



wwPDB X-ray Structure Validation Summary Report ⓘ

Jul 9, 2025 – 04:22 pm BST

PDB ID : 8RS8 / pdb_00008rs8
Title : Crystal structure of BRCA1 BRCTs in complex with a RIF1 phosphopeptide
Authors : Day, M.; Pearl, L.H.; Oliver, A.W.
Deposited on : 2024-01-24
Resolution : 1.31 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 Phenix2.0rc1
Mogul : 1.8.4, CSD as541be (2020)
Xtriage (Phenix) : 2.0rc1
EDS : 3.0
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4 : 9.0.003 (Gargrove)
Density-Fitness : 1.0.11
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.44

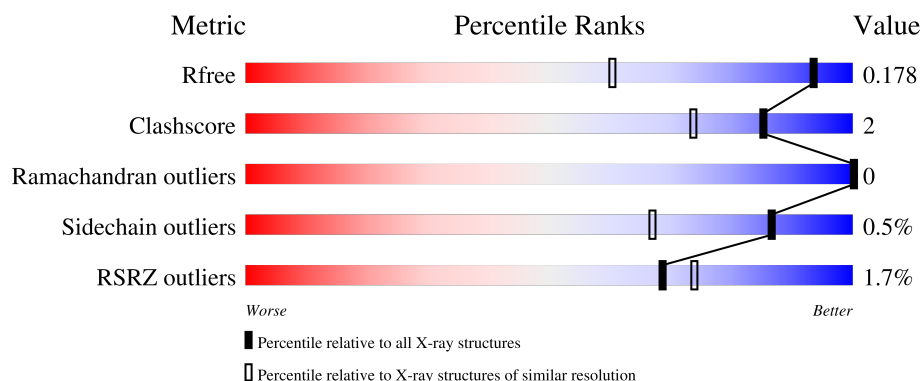
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.31 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}	164625	2202 (1.34-1.30)
Clashscore	180529	2378 (1.34-1.30)
Ramachandran outliers	177936	2325 (1.34-1.30)
Sidechain outliers	177891	2325 (1.34-1.30)
RSRZ outliers	164620	2199 (1.34-1.30)

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	217	<div> <div>%</div> <div>94%</div> <div>• •</div> </div>
1	B	217	<div> <div>2%</div> <div>91%</div> <div>• 6%</div> </div>
1	C	217	<div> <div>%</div> <div>91%</div> <div>6% •</div> </div>
1	D	217	<div> <div>%</div> <div>94%</div> <div>• •</div> </div>
2	E	11	<div> <div>18%</div> <div>73%</div> <div>18% 9%</div> </div>

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Mol	Chain	Length	Quality of chain
2	F	11	<div><div></div><div>9%</div><div>73%</div><div>18%</div><div>9%</div></div>
2	G	11	<div><div></div><div>82%</div><div>9%</div><div>9%</div></div>
2	H	11	<div><div></div><div>9%</div><div>82%</div><div>9%</div><div>9%</div></div>

2 Entry composition [i](#)

There are 6 unique types of molecules in this entry. The entry contains 15934 atoms, of which 7450 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 Breast cancer type 1 susceptibility protein.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	210	Total	C	H	N	O	S	0	11	0
			3444	1105	1707	294	323	15			
1	B	205	Total	C	H	N	O	S	0	9	0
			3368	1083	1669	288	312	16			
1	C	210	Total	C	H	N	O	S	0	15	0
			3516	1128	1745	304	324	15			
1	D	210	Total	C	H	N	O	S	0	21	0
			3554	1132	1771	307	327	17			

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1643	GLY	-	expression tag	UNP P38398
A	1644	PRO	-	expression tag	UNP P38398
A	1645	SER	-	expression tag	UNP P38398
B	1643	GLY	-	expression tag	UNP P38398
B	1644	PRO	-	expression tag	UNP P38398
B	1645	SER	-	expression tag	UNP P38398
C	1643	GLY	-	expression tag	UNP P38398
C	1644	PRO	-	expression tag	UNP P38398
C	1645	SER	-	expression tag	UNP P38398
D	1643	GLY	-	expression tag	UNP P38398
D	1644	PRO	-	expression tag	UNP P38398
D	1645	SER	-	expression tag	UNP P38398

- Molecule 2 is a protein called Telomere-associated protein RIF1.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
2	E	10	Total	C	H	N	O	P	0	0	0
			160	48	79	15	17	1			
2	F	10	Total	C	H	N	O	P	0	0	0
			160	48	79	15	17	1			

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Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
2	G	10	Total 160	C 48	H 79	N 15	O 17	P 1	0	0	0
2	H	10	Total 160	C 48	H 79	N 15	O 17	P 1	0	0	0

- Molecule 3 is 1,2-ETHANEDIOL (CCD ID: EDO) (formula: C₂H₆O₂).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	H	O	0	0
			10	2	6	2		
3	A	1	Total	C	H	O	0	0
			10	2	6	2		
3	A	1	Total	C	H	O	0	0
			10	2	6	2		
3	A	1	Total	C	H	O	0	0
			10	2	6	2		
3	A	1	Total	C	H	O	0	0
			10	2	6	2		
3	A	1	Total	C	H	O	0	0
			10	2	6	2		
3	A	1	Total	C	H	O	0	0
			10	2	6	2		

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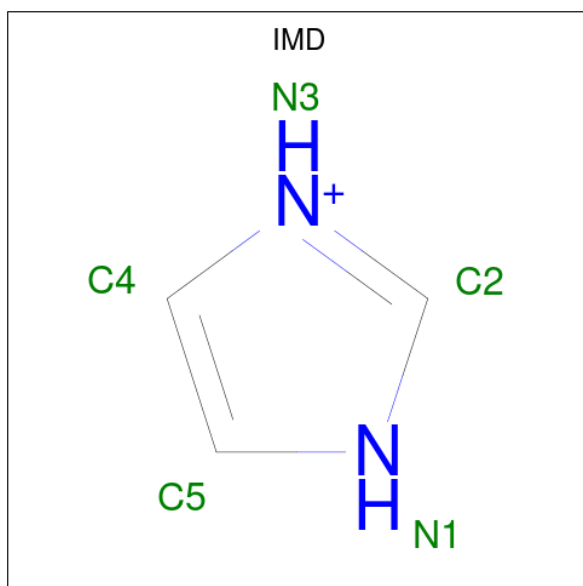
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	B	1	Total	C	H	O	0	0
			10	2	6	2		
3	B	1	Total	C	H	O	0	0
			10	2	6	2		
3	B	1	Total	C	H	O	0	0
			10	2	6	2		
3	B	1	Total	C	H	O	0	0
			10	2	6	2		
3	B	1	Total	C	H	O	0	0
			10	2	6	2		
3	B	1	Total	C	H	O	0	0
			10	2	6	2		
3	C	1	Total	C	H	O	0	0
			10	2	6	2		
3	C	1	Total	C	H	O	0	0
			10	2	6	2		
3	C	1	Total	C	H	O	0	0
			10	2	6	2		
3	C	1	Total	C	H	O	0	0
			10	2	6	2		
3	C	1	Total	C	H	O	0	0
			10	2	6	2		
3	C	1	Total	C	H	O	0	0
			10	2	6	2		
3	C	1	Total	C	H	O	0	0
			10	2	6	2		
3	C	1	Total	C	H	O	0	0
			10	2	6	2		
3	C	1	Total	C	H	O	0	0
			10	2	6	2		
3	D	1	Total	C	H	O	0	0
			10	2	6	2		
3	D	1	Total	C	H	O	0	0
			10	2	6	2		
3	D	1	Total	C	H	O	0	0
			10	2	6	2		

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	D	1	Total	C	H	O	0	0
			10	2	6	2		
3	D	1	Total	C	H	O	0	0
			10	2	6	2		
3	D	1	Total	C	H	O	0	0
			10	2	6	2		
3	D	1	Total	C	H	O	0	0
			10	2	6	2		
3	D	1	Total	C	H	O	0	0
			10	2	6	2		
3	G	1	Total	C	H	O	0	0
			10	2	6	2		
3	G	1	Total	C	H	O	0	0
			10	2	6	2		

- Molecule 4 is IMIDAZOLE (CCD ID: IMD) (formula: $C_3H_5N_2$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	B	1	Total	C	H	N	0	0
			10	3	5	2		
4	C	1	Total	C	H	N	0	0
			10	3	5	2		

- Molecule 5 is DI(HYDROXYETHYL)ETHER (CCD ID: PEG) (formula: $C_4H_{10}O_3$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	C	1	Total	C	H	O	0	0
			17	4	10	3		

- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	228	Total	O	0	1
			229	229		
6	B	195	Total	O	0	0
			195	195		
6	C	243	Total	O	0	1
			244	244		
6	D	255	Total	O	0	2
			257	257		
6	E	19	Total	O	0	0
			19	19		
6	F	25	Total	O	0	0
			25	25		
6	G	19	Total	O	0	0
			19	19		
6	H	17	Total	O	0	0
			17	17		

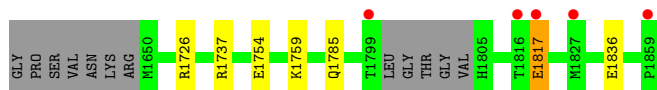
3 Residue-property plots [i](#)

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.

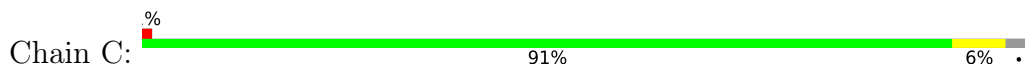
- Molecule 1: Breast cancer type 1 susceptibility protein



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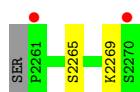
- Molecule 1: Breast cancer type 1 susceptibility protein



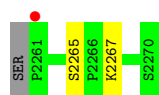
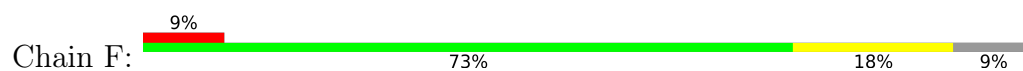
- Molecule 1: Breast cancer type 1 susceptibility protein



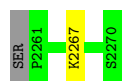
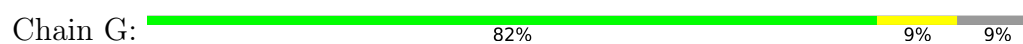
- Molecule 2: Telomere-associated protein RIF1



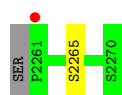
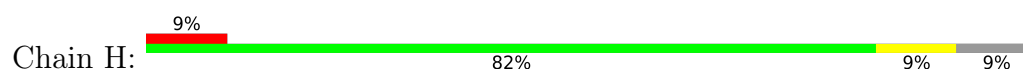
- Molecule 2: Telomere-associated protein RIF1



- Molecule 2: Telomere-associated protein RIF1



- Molecule 2: Telomere-associated protein RIF1



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	36.84Å 173.72Å 74.52Å 90.00° 89.05° 90.00°	Depositor
Resolution (Å)	56.55 – 1.31 56.55 – 1.31	Depositor EDS
% Data completeness (in resolution range)	98.1 (56.55-1.31) 98.1 (56.55-1.31)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.03 (at 1.31Å)	Xtriage
Refinement program	PHENIX 1.20.1_4487	Depositor
R, R_{free}	0.141 , 0.179 0.141 , 0.178	Depositor DCC
R_{free} test set	10849 reflections (4.95%)	wwPDB-VP
Wilson B-factor (Å ²)	18.6	Xtriage
Anisotropy	0.057	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.39 , 45.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.031 for h,-k,-l	Xtriage
F_o, F_c correlation	0.98	EDS
Total number of atoms	15934	wwPDB-VP
Average B, all atoms (Å ²)	28.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 19.48% 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: EDO, IMD, PEG, SEP

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	0.36	0/1819	0.55	0/2467
1	B	0.35	0/1768	0.53	0/2395
1	C	0.40	0/1854	0.58	0/2511
1	D	0.37	0/1899	0.56	0/2567
2	E	0.32	0/72	0.83	0/89
2	F	0.43	0/72	0.66	0/89
2	G	0.37	0/72	0.70	0/89
2	H	0.41	0/72	0.68	0/89
All	All	0.37	0/7628	0.56	0/10296

There are no bond length outliers.

There are no bond angle outliers.

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	1737	1707	1667	5	0
1	B	1699	1669	1630	5	3
1	C	1771	1745	1689	11	0
1	D	1783	1771	1669	4	0
2	E	81	79	79	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	F	81	79	79	1	0
2	G	81	79	79	1	0
2	H	81	79	79	0	0
3	A	36	54	54	0	0
3	B	28	42	42	1	0
3	C	44	66	66	4	0
3	D	32	48	48	1	0
3	G	8	12	12	0	0
4	B	5	5	5	1	0
4	C	5	5	5	0	0
5	C	7	10	10	0	0
6	A	229	0	0	3	0
6	B	195	0	0	4	4
6	C	244	0	0	4	0
6	D	257	0	0	3	0
6	E	19	0	0	1	0
6	F	25	0	0	1	0
6	G	19	0	0	1	0
6	H	17	0	0	0	0
All	All	8484	7450	7213	31	4

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 2.

The worst 5 of 31 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:1751[B]:ARG:NH1	6:C:2001[B]:HOH:O	1.85	1.07
1:C:1751[A]:ARG:NH1	6:C:2001[A]:HOH:O	1.88	1.05
1:B:1836:GLU:OE1	6:B:2001:HOH:O	1.92	0.88
3:D:1901:EDO:O1	6:D:2001:HOH:O	1.99	0.81
3:C:1911:EDO:O2	6:C:2002:HOH:O	1.99	0.80

All (4) 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)
6:B:2086:HOH:O	6:B:2195:HOH:O[1_655]	1.79	0.41
1:B:1817:GLU:OE2	6:B:2074:HOH:O[1_455]	1.81	0.39
1:B:1759:LYS:N	6:B:2195:HOH:O[1_655]	1.98	0.22

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1759:LYS:H	6:B:2195:HOH:O[1_655]	1.45	0.15

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	218/217 (100%)	214 (98%)	4 (2%)	0	100	100
1	B	209/217 (96%)	202 (97%)	7 (3%)	0	100	100
1	C	222/217 (102%)	216 (97%)	6 (3%)	0	100	100
1	D	228/217 (105%)	224 (98%)	4 (2%)	0	100	100
2	E	7/11 (64%)	7 (100%)	0	0	100	100
2	F	7/11 (64%)	6 (86%)	1 (14%)	0	100	100
2	G	7/11 (64%)	7 (100%)	0	0	100	100
2	H	7/11 (64%)	7 (100%)	0	0	100	100
All	All	905/912 (99%)	883 (98%)	22 (2%)	0	100	100

There are no Ramachandran outliers to report.

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	198/193 (103%)	197 (100%)	1 (0%)	86	67

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	B	193/193 (100%)	191 (99%)	2 (1%)	73	43
1	C	200/193 (104%)	200 (100%)	0	100	100
1	D	207/193 (107%)	205 (99%)	2 (1%)	73	43
2	E	8/9 (89%)	8 (100%)	0	100	100
2	F	8/9 (89%)	8 (100%)	0	100	100
2	G	8/9 (89%)	8 (100%)	0	100	100
2	H	8/9 (89%)	8 (100%)	0	100	100
All	All	830/808 (103%)	825 (99%)	5 (1%)	86	62

All (5) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1682	GLU
1	B	1726	ARG
1	B	1817	GLU
1	D	1791[A]	VAL
1	D	1791[B]	VAL

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

Mol	Chain	Res	Type
1	D	1774	ASN
1	D	1779	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

4 non-standard protein/DNA/RNA residues 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	SEP	F	2265	2	8,9,10	0.99	1 (12%)	8,12,14	0.89	0
2	SEP	E	2265	2	8,9,10	1.10	1 (12%)	8,12,14	0.99	0
2	SEP	H	2265	2	8,9,10	1.13	1 (12%)	8,12,14	1.03	0
2	SEP	G	2265	2	8,9,10	0.93	0	8,12,14	0.84	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	SEP	F	2265	2	-	0/5/8/10	-
2	SEP	E	2265	2	-	0/5/8/10	-
2	SEP	H	2265	2	-	0/5/8/10	-
2	SEP	G	2265	2	-	0/5/8/10	-

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	H	2265	SEP	P-O1P	2.79	1.59	1.50
2	E	2265	SEP	P-O1P	2.49	1.58	1.50
2	F	2265	SEP	P-O1P	2.29	1.57	1.50

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

40 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	EDO	A	1905	-	3,3,3	0.48	0	2,2,2	0.53	0
3	EDO	A	1904	-	3,3,3	0.40	0	2,2,2	0.42	0
3	EDO	B	1904	-	3,3,3	0.40	0	2,2,2	0.32	0
3	EDO	C	1909	-	3,3,3	0.55	0	2,2,2	0.36	0
3	EDO	C	1911	-	3,3,3	0.42	0	2,2,2	0.41	0
3	EDO	B	1901	-	3,3,3	0.50	0	2,2,2	0.31	0
4	IMD	B	1908	-	3,5,5	0.44	0	4,5,5	0.49	0
3	EDO	B	1902	-	3,3,3	0.43	0	2,2,2	0.27	0
3	EDO	G	2301	-	3,3,3	0.54	0	2,2,2	0.17	0
3	EDO	D	1905	-	3,3,3	0.49	0	2,2,2	0.28	0
3	EDO	C	1907	-	3,3,3	0.46	0	2,2,2	0.47	0
3	EDO	A	1902	-	3,3,3	0.46	0	2,2,2	0.32	0
3	EDO	B	1905	-	3,3,3	0.42	0	2,2,2	0.44	0
3	EDO	D	1903	-	3,3,3	0.48	0	2,2,2	0.44	0
3	EDO	D	1904	-	3,3,3	0.46	0	2,2,2	0.48	0
3	EDO	C	1901	-	3,3,3	0.44	0	2,2,2	0.19	0
4	IMD	C	1913	-	3,5,5	0.40	0	4,5,5	0.55	0
3	EDO	C	1910	-	3,3,3	0.46	0	2,2,2	0.24	0
3	EDO	C	1908	-	3,3,3	0.46	0	2,2,2	0.32	0
3	EDO	G	2302	-	3,3,3	0.50	0	2,2,2	0.20	0
3	EDO	C	1902	-	3,3,3	0.37	0	2,2,2	0.42	0
3	EDO	B	1907	-	3,3,3	0.39	0	2,2,2	0.53	0
3	EDO	B	1906	-	3,3,3	0.40	0	2,2,2	0.58	0
3	EDO	A	1907	-	3,3,3	0.49	0	2,2,2	0.16	0
3	EDO	D	1906	-	3,3,3	0.38	0	2,2,2	0.41	0
3	EDO	A	1901	-	3,3,3	0.43	0	2,2,2	0.50	0
3	EDO	C	1903	-	3,3,3	0.50	0	2,2,2	0.28	0
3	EDO	C	1906	-	3,3,3	0.51	0	2,2,2	0.57	0
3	EDO	A	1903	-	3,3,3	0.53	0	2,2,2	0.55	0
3	EDO	D	1907	-	3,3,3	0.51	0	2,2,2	0.44	0
3	EDO	D	1902	-	3,3,3	0.50	0	2,2,2	0.48	0
3	EDO	C	1905	-	3,3,3	0.64	0	2,2,2	0.30	0
5	PEG	C	1912	-	6,6,6	0.15	0	5,5,5	0.11	0
3	EDO	A	1908	-	3,3,3	0.48	0	2,2,2	0.32	0
3	EDO	C	1904	-	3,3,3	0.46	0	2,2,2	0.13	0
3	EDO	A	1906	-	3,3,3	0.42	0	2,2,2	0.51	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	EDO	D	1901	-	3,3,3	0.53	0	2,2,2	0.30	0
3	EDO	D	1908	-	3,3,3	0.44	0	2,2,2	0.46	0
3	EDO	A	1909	-	3,3,3	0.41	0	2,2,2	0.42	0
3	EDO	B	1903	-	3,3,3	0.41	0	2,2,2	0.20	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
3	EDO	A	1905	-	-	1/1/1/1	-
3	EDO	A	1904	-	-	0/1/1/1	-
3	EDO	B	1904	-	-	0/1/1/1	-
3	EDO	C	1909	-	-	0/1/1/1	-
3	EDO	C	1911	-	-	0/1/1/1	-
3	EDO	B	1901	-	-	0/1/1/1	-
4	IMD	B	1908	-	-	-	0/1/1/1
3	EDO	B	1902	-	-	0/1/1/1	-
3	EDO	G	2301	-	-	0/1/1/1	-
3	EDO	D	1905	-	-	0/1/1/1	-
3	EDO	C	1907	-	-	0/1/1/1	-
3	EDO	A	1902	-	-	0/1/1/1	-
3	EDO	B	1905	-	-	1/1/1/1	-
3	EDO	D	1903	-	-	0/1/1/1	-
3	EDO	D	1904	-	-	1/1/1/1	-
3	EDO	C	1901	-	-	1/1/1/1	-
4	IMD	C	1913	-	-	-	0/1/1/1
3	EDO	C	1910	-	-	0/1/1/1	-
3	EDO	C	1908	-	-	0/1/1/1	-
3	EDO	G	2302	-	-	0/1/1/1	-
3	EDO	C	1902	-	-	1/1/1/1	-
3	EDO	B	1907	-	-	0/1/1/1	-
3	EDO	B	1906	-	-	1/1/1/1	-
3	EDO	A	1907	-	-	0/1/1/1	-
3	EDO	D	1906	-	-	0/1/1/1	-
3	EDO	A	1901	-	-	0/1/1/1	-
3	EDO	C	1903	-	-	0/1/1/1	-
3	EDO	C	1906	-	-	0/1/1/1	-
3	EDO	A	1903	-	-	0/1/1/1	-
3	EDO	D	1907	-	-	0/1/1/1	-
3	EDO	D	1902	-	-	0/1/1/1	-
3	EDO	C	1905	-	-	0/1/1/1	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	PEG	C	1912	-	-	0/4/4/4	-
3	EDO	A	1908	-	-	0/1/1/1	-
3	EDO	C	1904	-	-	0/1/1/1	-
3	EDO	A	1906	-	-	0/1/1/1	-
3	EDO	D	1901	-	-	0/1/1/1	-
3	EDO	D	1908	-	-	1/1/1/1	-
3	EDO	A	1909	-	-	1/1/1/1	-
3	EDO	B	1903	-	-	1/1/1/1	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

5 of 9 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	D	1904	EDO	O1-C1-C2-O2
3	A	1909	EDO	O1-C1-C2-O2
3	C	1902	EDO	O1-C1-C2-O2
3	A	1905	EDO	O1-C1-C2-O2
3	B	1903	EDO	O1-C1-C2-O2

There are no ring outliers.

6 monomers are involved in 7 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	C	1911	EDO	1	0
4	B	1908	IMD	1	0
3	B	1902	EDO	1	0
3	C	1903	EDO	1	0
3	C	1904	EDO	2	0
3	D	1901	EDO	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, 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	210/217 (96%)	-0.19	2 (0%) 79 83	10, 25, 42, 54	6 (2%)
1	B	205/217 (94%)	-0.13	5 (2%) 59 65	16, 27, 46, 65	5 (2%)
1	C	210/217 (96%)	-0.38	2 (0%) 79 83	10, 22, 38, 55	9 (4%)
1	D	210/217 (96%)	-0.30	2 (0%) 79 83	11, 23, 41, 59	11 (5%)
2	E	9/11 (81%)	0.61	2 (22%) 3 3	22, 35, 55, 58	0
2	F	9/11 (81%)	0.56	1 (11%) 12 12	20, 30, 46, 54	0
2	G	9/11 (81%)	0.25	0 100 100	19, 29, 39, 56	0
2	H	9/11 (81%)	0.64	1 (11%) 12 12	19, 29, 52, 56	0
All	All	871/912 (95%)	-0.22	15 (1%) 69 74	10, 25, 44, 65	31 (3%)

The worst 5 of 15 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	F	2261	PRO	4.5
2	H	2261	PRO	3.9
1	B	1816	THR	3.4
2	E	2261	PRO	3.3
2	E	2270	SER	3.2

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

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(Å ²)	Q<0.9
2	SEP	E	2265	10/11	0.99	0.05	19,22,27,29	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
2	SEP	F	2265	10/11	0.99	0.04	17,19,24,27	0
2	SEP	G	2265	10/11	0.99	0.05	17,19,23,23	0
2	SEP	H	2265	10/11	0.99	0.05	18,20,25,28	0

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(\AA^2)	Q<0.9
3	EDO	D	1903	4/4	0.79	0.16	48,57,64,71	0
3	EDO	B	1907	4/4	0.81	0.14	48,58,61,63	0
5	PEG	C	1912	7/7	0.81	0.15	45,54,65,67	0
3	EDO	A	1909	4/4	0.83	0.13	51,61,63,64	0
3	EDO	D	1904	4/4	0.83	0.16	46,56,57,59	0
3	EDO	C	1906	4/4	0.83	0.14	37,45,46,50	0
3	EDO	C	1904	4/4	0.84	0.14	40,48,54,61	0
3	EDO	D	1908	4/4	0.85	0.14	41,50,58,61	0
4	IMD	B	1908	5/5	0.85	0.12	51,53,63,63	0
3	EDO	B	1906	4/4	0.85	0.15	50,60,62,65	0
3	EDO	C	1909	4/4	0.86	0.14	33,39,40,42	0
3	EDO	A	1905	4/4	0.86	0.14	38,50,57,62	0
3	EDO	A	1903	4/4	0.87	0.13	32,39,39,41	0
4	IMD	C	1913	5/5	0.87	0.11	46,51,61,62	0
3	EDO	C	1907	4/4	0.87	0.13	39,47,53,57	0
3	EDO	C	1910	4/4	0.88	0.12	50,60,61,63	0
3	EDO	G	2302	4/4	0.88	0.12	51,61,66,68	0
3	EDO	C	1911	4/4	0.88	0.11	46,55,58,60	0
3	EDO	A	1908	4/4	0.88	0.11	47,56,57,63	0
3	EDO	C	1902	4/4	0.88	0.13	47,57,60,63	0
3	EDO	C	1908	4/4	0.89	0.10	55,66,69,70	0
3	EDO	C	1905	4/4	0.90	0.12	29,35,39,39	0
3	EDO	A	1907	4/4	0.90	0.10	47,57,59,60	0
3	EDO	A	1906	4/4	0.91	0.10	28,35,37,44	0
3	EDO	A	1904	4/4	0.92	0.10	30,36,40,42	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
3	EDO	B	1905	4/4	0.92	0.14	59,70,73,75	0
3	EDO	C	1903	4/4	0.93	0.10	29,40,45,51	0
3	EDO	D	1906	4/4	0.94	0.08	34,43,48,55	0
3	EDO	B	1903	4/4	0.94	0.10	39,47,49,49	0
3	EDO	D	1902	4/4	0.94	0.08	30,37,39,40	0
3	EDO	D	1901	4/4	0.95	0.08	20,35,43,45	0
3	EDO	B	1904	4/4	0.95	0.08	33,45,50,55	0
3	EDO	D	1905	4/4	0.95	0.09	24,35,42,42	0
3	EDO	D	1907	4/4	0.96	0.08	31,42,46,50	0
3	EDO	B	1902	4/4	0.96	0.08	32,41,50,52	0
3	EDO	A	1901	4/4	0.97	0.06	24,28,30,31	0
3	EDO	G	2301	4/4	0.97	0.07	20,30,38,39	0
3	EDO	A	1902	4/4	0.97	0.06	29,35,36,37	0
3	EDO	C	1901	4/4	0.99	0.04	25,30,34,34	0
3	EDO	B	1901	4/4	0.99	0.03	19,23,25,26	0

6.5 Other polymers ⓘ

There are no such residues in this entry.