



# Full wwPDB X-ray Structure Validation Report ⓘ

Nov 13, 2023 – 04:06 PM EST

PDB ID : 8TRS  
Title : Structure of the EphA2 CRD bound to FabS1CE\_C1, trigonal form  
Authors : Singer, A.U.; Bruce, H.A.; Blazer, L.; Adams, J.J.; Sicheri, F.; Sidhu, S.S.  
Deposited on : 2023-08-10  
Resolution : 1.90 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

<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>.

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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 : 1.8.5 (274361), CSD as541be (2020)  
Xtrriage (Phenix) : 1.13  
EDS : 2.36  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
Refmac : 5.8.0158  
CCP4 : 7.0.044 (Gargrove)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.36

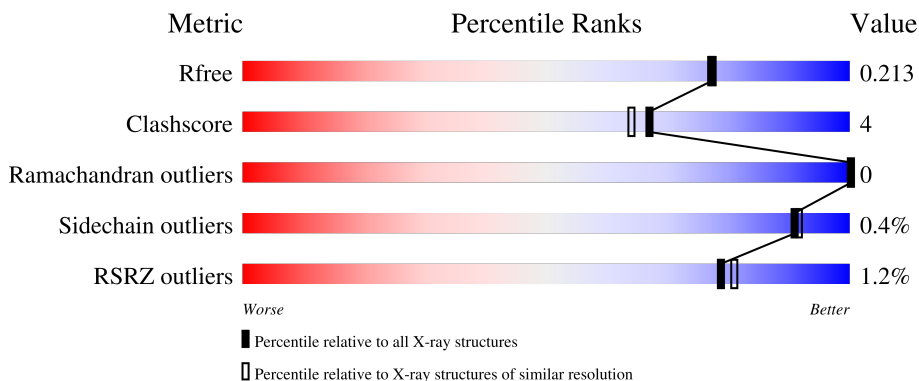
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 1.90 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))
$R_{free}$	130704	6207 (1.90-1.90)
Clashscore	141614	6847 (1.90-1.90)
Ramachandran outliers	138981	6760 (1.90-1.90)
Sidechain outliers	138945	6760 (1.90-1.90)
RSRZ outliers	127900	6082 (1.90-1.90)

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  $\geq 3$ , 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	222	 89% 8% .
2	G	215	 94% 6%
3	D	132	 5% 90% 9% .

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
6	CL	A	317	-	-	X	-

## 2 Entry composition

There are 8 unique types of molecules in this entry. The entry contains 4598 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 S1CE variant of Fab C1 heavy chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	216	1614	1029	263	315	7	0	0	0

- Molecule 2 is a protein called S1CE variant of Fab C1 light chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	G	215	1658	1040	270	342	6	0	4	0

- Molecule 3 is a protein called Ephrin type-A receptor 2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
3	D	131	942	589	153	186	14	0	0	0

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
D	327	LEU	-	expression tag	UNP P29317
D	328	VAL	-	expression tag	UNP P29317
D	329	PRO	-	expression tag	UNP P29317
D	330	ARG	-	expression tag	UNP P29317

- Molecule 4 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: C<sub>2</sub>H<sub>6</sub>O<sub>2</sub>).



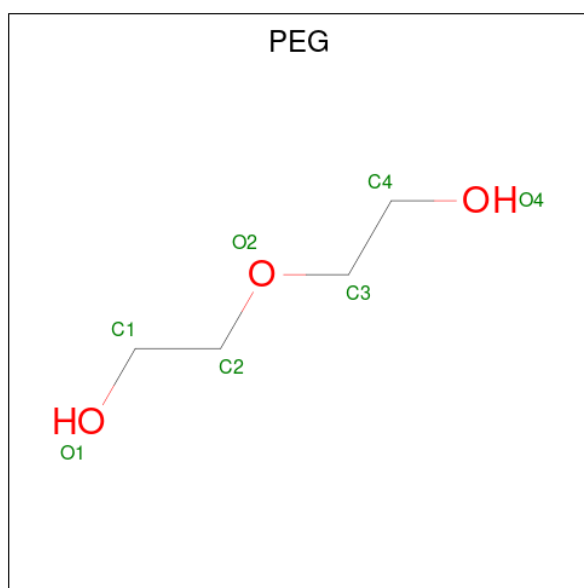
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total C O 4 2 2	0	0
4	A	1	Total C O 4 2 2	0	0
4	A	1	Total C O 4 2 2	0	0
4	A	1	Total C O 4 2 2	0	0
4	A	1	Total C O 4 2 2	0	0
4	A	1	Total C O 4 2 2	0	0
4	A	1	Total C O 4 2 2	0	0
4	A	1	Total C O 4 2 2	0	0
4	A	1	Total C O 4 2 2	0	0
4	A	1	Total C O 4 2 2	0	0
4	G	1	Total C O 4 2 2	0	0
4	G	1	Total C O 4 2 2	0	0
4	G	1	Total C O 4 2 2	0	0
4	G	1	Total C O 4 2 2	0	0
4	G	1	Total C O 4 2 2	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	G	1	Total C O 4 2 2	0	0
4	G	1	Total C O 4 2 2	0	0
4	G	1	Total C O 4 2 2	0	0
4	G	1	Total C O 4 2 2	0	0
4	D	1	Total C O 4 2 2	0	0

- Molecule 5 is DI(HYDROXYETHYL)ETHER (three-letter code: PEG) (formula: C<sub>4</sub>H<sub>10</sub>O<sub>3</sub>).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	1	Total C O 7 4 3	0	0
5	A	1	Total C O 7 4 3	0	0
5	G	1	Total C O 7 4 3	0	0
5	G	1	Total C O 7 4 3	0	0
5	G	1	Total C O 7 4 3	0	0
5	G	1	Total C O 7 4 3	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	G	1	Total	C O	0	0
			7	4 3		

- Molecule 6 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	7	Total	Cl	0	1
			8	8		
6	G	8	Total	Cl	0	0
			8	8		
6	D	2	Total	Cl	0	0
			2	2		

- Molecule 7 is SODIUM ION (three-letter code: NA) (formula: Na).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	D	1	Total	Na	0	0
			1	1		


- Molecule 8 is water.

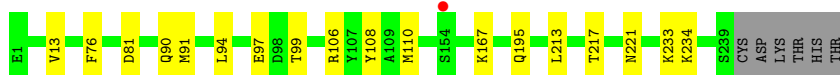
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	A	93	Total	O	0	1
			94	94		
8	G	108	Total	O	0	1
			109	109		
8	D	36	Total	O	0	1
			37	37		

### 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: S1CE variant of Fab C1 heavy chain

Chain A:  89% 8%

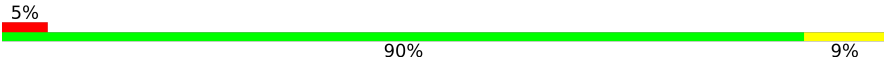


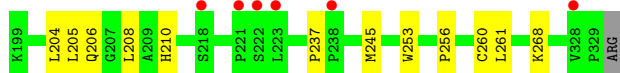
- Molecule 2: S1CE variant of Fab C1 light chain

Chain G:  94% 6%



- Molecule 3: Ephrin type-A receptor 2

Chain D:  5% 90% 9%





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 32 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	71.38Å 71.38Å 235.01Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	61.81 – 1.90 61.81 – 1.90	Depositor EDS
% Data completeness (in resolution range)	100.0 (61.81-1.90) 100.0 (61.81-1.90)	Depositor EDS
$R_{merge}$	0.05	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.31 (at 1.90Å)	Xtrriage
Refinement program	PHENIX 1.20.1_4487	Depositor
R, $R_{free}$	0.180 , 0.214 0.180 , 0.213	Depositor DCC
$R_{free}$ test set	2734 reflections (4.89%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	41.8	Xtrriage
Anisotropy	0.188	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.34 , 53.8	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.33$	Xtrriage
Estimated twinning fraction	0.024 for -h,-k,l	Xtrriage
$F_o, F_c$ correlation	0.97	EDS
Total number of atoms	4598	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	50.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.83% 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 [i](#)

### 5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: PEG, NA, EDO, CL

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	0.41	0/1657	0.63	0/2264
2	G	0.39	0/1698	0.63	0/2311
3	D	0.36	0/970	0.57	0/1329
All	All	0.39	0/4325	0.61	0/5904

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	1614	0	1547	14	0
2	G	1658	0	1579	11	0
3	D	942	0	853	6	0
4	A	36	0	54	3	0
4	D	4	0	6	0	0
4	G	36	0	54	2	0
5	A	14	0	20	3	0
5	G	35	0	50	4	0
6	A	8	0	0	2	0
6	D	2	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	G	8	0	0	1	0
7	D	1	0	0	0	0
8	A	94	0	0	0	0
8	D	37	0	0	0	0
8	G	109	0	0	2	0
All	All	4598	0	4163	33	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 4.

All (33) 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)
3:D:245:MET:HG2	3:D:253:TRP:CE3	2.25	0.70
2:G:217:GLY:H	5:G:306:PEG:H12	1.59	0.68
1:A:90:GLN:HG2	5:A:308:PEG:H41	1.79	0.63
3:D:208:LEU:HD21	3:D:268:LYS:HG3	1.79	0.62
1:A:97:GLU:N	6:A:317:CL:CL	2.66	0.61
3:D:206:GLN:HG2	3:D:256:PRO:HG3	1.85	0.59
1:A:217:THR:HG23	1:A:234:LYS:HE2	1.85	0.58
2:G:22[B]:THR:HG22	2:G:88[B]:THR:HB	1.85	0.58
2:G:118:GLN:HG3	6:G:319:CL:CL	2.45	0.52
1:A:108:TYR:CD1	2:G:114(A):ILE:HD11	2.45	0.52
3:D:204:LEU:HD22	3:D:253:TRP:CD1	2.46	0.51
1:A:13:VAL:HG11	1:A:94:LEU:HD13	1.96	0.47
2:G:140:ASP:O	2:G:144:LYS:HD2	2.15	0.47
1:A:167:LYS:NZ	1:A:195:GLN:OE1	2.48	0.47
5:G:305:PEG:H32	8:G:413:HOH:O	2.14	0.47
1:A:81:ASP:HB2	5:A:309:PEG:H31	1.97	0.46
3:D:205:LEU:HD23	3:D:210:HIS:HA	1.97	0.46
2:G:96[B]:PRO:HB3	5:G:308:PEG:H41	1.97	0.45
1:A:221:ASN:HB2	4:A:310:EDO:H22	1.99	0.45
5:G:312:PEG:H22	5:G:312:PEG:H41	1.62	0.43
3:D:260:CYS:O	3:D:261:LEU:HD23	2.19	0.43
1:A:99:THR:OG1	4:A:306:EDO:H21	2.19	0.42
2:G:125:LYS:HB3	2:G:125:LYS:HE2	1.89	0.42
1:A:97:GLU:CB	6:A:317:CL:CL	3.05	0.41
1:A:213:LEU:HD23	1:A:213:LEU:HA	1.88	0.41
1:A:76:PHE:CE1	1:A:91:MET:HB3	2.56	0.41
1:A:106:ARG:O	1:A:110:MET:HA	2.21	0.41
2:G:216:GLN:HG3	8:G:405:HOH:O	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:303:EDO:H21	4:A:305:EDO:H22	2.03	0.41
5:A:309:PEG:H12	5:A:309:PEG:H32	1.28	0.40
2:G:231:GLU:O	4:G:313:EDO:H22	2.21	0.40
1:A:108:TYR:CE1	2:G:114(A):ILE:HD11	2.57	0.40
2:G:163:LYS:HG3	4:G:309:EDO:H21	2.03	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	214/222 (96%)	212 (99%)	2 (1%)	0	100	100
2	G	217/215 (101%)	212 (98%)	5 (2%)	0	100	100
3	D	129/132 (98%)	126 (98%)	3 (2%)	0	100	100
All	All	560/569 (98%)	550 (98%)	10 (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	174/186 (94%)	173 (99%)	1 (1%)	86	87
2	G	186/187 (100%)	186 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
3	D	101/107 (94%)	100 (99%)	1 (1%)	76	76
All	All	461/480 (96%)	459 (100%)	2 (0%)	91	91

All (2) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	233	LYS
3	D	237	PRO

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

### 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 monosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

Of 45 ligands modelled in this entry, 19 are monoatomic - leaving 26 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	$\# Z  > 2$
4	EDO	D	401	-	3,3,3	0.48	0	2,2,2	0.22	0
5	PEG	G	308	-	6,6,6	0.17	0	5,5,5	0.12	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
5	PEG	G	312	-	6,6,6	0.12	0	5,5,5	0.14	0
4	EDO	G	307	-	3,3,3	0.52	0	2,2,2	0.05	0
4	EDO	G	311	-	3,3,3	0.50	0	2,2,2	0.38	0
4	EDO	A	310	-	3,3,3	0.56	0	2,2,2	0.23	0
4	EDO	G	301	-	3,3,3	0.65	0	2,2,2	0.29	0
4	EDO	A	307	-	3,3,3	0.57	0	2,2,2	0.27	0
4	EDO	A	304	-	3,3,3	0.41	0	2,2,2	0.61	0
4	EDO	A	301	-	3,3,3	0.44	0	2,2,2	0.75	0
4	EDO	A	302	-	3,3,3	0.68	0	2,2,2	0.29	0
4	EDO	G	309	-	3,3,3	0.45	0	2,2,2	0.47	0
4	EDO	A	303	-	3,3,3	0.46	0	2,2,2	0.44	0
4	EDO	A	306	-	3,3,3	0.46	0	2,2,2	0.48	0
4	EDO	A	305	-	3,3,3	0.52	0	2,2,2	0.34	0
4	EDO	A	311	-	3,3,3	0.53	0	2,2,2	0.28	0
5	PEG	A	309	-	6,6,6	0.24	0	5,5,5	0.14	0
5	PEG	A	308	-	6,6,6	0.24	0	5,5,5	0.22	0
5	PEG	G	306	-	6,6,6	0.15	0	5,5,5	0.11	0
4	EDO	G	314	-	3,3,3	0.52	0	2,2,2	0.29	0
4	EDO	G	313	-	3,3,3	0.55	0	2,2,2	0.16	0
4	EDO	G	310	-	3,3,3	0.50	0	2,2,2	0.33	0
5	PEG	G	304	-	6,6,6	0.14	0	5,5,5	0.08	0
4	EDO	G	302	-	3,3,3	0.45	0	2,2,2	0.37	0
5	PEG	G	305	-	6,6,6	0.11	0	5,5,5	0.09	0
4	EDO	G	303	-	3,3,3	0.58	0	2,2,2	0.07	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
4	EDO	D	401	-	-	0/1/1/1	-
5	PEG	G	308	-	-	1/4/4/4	-
5	PEG	G	312	-	-	2/4/4/4	-
4	EDO	G	307	-	-	0/1/1/1	-
4	EDO	G	311	-	-	1/1/1/1	-
4	EDO	A	310	-	-	0/1/1/1	-
4	EDO	G	301	-	-	0/1/1/1	-
4	EDO	A	307	-	-	0/1/1/1	-
4	EDO	A	304	-	-	0/1/1/1	-
4	EDO	A	301	-	-	0/1/1/1	-
4	EDO	A	302	-	-	1/1/1/1	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	EDO	G	309	-	-	0/1/1/1	-
4	EDO	A	303	-	-	0/1/1/1	-
4	EDO	A	306	-	-	1/1/1/1	-
4	EDO	A	305	-	-	1/1/1/1	-
4	EDO	A	311	-	-	0/1/1/1	-
5	PEG	A	309	-	-	2/4/4/4	-
5	PEG	A	308	-	-	3/4/4/4	-
5	PEG	G	306	-	-	3/4/4/4	-
4	EDO	G	314	-	-	1/1/1/1	-
4	EDO	G	313	-	-	1/1/1/1	-
4	EDO	G	310	-	-	0/1/1/1	-
5	PEG	G	304	-	-	1/4/4/4	-
4	EDO	G	302	-	-	0/1/1/1	-
5	PEG	G	305	-	-	3/4/4/4	-
4	EDO	G	303	-	-	1/1/1/1	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (22) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	A	309	PEG	C1-C2-O2-C3
5	A	308	PEG	O1-C1-C2-O2
5	A	309	PEG	O1-C1-C2-O2
5	G	312	PEG	O1-C1-C2-O2
5	G	312	PEG	C4-C3-O2-C2
5	G	304	PEG	O2-C3-C4-O4
5	G	306	PEG	O1-C1-C2-O2
5	G	305	PEG	C1-C2-O2-C3
5	G	305	PEG	O1-C1-C2-O2
4	A	306	EDO	O1-C1-C2-O2
5	A	308	PEG	C1-C2-O2-C3
4	G	314	EDO	O1-C1-C2-O2
4	G	313	EDO	O1-C1-C2-O2
5	G	306	PEG	C4-C3-O2-C2
4	G	303	EDO	O1-C1-C2-O2
5	A	308	PEG	O2-C3-C4-O4
5	G	306	PEG	C1-C2-O2-C3
5	G	308	PEG	C1-C2-O2-C3

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Mol	Chain	Res	Type	Atoms
4	A	302	EDO	O1-C1-C2-O2
4	G	311	EDO	O1-C1-C2-O2
5	G	305	PEG	O2-C3-C4-O4
4	A	305	EDO	O1-C1-C2-O2

There are no ring outliers.

12 monomers are involved in 12 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	G	308	PEG	1	0
5	G	312	PEG	1	0
4	A	310	EDO	1	0
4	G	309	EDO	1	0
4	A	303	EDO	1	0
4	A	306	EDO	1	0
4	A	305	EDO	1	0
5	A	309	PEG	2	0
5	A	308	PEG	1	0
5	G	306	PEG	1	0
4	G	313	EDO	1	0
5	G	305	PEG	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 [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, 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	216/222 (97%)	-0.18	1 (0%) 91   92	32, 43, 62, 86	0
2	G	215/215 (100%)	-0.16	0 100   100	32, 45, 67, 103	0
3	D	131/132 (99%)	0.17	6 (4%) 32   35	37, 61, 95, 108	0
All	All	562/569 (98%)	-0.09	7 (1%) 79   81	32, 46, 78, 108	0

All (7) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	D	238	PRO	6.4
3	D	222	SER	4.0
3	D	218	SER	2.8
3	D	221	PRO	2.6
3	D	328	VAL	2.4
1	A	154	SER	2.4
3	D	223	LEU	2.1

### 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 monosaccharides 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, 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	B-factors(Å <sup>2</sup> )	Q<0.9
6	CL	A	314	1/1	0.54	0.11	82,82,82,82	0
5	PEG	G	306	7/7	0.69	0.21	63,64,71,74	0
6	CL	G	322	1/1	0.70	0.09	84,84,84,84	0
4	EDO	A	305	4/4	0.71	0.26	55,57,69,71	0
6	CL	A	316	1/1	0.71	0.12	87,87,87,87	0
4	EDO	A	302	4/4	0.71	0.16	42,48,57,60	0
6	CL	D	403	1/1	0.71	0.16	90,90,90,90	0
4	EDO	G	307	4/4	0.73	0.16	63,64,70,74	0
4	EDO	A	311	4/4	0.75	0.18	58,61,64,69	0
6	CL	G	316	1/1	0.75	0.17	87,87,87,87	0
6	CL	A	318[B]	1/1	0.76	0.11	55,55,55,55	1
6	CL	A	318[A]	1/1	0.76	0.11	65,65,65,65	1
4	EDO	A	307	4/4	0.78	0.22	55,58,60,63	0
4	EDO	G	314	4/4	0.78	0.25	58,58,63,67	0
6	CL	A	312	1/1	0.79	0.10	70,70,70,70	0
6	CL	A	315	1/1	0.81	0.08	82,82,82,82	0
4	EDO	A	303	4/4	0.82	0.26	55,57,58,66	0
5	PEG	A	308	7/7	0.82	0.26	34,56,67,72	0
5	PEG	G	308	7/7	0.83	0.18	58,64,69,74	0
5	PEG	G	312	7/7	0.84	0.24	69,69,73,83	0
4	EDO	G	313	4/4	0.84	0.14	68,70,71,86	0
6	CL	A	317	1/1	0.85	0.10	73,73,73,73	0
5	PEG	A	309	7/7	0.85	0.27	50,57,66,71	0
4	EDO	A	306	4/4	0.85	0.36	54,57,63,69	0
4	EDO	G	310	4/4	0.86	0.12	62,63,69,71	0
4	EDO	A	310	4/4	0.87	0.21	47,49,61,67	0
5	PEG	G	304	7/7	0.88	0.11	58,62,71,71	0
6	CL	G	317	1/1	0.88	0.06	82,82,82,82	0
4	EDO	G	303	4/4	0.89	0.12	48,54,56,59	0
4	EDO	G	311	4/4	0.90	0.15	56,58,66,66	0
5	PEG	G	305	7/7	0.91	0.10	53,53,67,68	0
6	CL	G	321	1/1	0.91	0.10	76,76,76,76	0
6	CL	G	315	1/1	0.91	0.09	79,79,79,79	0
4	EDO	G	309	4/4	0.91	0.20	54,66,66,73	0
6	CL	G	318	1/1	0.92	0.07	85,85,85,85	0
4	EDO	G	301	4/4	0.92	0.15	35,47,51,61	0
7	NA	D	404	1/1	0.92	0.18	75,75,75,75	0
6	CL	D	402	1/1	0.93	0.07	76,76,76,76	0
4	EDO	D	401	4/4	0.93	0.10	58,60,60,62	0
6	CL	A	313	1/1	0.93	0.15	75,75,75,75	0
6	CL	G	320	1/1	0.96	0.09	69,69,69,69	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
4	EDO	G	302	4/4	0.96	0.12	39,49,57,70	0
4	EDO	A	301	4/4	0.97	0.11	36,38,39,39	0
6	CL	G	319	1/1	0.97	0.19	67,67,67,67	0
4	EDO	A	304	4/4	0.98	0.11	39,40,46,52	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.