	C874	R804	K719	A642
I1122	E1036	H948	I875	E805	F720	F643
L1125	M1037	E951	D876	L806	L723	V646
R1128	E1038	E952	T879	R807	G724	K650
K1129	L1039	R953	N881	R808	L725	V654
T1130	E1040	G956	T882	Q811	L726	L655
R1131	K1043	Q963	I883	Y816	L727	V656
L1132	E1044	S964	I884	N817	K739	P657
E1133	E1045	M967	T885	D818	A744	T658
R1136	L1046	E968	E886	V819	M745	L661
M1139	I1047	T969	R887	E820	R746	A662
R1140	A1051	I974	A888	N821	A747	Q663
E1141	L1052	Y975	D889	I822	M748	Q664
L1142	L1053	M976	H890	Q823	V749	H665
E1143	D1055	E977	L893	E827	M749	Y666
E1144	P1056	L978	A894	R828	R750	D667
E1147	A1057	E979	L896	L829	A751	V668
ALA	R1058	Y976	Q897	A830	A753	F669
	L1059	M977	Q898	E831	L754	B670
	L1060	E978	L899	L832	T755	D671
	L1066	L979	R900	P834	A756	B672
	R1067	E980	G901	E835	T757	I680
	Q1068	N981	R902	E836		
	Q1071	A982	V903	R837		
	K1072	V983	G904	I838		
			R905	A839		
			S906	I840		

4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	151.87Å 161.99Å 161.73Å 90.00° 105.09° 90.00°	Depositor
Resolution (Å)	40.00 – 3.20 40.00 – 3.20	Depositor EDS
% Data completeness (in resolution range)	(Not available) (40.00-3.20) 98.2 (40.00-3.20)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.59 (at 3.18Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.234 , 0.295 0.222 , 0.278	Depositor DCC
R_{free} test set	3095 reflections (5.04%)	wwPDB-VP
Wilson B-factor (Å ²)	63.1	Xtriage
Anisotropy	0.045	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.28 , 45.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	18063	wwPDB-VP
Average B, all atoms (Å ²)	50.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.00% 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, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality [i](#)

5.1 Standard geometry [i](#)

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

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	0.63	0/9162	1.12	66/12429 (0.5%)
1	B	0.60	0/9051	1.06	55/12284 (0.4%)
All	All	0.62	0/18213	1.09	121/24713 (0.5%)

There are no bond length outliers.

The worst 5 of 121 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	85	GLN	OE1-CD-NE2	-9.77	112.83	122.60
1	A	838	ILE	N-CA-C	9.09	121.57	109.21
1	B	40	GLY	CA-C-N	9.06	129.42	119.90
1	B	40	GLY	C-N-CA	9.06	129.42	119.90
1	B	422	GLY	N-CA-C	8.96	134.41	113.18

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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	8980	0	8865	629	0
1	B	8873	0	8675	602	0
2	A	10	0	0	0	0
2	B	5	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	A	30	0	36	10	0
3	B	45	0	54	26	0
4	A	68	0	0	5	0
4	B	52	0	0	3	0
All	All	18063	0	17630	1227	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 34.

The worst 5 of 1227 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:B:254:PRO:HD2	1:B:257:ILE:HD12	1.17	1.15
1:A:474:LEU:HD21	1:A:1028:LYS:HG3	1.31	1.07
1:B:117:VAL:HG12	1:B:118:CYS:H	1.16	1.05
1:A:116:ARG:HG3	1:A:320:LEU:O	1.57	1.04
1:B:386:VAL:HB	1:B:443:LEU:HD12	1.39	1.03

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	1144/1151 (99%)	941 (82%)	153 (13%)	50 (4%)	2	15
1	B	1141/1151 (99%)	942 (83%)	153 (13%)	46 (4%)	2	17
All	All	2285/2302 (99%)	1883 (82%)	306 (13%)	96 (4%)	2	16

5 of 96 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	24	GLY
1	A	25	ALA
1	A	38	HIS
1	A	132	LYS
1	A	187	ASP

5.3.2 Protein sidechains [i](#)

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	930/975 (95%)	840 (90%)	90 (10%)	8	32
1	B	904/975 (93%)	834 (92%)	70 (8%)	12	41
All	All	1834/1950 (94%)	1674 (91%)	160 (9%)	9	36

5 of 160 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	330	GLU
1	B	845	MET
1	B	404	ARG
1	B	635	THR
1	B	991	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 49 such sidechains are listed below:

Mol	Chain	Res	Type
1	B	243	HIS
1	B	543	HIS
1	B	279	ASN
1	B	432	HIS
1	B	692	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 oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

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$
3	EPE	B	1152	-	15,15,15	1.07	0	19,20,20	1.26	2 (10%)
3	EPE	B	1150	-	15,15,15	0.96	0	19,20,20	1.43	2 (10%)
3	EPE	A	1152	-	15,15,15	1.06	0	19,20,20	1.39	3 (15%)
2	SO4	A	1149	-	4,4,4	0.36	0	6,6,6	0.27	0
3	EPE	A	1151	-	15,15,15	1.15	0	19,20,20	1.41	2 (10%)
2	SO4	B	1149	-	4,4,4	0.38	0	6,6,6	0.22	0
2	SO4	A	1150	-	4,4,4	0.34	0	6,6,6	0.23	0
3	EPE	B	1151	-	15,15,15	1.39	1 (6%)	19,20,20	1.42	2 (10%)

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
3	EPE	B	1152	-	-	0/9/19/19	0/1/1/1
3	EPE	B	1150	-	-	1/9/19/19	0/1/1/1
3	EPE	A	1152	-	-	1/9/19/19	0/1/1/1
3	EPE	A	1151	-	-	1/9/19/19	0/1/1/1
3	EPE	B	1151	-	-	1/9/19/19	0/1/1/1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	1151	EPE	C10-S	2.83	1.81	1.77

The worst 5 of 11 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	1152	EPE	O1S-S-C10	4.29	113.21	106.73
3	A	1151	EPE	O1S-S-C10	4.24	113.13	106.73
3	B	1151	EPE	O1S-S-C10	3.92	112.65	106.73
3	B	1150	EPE	O1S-S-C10	3.88	112.59	106.73
3	B	1152	EPE	O1S-S-C10	3.64	112.23	106.73

There are no chirality outliers.

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	B	1151	EPE	N4-C7-C8-O8
3	A	1151	EPE	N4-C7-C8-O8
3	A	1152	EPE	N4-C7-C8-O8
3	B	1150	EPE	N4-C7-C8-O8

There are no ring outliers.

4 monomers are involved in 36 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	1150	EPE	14	0
3	A	1152	EPE	1	0
3	A	1151	EPE	9	0
3	B	1151	EPE	12	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 [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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	1146/1151 (99%)	-0.16	16 (1%) 73 54	4, 44, 83, 109	0
1	B	1143/1151 (99%)	0.08	44 (3%) 44 27	4, 53, 105, 123	0
All	All	2289/2302 (99%)	-0.04	60 (2%) 57 37	4, 48, 100, 123	0

The worst 5 of 60 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	282	LEU	4.4
1	B	630	VAL	3.5
1	B	353	LEU	3.4
1	B	283	VAL	3.3
1	B	284	ASN	3.3

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 oligosaccharides 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. 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	B-factors($\text{\AA}^2$)	Q<0.9
2	SO4	B	1149	5/5	0.54	0.13	120,120,120,121	0
3	EPE	B	1152	15/15	0.62	0.21	95,95,98,98	0
3	EPE	B	1151	15/15	0.66	0.22	105,108,109,109	0
2	SO4	A	1150	5/5	0.67	0.13	104,104,105,105	0
3	EPE	A	1152	15/15	0.72	0.19	88,89,91,92	0
3	EPE	B	1150	15/15	0.81	0.21	81,89,91,92	0
3	EPE	A	1151	15/15	0.84	0.15	104,105,105,106	0
2	SO4	A	1149	5/5	0.88	0.10	89,89,89,89	0

6.5 Other polymers [i](#)

There are no such residues in this entry.