



# wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 6, 2026 – 01:24 AM UTC

PDB ID : 6UJ9 / pdb\_00006uj9  
Title : Crystal structure of HLA-B\*07:02 with R140Q mutant IDH2 peptide in complex with Fab  
Authors : Miller, M.S.; Thirawatananond, P.; Aytenfisu, T.Y.; Wright, K.; Gabelli, S.B.  
Deposited on : 2019-10-02  
Resolution : 2.90 Å(reported)

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

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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 : 4-5-2 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

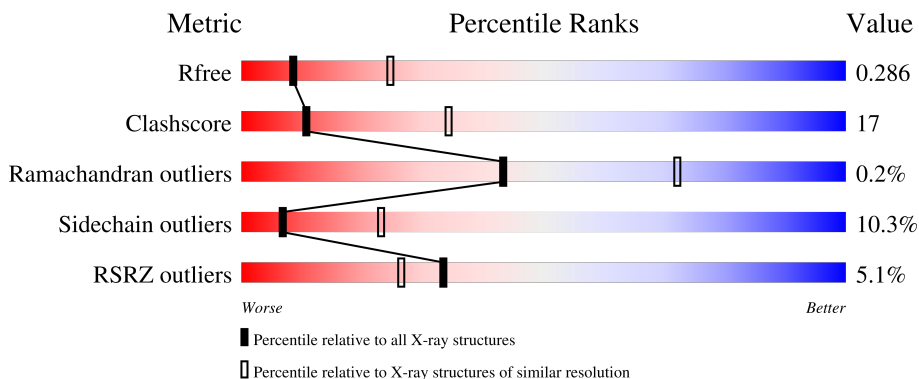
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.90 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))
$R_{free}$	180053	2481 (2.90-2.90)
Clashscore	190562	2690 (2.90-2.90)
Ramachandran outliers	187476	2623 (2.90-2.90)
Sidechain outliers	187428	2625 (2.90-2.90)
RSRZ outliers	180081	2481 (2.90-2.90)

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	298	 10% 59% 28% 6% 7%
2	B	119	 2% 56% 24% 16%
3	C	10	 60% 40%
4	L	214	 74% 22%
5	H	218	 3% 68% 26% 6%

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:

<b>Mol</b>	<b>Type</b>	<b>Chain</b>	<b>Res</b>	<b>Chirality</b>	<b>Geometry</b>	<b>Clashes</b>	<b>Electron density</b>
6	PEG	B	501	-	-	X	-

## 2 Entry composition

There are 9 unique types of molecules in this entry. The entry contains 6557 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 HLA class I histocompatibility antigen, B-7 alpha chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	277	2270	1409	415	439	7	0	0	0

There are 18 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	0	MET	-	initiating methionine	UNP P01889
A	281	GLY	-	expression tag	UNP P01889
A	282	SER	-	expression tag	UNP P01889
A	283	LEU	-	expression tag	UNP P01889
A	284	HIS	-	expression tag	UNP P01889
A	285	HIS	-	expression tag	UNP P01889
A	286	ILE	-	expression tag	UNP P01889
A	287	LEU	-	expression tag	UNP P01889
A	288	ASP	-	expression tag	UNP P01889
A	289	ALA	-	expression tag	UNP P01889
A	290	GLN	-	expression tag	UNP P01889
A	291	LYS	-	expression tag	UNP P01889
A	292	MET	-	expression tag	UNP P01889
A	293	VAL	-	expression tag	UNP P01889
A	294	TRP	-	expression tag	UNP P01889
A	295	ASN	-	expression tag	UNP P01889
A	296	HIS	-	expression tag	UNP P01889
A	297	ARG	-	expression tag	UNP P01889

- Molecule 2 is a protein called Beta-2-microglobulin.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	B	100	834	531	141	159	3	0	0	0

- Molecule 3 is a protein called Isocitrate dehydrogenase [NADP], mitochondrial.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
3	C	10	74	45	13	16	0	0	0

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	7	GLN	ARG	engineered mutation	UNP P48735

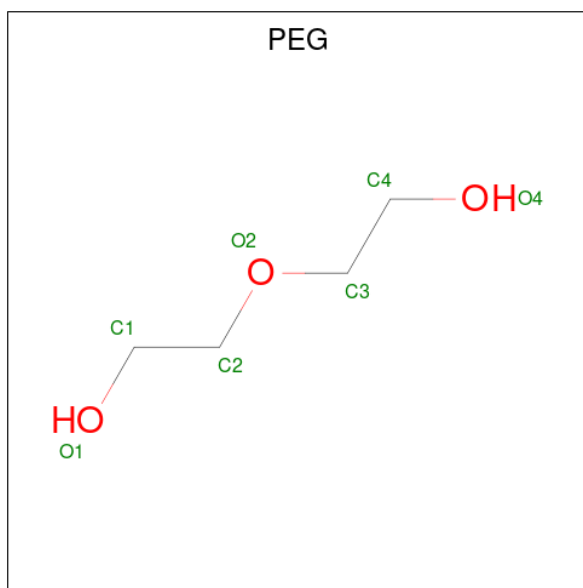
- Molecule 4 is a protein called Fab light chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
4	L	213	1642	1030	274	333	5	0	0	0

- Molecule 5 is a protein called Fab heavy chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
5	H	218	1640	1040	272	321	7	0	0	0

- Molecule 6 is DI(HYDROXYETHYL)ETHER (CCD ID: PEG) (formula: C<sub>4</sub>H<sub>10</sub>O<sub>3</sub>).



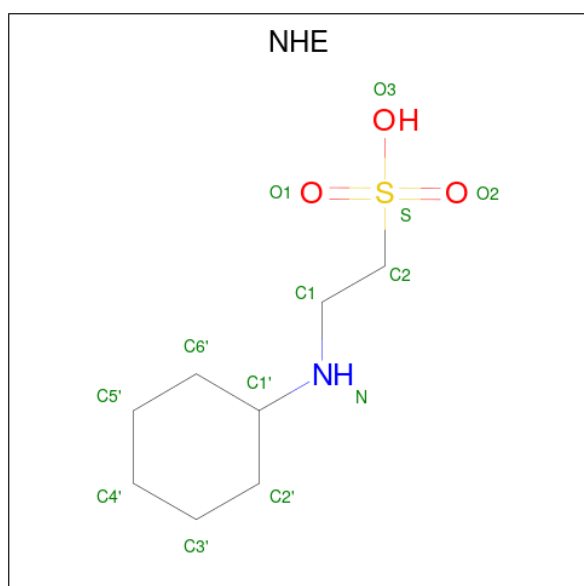
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	C	O		
6	A	1	7	4	3	0	0
6	A	1	7	4	3	0	0

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	A	1	Total	C	O	0	0
			7	4	3		
6	B	1	Total	C	O	0	0
			7	4	3		
6	L	1	Total	C	O	0	0
			7	4	3		
6	L	1	Total	C	O	0	0
			7	4	3		

- Molecule 7 is 2-[N-CYCLOHEXYLAMINO]ETHANE SULFONIC ACID (CCD ID: NHE) (formula: C<sub>8</sub>H<sub>17</sub>NO<sub>3</sub>S).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
7	A	1	Total	C	N	O	S	0	0
			13	8	1	3	1		

- Molecule 8 is SULFATE ION (CCD ID: SO4) (formula: O<sub>4</sub>S).



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

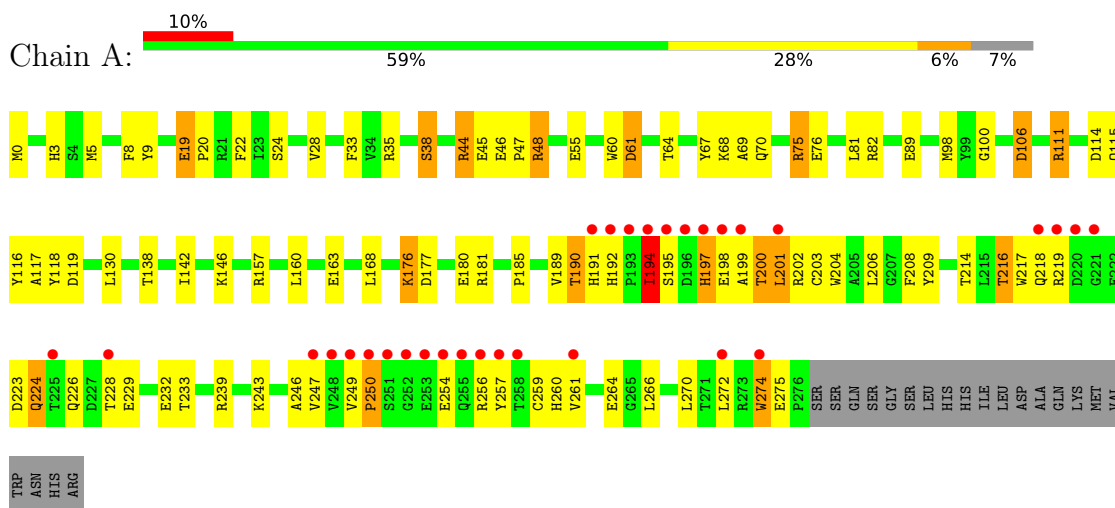
- Molecule 9 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
9	C	1	Total O 1 1	0	0
9	H	1	Total O 1 1	0	0

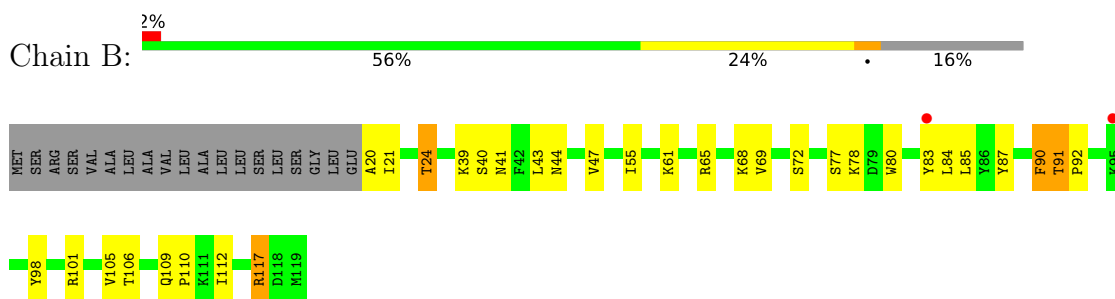
### 3 Residue-property plots [i](#)

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: HLA class I histocompatibility antigen, B-7 alpha chain



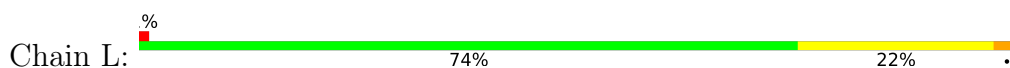
- Molecule 2: Beta-2-microglobulin

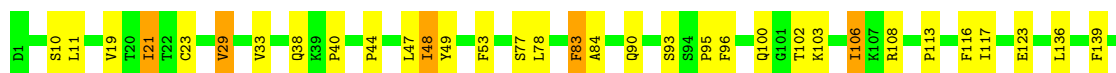


- Molecule 3: Isocitrate dehydrogenase [NADP], mitochondrial

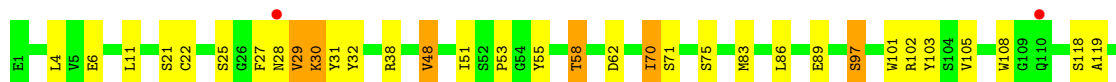


- Molecule 4: Fab light chain





- Molecule 5: Fab heavy chain



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	83.61Å 42.01Å 125.18Å 90.00° 92.75° 90.00°	Depositor
Resolution (Å)	48.93 – 2.90 48.93 – 2.90	Depositor EDS
% Data completeness (in resolution range)	98.2 (48.93-2.90) 98.2 (48.93-2.90)	Depositor EDS
$R_{merge}$	0.15	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.80 (at 2.91Å)	Xtrriage
Refinement program	REFMAC 5.8.0257	Depositor
R, $R_{free}$	0.214 , 0.287 0.222 , 0.286	Depositor DCC
$R_{free}$ test set	973 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	44.2	Xtrriage
Anisotropy	0.396	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.33 , 32.2	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.33$	Xtrriage
Estimated twinning fraction	0.014 for h,-k,-l	Xtrriage
$F_o, F_c$ correlation	0.91	EDS
Total number of atoms	6557	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	44.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 7.08% 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, SO4, NHE

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	1.02	0/2333	1.48	13/3169 (0.4%)
2	B	0.95	0/857	1.26	0/1159
3	C	0.98	0/74	1.27	0/99
4	L	0.99	0/1678	1.33	5/2279 (0.2%)
5	H	1.01	1/1683 (0.1%)	1.29	3/2297 (0.1%)
All	All	1.00	1/6625 (0.0%)	1.36	21/9003 (0.2%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	H	101	TRP	C-O	-5.46	1.17	1.24

The worst 5 of 21 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	H	53	PRO	CB-CA-C	-7.42	102.29	111.64
1	A	61	ASP	CA-CB-CG	6.82	119.42	112.60
1	A	250	PRO	CA-C-N	6.32	129.84	120.87
1	A	250	PRO	C-N-CA	6.32	129.84	120.87
4	L	95	PRO	N-CD-CG	-6.24	96.32	103.80

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	2270	0	2114	111	0
2	B	834	0	796	32	0
3	C	74	0	77	4	0
4	L	1642	0	1595	36	0
5	H	1640	0	1598	51	0
6	A	21	0	30	1	0
6	B	7	0	10	4	0
6	L	14	0	20	0	0
7	A	13	0	17	3	0
8	A	25	0	0	0	0
8	B	5	0	0	0	0
8	H	10	0	0	0	0
9	C	1	0	0	0	0
9	H	1	0	0	0	0
All	All	6557	0	6257	214	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 17.

The worst 5 of 214 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:249:VAL:HG21	1:A:257:TYR:CE1	1.67	1.28
1:A:249:VAL:HG22	1:A:250:PRO:HD2	1.26	1.12
1:A:249:VAL:CG2	1:A:250:PRO:HD2	1.82	1.10
1:A:76:GLU:HG3	5:H:103:TYR:OH	1.60	1.01
1:A:119:ASP:HB3	2:B:20:ALA:CB	1.93	0.97

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	275/298 (92%)	264 (96%)	10 (4%)	1 (0%)	30	59
2	B	98/119 (82%)	96 (98%)	2 (2%)	0	100	100
3	C	8/10 (80%)	8 (100%)	0	0	100	100
4	L	211/214 (99%)	206 (98%)	5 (2%)	0	100	100
5	H	216/218 (99%)	206 (95%)	9 (4%)	1 (0%)	24	54
All	All	808/859 (94%)	780 (96%)	26 (3%)	2 (0%)	43	72

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	194	ILE
5	H	29	VAL

### 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	235/254 (92%)	214 (91%)	21 (9%)	9	28
2	B	94/109 (86%)	84 (89%)	10 (11%)	6	22
3	C	9/9 (100%)	8 (89%)	1 (11%)	6	20
4	L	188/189 (100%)	175 (93%)	13 (7%)	14	41
5	H	182/182 (100%)	154 (85%)	28 (15%)	2	9
All	All	708/743 (95%)	635 (90%)	73 (10%)	7	23

5 of 73 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
5	H	132	SER
5	H	214	LYS
5	H	154	PRO
5	H	188	THR
2	B	68	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	32	GLN
1	A	144	GLN
1	A	155	GLN
3	C	3	ASN
4	L	199	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](#)

15 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	$\# Z  > 2$
8	SO4	A	309	-	4,4,4	0.34	0	6,6,6	0.07	0
8	SO4	A	308	-	4,4,4	0.31	0	6,6,6	0.10	0
8	SO4	H	301	-	4,4,4	0.59	0	6,6,6	0.21	0
6	PEG	A	303	-	6,6,6	0.19	0	5,5,5	0.09	0
6	PEG	B	501	-	6,6,6	0.17	0	5,5,5	0.09	0
6	PEG	L	302	-	6,6,6	0.14	0	5,5,5	0.10	0
8	SO4	A	305	-	4,4,4	0.32	0	6,6,6	0.09	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
7	NHE	A	304	-	13,13,13	2.71	2 (15%)	16,17,17	2.40	7 (43%)
8	SO4	A	306	-	4,4,4	0.31	0	6,6,6	0.09	0
8	SO4	H	302	-	4,4,4	0.33	0	6,6,6	0.05	0
8	SO4	B	502	-	4,4,4	0.32	0	6,6,6	0.08	0
8	SO4	A	307	-	4,4,4	0.32	0	6,6,6	0.14	0
6	PEG	A	302	-	6,6,6	0.15	0	5,5,5	0.10	0
6	PEG	A	301	-	6,6,6	0.18	0	5,5,5	0.20	0
6	PEG	L	301	-	6,6,6	0.14	0	5,5,5	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
6	PEG	A	303	-	-	0/4/4/4	-
6	PEG	B	501	-	-	2/4/4/4	-
6	PEG	L	302	-	-	0/4/4/4	-
7	NHE	A	304	-	-	2/7/15/15	0/1/1/1
6	PEG	A	302	-	-	0/4/4/4	-
6	PEG	A	301	-	-	1/4/4/4	-
6	PEG	L	301	-	-	3/4/4/4	-

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	A	304	NHE	C2-S	-8.17	1.66	1.77
7	A	304	NHE	O3-S	4.97	1.65	1.47

The worst 5 of 7 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	A	304	NHE	C1-N-C1'	4.75	123.32	114.18
7	A	304	NHE	C5'-C6'-C1'	3.76	117.84	111.09
7	A	304	NHE	O1-S-C2	3.69	112.31	106.73
7	A	304	NHE	O3-S-C2	3.68	113.20	106.00
7	A	304	NHE	O2-S-C2	-2.89	102.36	106.73

There are no chirality outliers.

5 of 8 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
7	A	304	NHE	N-C1-C2-S
6	L	301	PEG	O2-C3-C4-O4
6	L	301	PEG	O1-C1-C2-O2
6	B	501	PEG	C4-C3-O2-C2
7	A	304	NHE	C2-C1-N-C1'

There are no ring outliers.

3 monomers are involved in 8 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	B	501	PEG	4	0
7	A	304	NHE	3	0
6	A	302	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	277/298 (92%)	0.60	31 (11%) 10 9	20, 42, 114, 155	0
2	B	100/119 (84%)	0.25	2 (2%) 65 56	25, 45, 66, 84	0
3	C	10/10 (100%)	-0.02	0 100 100	24, 26, 35, 41	0
4	L	213/214 (99%)	0.04	2 (0%) 81 75	22, 35, 55, 68	0
5	H	218/218 (100%)	0.13	7 (3%) 50 41	22, 38, 63, 95	0
All	All	818/859 (95%)	0.28	42 (5%) 33 26	20, 38, 79, 155	0

The worst 5 of 42 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	254	GLU	5.5
1	A	257	TYR	5.4
5	H	133	SER	5.3
1	A	221	GLY	4.7
1	A	250	PRO	4.5

### 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, 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	PEG	L	301	7/7	0.64	0.21	57,57,59,65	0
8	SO4	A	309	5/5	0.64	0.09	124,127,128,129	0
8	SO4	A	307	5/5	0.68	0.24	108,110,117,123	0
8	SO4	H	302	5/5	0.70	0.14	99,100,108,109	0
7	NHE	A	304	13/13	0.74	0.27	92,96,118,127	0
6	PEG	L	302	7/7	0.75	0.16	70,73,77,78	0
6	PEG	A	301	7/7	0.76	0.17	47,53,55,58	0
6	PEG	B	501	7/7	0.76	0.20	76,78,80,80	0
8	SO4	A	308	5/5	0.78	0.18	113,115,121,123	0
8	SO4	H	301	5/5	0.82	0.19	89,91,94,97	0
8	SO4	B	502	5/5	0.82	0.17	79,84,87,89	0
8	SO4	A	305	5/5	0.83	0.20	84,89,95,96	0
8	SO4	A	306	5/5	0.84	0.20	79,80,85,85	0
6	PEG	A	302	7/7	0.85	0.14	60,61,62,62	0
6	PEG	A	303	7/7	0.88	0.14	48,54,59,59	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.