



# Full wwPDB X-ray Structure Validation Report ⓘ

Jun 18, 2026 – 12:12 PM EDT

PDB ID : 9EK4 / pdb\_00009ek4  
Title : Crystal structure of HLA-B\*07:02 with the 9-mer TP53 mutant peptide MPILTIITL  
Authors : Tan, K.; Maillis, R.J.; Reinherz, E.L.  
Deposited on : 2024-11-30  
Resolution : 2.05 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>.

---

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

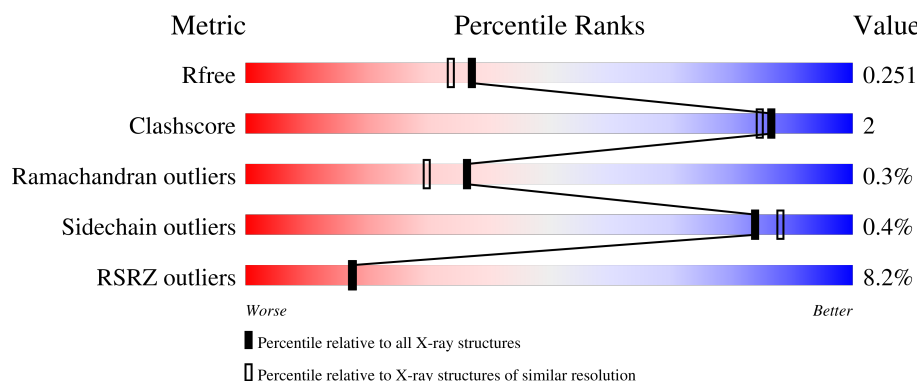
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.05 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	2260 (2.04-2.04)
Clashscore	190562	2333 (2.04-2.04)
Ramachandran outliers	187476	2318 (2.04-2.04)
Sidechain outliers	187428	2318 (2.04-2.04)
RSRZ outliers	180081	2260 (2.04-2.04)

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	277	<div> <div>12%</div> <div>94%</div> <div>5%</div> </div>
1	D	277	<div> <div>8%</div> <div>95%</div> <div>5%</div> </div>
2	B	100	<div> <div>3%</div> <div>92%</div> <div>8%</div> </div>
2	E	100	<div> <div>4%</div> <div>93%</div> <div>7%</div> </div>
3	C	9	<div> <div>11%</div> <div>89%</div> <div>11%</div> </div>

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Length	Quality of chain
3	F	9	<div><div>11%</div><div></div><div>100%</div></div>

## 2 Entry composition

There are 10 unique types of molecules in this entry. The entry contains 6731 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 alpha chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	276	Total	C	N	O	S	0	1	0
			2268	1407	415	440	6			
1	D	276	Total	C	N	O	S	0	0	0
			2262	1404	414	438	6			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	0	MET	-	initiating methionine	UNP P01889
D	0	MET	-	initiating methionine	UNP P01889

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	100	Total	C	N	O	S	0	1	0
			844	537	142	161	4			
2	E	100	Total	C	N	O	S	0	1	0
			844	538	142	160	4			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	0	MET	-	initiating methionine	UNP P61769
E	0	MET	-	initiating methionine	UNP P61769

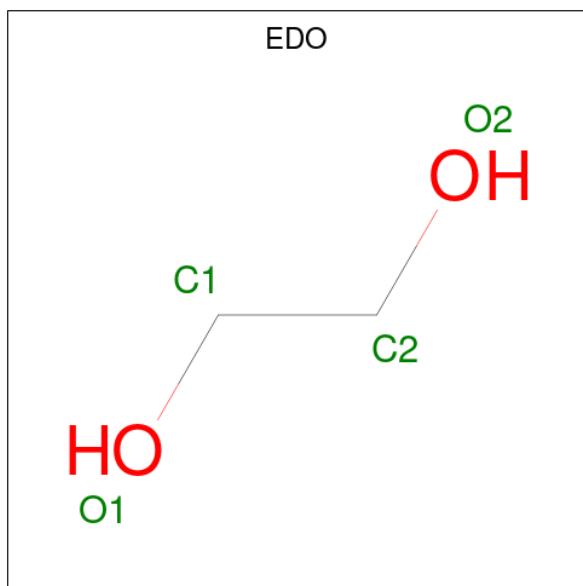
- Molecule 3 is a protein called Mutant peptide from Cellular tumor antigen p53.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	9	Total	C	N	O	S	0	0	0
			70	48	9	12	1			
3	F	9	Total	C	N	O	S	0	0	0
			70	48	9	12	1			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	1	MET	ARG	engineered mutation	UNP P04637
F	1	MET	ARG	engineered mutation	UNP P04637

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



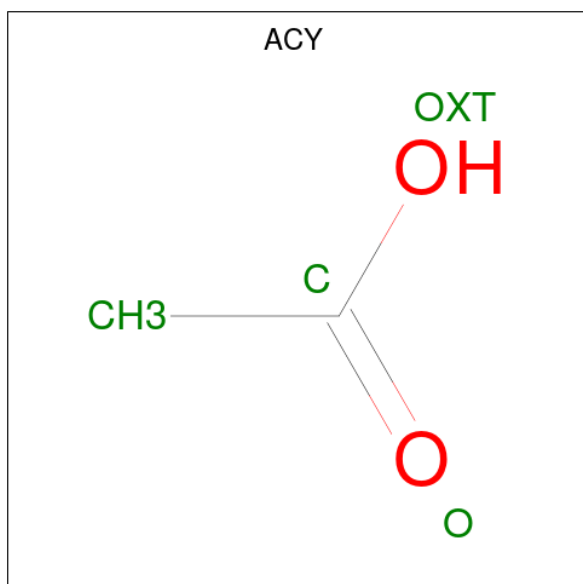
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total C O 4 2 2	0	0
4	A	1	Total C O 4 2 2	0	0
4	A	1	Total C O 4 2 2	0	0
4	A	1	Total C O 4 2 2	0	0
4	A	1	Total C O 4 2 2	0	0
4	A	1	Total C O 4 2 2	0	0
4	B	1	Total C O 4 2 2	0	0
4	B	1	Total C O 4 2 2	0	0
4	C	1	Total C O 4 2 2	0	0
4	C	1	Total C O 4 2 2	0	0

*Continued on next page...*

Continued from previous page...

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

- Molecule 5 is ACETIC ACID (CCD ID: ACY) (formula:  $C_2H_4O_2$ ).

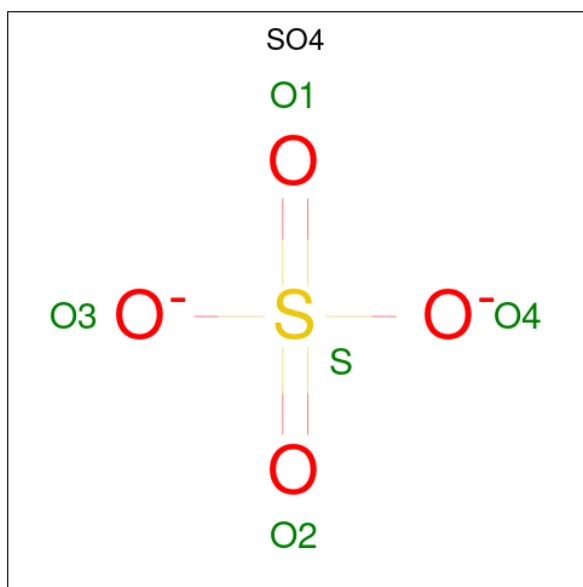


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	C	O	0	0
			4	2	2		
5	D	1	Total	C	O	0	0
			4	2	2		
5	D	1	Total	C	O	0	0
			4	2	2		
5	D	1	Total	C	O	0	0
			4	2	2		

- Molecule 6 is NICKEL (II) ION (CCD ID: NI) (formula: Ni).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	1	Total Ni 1 1	0	0
6	D	1	Total Ni 1 1	0	0

- Molecule 7 is SULFATE ION (CCD ID: SO4) (formula: O<sub>4</sub>S).



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

- Molecule 8 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
8	B	1	Total Zn 1 1	0	0
8	D	1	Total Zn 1 1	0	0

- Molecule 9 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
9	B	1	Total 1	Cl 1	0	0
9	E	2	Total 2	Cl 2	0	0

- Molecule 10 is water.

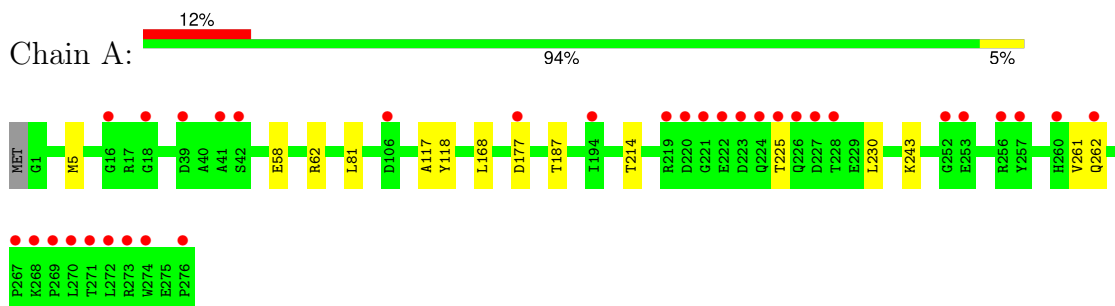
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
10	A	98	Total 98	O 98	0	0
10	B	42	Total 42	O 42	0	0
10	C	4	Total 4	O 4	0	0
10	D	74	Total 74	O 74	0	0
10	E	43	Total 43	O 43	0	0
10	F	5	Total 5	O 5	0	0



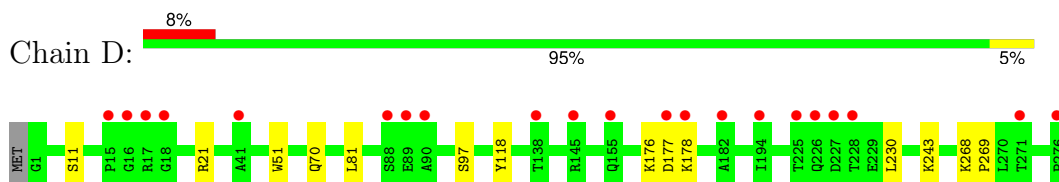
### 3 Residue-property plots

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.

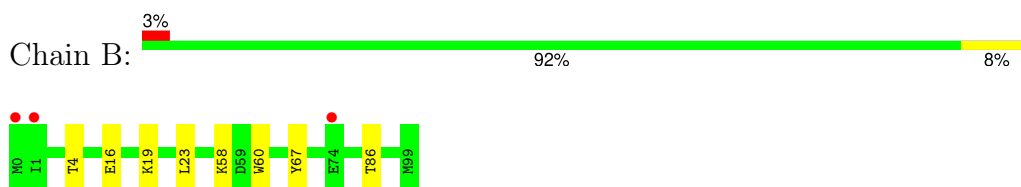
- Molecule 1: HLA class I histocompatibility antigen, B alpha chain



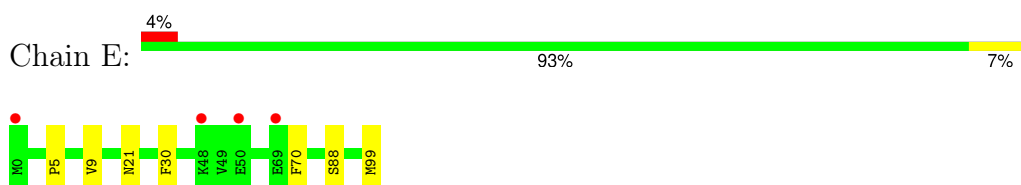
- Molecule 1: HLA class I histocompatibility antigen, B alpha chain



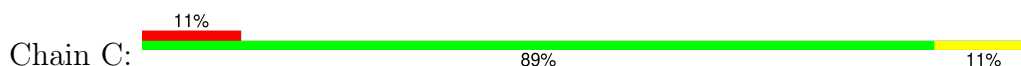
- Molecule 2: Beta-2-microglobulin

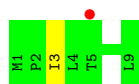


- Molecule 2: Beta-2-microglobulin

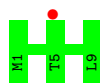


- Molecule 3: Mutant peptide from Cellular tumor antigen p53





- Molecule 3: Mutant peptide from Cellular tumor antigen p53



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	46.98Å 92.67Å 108.55Å 90.00° 94.18° 90.00°	Depositor
Resolution (Å)	46.74 – 2.05 46.74 – 2.05	Depositor EDS
% Data completeness (in resolution range)	98.7 (46.74-2.05) 98.8 (46.74-2.05)	Depositor EDS
$R_{merge}$	0.14	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.86 (at 2.05Å)	Xtriage
Refinement program	PHENIX 1.21.2_5419	Depositor
R, $R_{free}$	0.210 , 0.251 0.210 , 0.251	Depositor DCC
$R_{free}$ test set	2747 reflections (4.73%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	27.6	Xtriage
Anisotropy	0.227	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.32 , 36.3	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.93	EDS
Total number of atoms	6731	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	37.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 13.91% 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: CL, EDO, SO4, ACY, NI, ZN

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	0.12	0/2331	0.30	0/3167
1	D	0.11	0/2325	0.28	0/3159
2	B	0.11	0/867	0.31	0/1173
2	E	0.12	0/867	0.33	0/1172
3	C	0.14	0/70	0.33	0/94
3	F	0.11	0/70	0.26	0/94
All	All	0.12	0/6530	0.30	0/8859

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	2268	0	2109	8	0
1	D	2262	0	2105	7	0
2	B	844	0	810	6	0
2	E	844	0	810	4	0
3	C	70	0	87	1	0
3	F	70	0	87	0	0
4	A	24	0	36	2	0

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	B	8	0	12	1	0
4	C	8	0	12	2	0
4	D	16	0	24	1	0
4	E	8	0	11	2	0
5	A	4	0	3	0	0
5	D	12	0	9	0	0
6	A	1	0	0	0	0
6	D	1	0	0	0	0
7	A	10	0	0	0	0
7	B	5	0	0	0	0
7	D	5	0	0	0	0
8	B	1	0	0	0	0
8	D	1	0	0	0	0
9	B	1	0	0	0	0
9	E	2	0	0	0	0
10	A	98	0	0	0	0
10	B	42	0	0	0	0
10	C	4	0	0	0	0
10	D	74	0	0	1	0
10	E	43	0	0	0	0
10	F	5	0	0	0	0
All	All	6731	0	6115	26	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 2.

All (26) 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:D:230:LEU:HD22	1:D:243:LYS:HE3	1.73	0.70
3:C:3:ILE:HA	4:C:102:EDO:H21	1.81	0.62
1:D:268:LYS:HG3	1:D:269:PRO:HD2	1.86	0.58
2:E:9:VAL:O	4:E:101:EDO:H21	2.04	0.57
1:A:187:THR:HG21	1:A:261:VAL:HG21	1.89	0.55
1:A:230:LEU:HD11	1:A:243:LYS:HE3	1.90	0.53
2:B:16:GLU:HB2	2:B:19:LYS:HE3	1.90	0.53
1:D:178:LYS:HE3	10:D:401:HOH:O	2.09	0.52
1:A:58:GLU:O	1:A:62:ARG:HB2	2.11	0.50
1:A:5:MET:HB2	1:A:168:LEU:HD13	1.95	0.49
2:E:99:MET:HB2	4:E:101:EDO:H22	1.95	0.48
2:B:58:LYS:HA	4:B:102:EDO:H11	1.96	0.47

*Continued on next page...*

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:177:ASP:HB2	4:A:303:EDO:H22	1.96	0.47
2:B:4[A]:THR:HG22	2:B:86:THR:HB	1.97	0.46
1:D:70:GLN:NE2	4:D:305:EDO:H12	2.31	0.45
1:A:214:THR:OG1	1:A:262:GLN:HB2	2.17	0.45
4:A:304:EDO:H11	2:B:58:LYS:O	2.18	0.44
4:C:101:EDO:O1	4:C:102:EDO:H22	2.18	0.44
2:E:5:PRO:HB3	2:E:30:PHE:HB3	2.01	0.43
1:D:81:LEU:HD13	1:D:118:TYR:CD1	2.55	0.42
1:D:51:TRP:HE1	1:D:178:LYS:HE2	1.83	0.41
1:A:81:LEU:HD13	1:A:118:TYR:CD1	2.56	0.41
1:A:117:ALA:HB2	2:B:60:TRP:CE2	2.55	0.41
2:B:23:LEU:O	2:B:67:TYR:HA	2.22	0.40
1:D:11:SER:HA	1:D:21:ARG:O	2.21	0.40
2:E:21:ASN:HB3	2:E:70:PHE:CE1	2.56	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	275/277 (99%)	265 (96%)	9 (3%)	1 (0%)	30	22
1	D	274/277 (99%)	268 (98%)	5 (2%)	1 (0%)	30	22
2	B	99/100 (99%)	98 (99%)	1 (1%)	0	100	100
2	E	99/100 (99%)	97 (98%)	2 (2%)	0	100	100
3	C	7/9 (78%)	7 (100%)	0	0	100	100
3	F	7/9 (78%)	7 (100%)	0	0	100	100
All	All	761/772 (99%)	742 (98%)	17 (2%)	2 (0%)	36	30

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	176	LYS
1	A	225	THR

### 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	235/235 (100%)	235 (100%)	0	100	100
1	D	234/235 (100%)	232 (99%)	2 (1%)	70	75
2	B	96/95 (101%)	96 (100%)	0	100	100
2	E	96/95 (101%)	95 (99%)	1 (1%)	68	72
3	C	9/9 (100%)	9 (100%)	0	100	100
3	F	9/9 (100%)	9 (100%)	0	100	100
All	All	679/678 (100%)	676 (100%)	3 (0%)	84	88

All (3) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	D	97	SER
1	D	177	ASP
2	E	88	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (9) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	54	GLN
1	A	255	GLN
1	A	260	HIS
2	B	2	GLN
2	B	13	HIS
1	D	70	GLN
1	D	127	ASN
1	D	141	GLN
2	E	13	HIS

### 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](#)

Of 31 ligands modelled in this entry, 7 are monoatomic - leaving 24 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	306	-	3,3,3	0.25	0	2,2,2	0.32	0
7	SO4	A	309	-	4,4,4	0.65	0	6,6,6	0.09	0
7	SO4	A	310	-	4,4,4	0.67	0	6,6,6	0.08	0
4	EDO	D	305	-	3,3,3	0.25	0	2,2,2	0.29	0
4	EDO	A	303	-	3,3,3	0.25	0	2,2,2	0.34	0
5	ACY	D	301	6	3,3,3	1.12	0	3,3,3	0.99	0
4	EDO	D	303	-	3,3,3	0.25	0	2,2,2	0.33	0
5	ACY	A	305	6	3,3,3	1.10	0	3,3,3	1.04	0
5	ACY	D	304	-	3,3,3	1.14	0	3,3,3	0.93	0
4	EDO	A	306	-	3,3,3	0.25	0	2,2,2	0.29	0
4	EDO	A	302	-	3,3,3	0.25	0	2,2,2	0.32	0
4	EDO	E	102	-	3,3,3	0.25	0	2,2,2	0.28	0
4	EDO	A	304	-	3,3,3	0.25	0	2,2,2	0.30	0
4	EDO	A	307	-	3,3,3	0.24	0	2,2,2	0.40	0
4	EDO	A	301	-	3,3,3	0.25	0	2,2,2	0.33	0
4	EDO	D	307	-	3,3,3	0.25	0	2,2,2	0.24	0
4	EDO	B	101	-	3,3,3	0.25	0	2,2,2	0.35	0
4	EDO	E	101	-	3,3,3	0.24	0	2,2,2	0.22	0



Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
4	EDO	C	101	-	3,3,3	0.24	0	2,2,2	0.32	0
4	EDO	B	102	-	3,3,3	0.25	0	2,2,2	0.31	0
5	ACY	D	302	-	3,3,3	1.11	0	3,3,3	1.02	0
7	SO4	D	310	-	4,4,4	0.67	0	6,6,6	0.20	0
4	EDO	C	102	-	3,3,3	0.25	0	2,2,2	0.33	0
7	SO4	B	105	-	4,4,4	0.67	0	6,6,6	0.08	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	A	303	-	-	0/1/1/1	-
4	EDO	D	306	-	-	1/1/1/1	-
4	EDO	C	101	-	-	1/1/1/1	-
4	EDO	B	102	-	-	0/1/1/1	-
4	EDO	A	306	-	-	1/1/1/1	-
4	EDO	A	302	-	-	0/1/1/1	-
4	EDO	C	102	-	-	1/1/1/1	-
4	EDO	E	102	-	-	1/1/1/1	-
4	EDO	A	304	-	-	1/1/1/1	-
4	EDO	A	307	-	-	0/1/1/1	-
4	EDO	D	303	-	-	0/1/1/1	-
4	EDO	D	305	-	-	1/1/1/1	-
4	EDO	A	301	-	-	1/1/1/1	-
4	EDO	D	307	-	-	1/1/1/1	-
4	EDO	B	101	-	-	0/1/1/1	-
4	EDO	E	101	-	-	1/1/1/1	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (10) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	C	101	EDO	O1-C1-C2-O2
4	A	301	EDO	O1-C1-C2-O2
4	E	101	EDO	O1-C1-C2-O2
4	D	305	EDO	O1-C1-C2-O2
4	E	102	EDO	O1-C1-C2-O2

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms
4	A	306	EDO	O1-C1-C2-O2
4	D	306	EDO	O1-C1-C2-O2
4	C	102	EDO	O1-C1-C2-O2
4	A	304	EDO	O1-C1-C2-O2
4	D	307	EDO	O1-C1-C2-O2

There are no ring outliers.

7 monomers are involved in 8 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	D	305	EDO	1	0
4	A	303	EDO	1	0
4	A	304	EDO	1	0
4	E	101	EDO	2	0
4	C	101	EDO	1	0
4	B	102	EDO	1	0
4	C	102	EDO	2	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, 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	276/277 (99%)	0.57	33 (11%) 9 8	9, 33, 80, 96	1 (0%)
1	D	276/277 (99%)	0.54	21 (7%) 20 20	21, 37, 59, 88	0
2	B	100/100 (100%)	0.37	3 (3%) 52 53	15, 34, 57, 71	1 (1%)
2	E	100/100 (100%)	0.55	4 (4%) 42 42	12, 35, 60, 82	1 (1%)
3	C	9/9 (100%)	0.46	1 (11%) 10 10	20, 25, 28, 40	0
3	F	9/9 (100%)	0.52	1 (11%) 10 10	24, 29, 35, 48	0
All	All	770/772 (99%)	0.53	63 (8%) 17 18	9, 35, 65, 96	3 (0%)

All (63) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	270	LEU	4.6
1	A	224	GLN	4.5
1	A	271	THR	4.0
1	A	269	PRO	4.0
1	A	41	ALA	3.9
1	A	221	GLY	3.7
1	A	252	GLY	3.6
1	A	276	PRO	3.4
1	A	222	GLU	3.4
1	D	16	GLY	3.4
1	A	177	ASP	3.2
1	A	223	ASP	3.2
1	A	227	ASP	3.1
2	B	1	ILE	3.0
1	A	225	THR	3.0
1	D	41	ALA	2.9
1	A	220	ASP	2.9
2	B	0	MET	2.8
1	D	228	THR	2.8

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
1	A	194	ILE	2.8
2	E	48	LYS	2.8
1	A	219	ARG	2.7
1	D	182	ALA	2.7
1	D	178	LYS	2.7
1	D	15	PRO	2.7
1	D	89	GLU	2.7
1	A	106	ASP	2.7
1	A	16	GLY	2.6
1	D	194	ILE	2.6
1	A	253	GLU	2.6
3	C	5	THR	2.6
1	A	42	SER	2.6
1	A	226	GLN	2.6
1	A	260	HIS	2.5
1	D	271	THR	2.5
1	A	274	TRP	2.5
1	A	268	LYS	2.5
1	D	177	ASP	2.4
2	E	50	GLU	2.4
1	D	276	PRO	2.4
2	E	0	MET	2.4
1	A	228	THR	2.4
1	D	155	GLN	2.3
3	F	5	THR	2.3
1	D	225	THR	2.3
1	D	90	ALA	2.3
1	D	17	ARG	2.2
1	A	257	TYR	2.2
1	A	18	GLY	2.2
1	A	272	LEU	2.2
1	D	88	SER	2.2
1	A	39	ASP	2.2
2	B	74	GLU	2.1
1	D	226	GLN	2.1
1	D	227	ASP	2.1
1	A	256	ARG	2.1
2	E	69	GLU	2.1
1	D	138	THR	2.1
1	A	273	ARG	2.1
1	A	262	GLN	2.0
1	D	145	ARG	2.0

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
1	A	267	PRO	2.0
1	D	18	GLY	2.0

## 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
4	EDO	A	303	4/4	0.50	0.20	65,66,67,69	0
4	EDO	E	101	4/4	0.65	0.26	33,38,44,48	0
4	EDO	A	304	4/4	0.68	0.23	42,45,46,46	0
5	ACY	D	302	4/4	0.74	0.17	52,53,56,56	0
4	EDO	B	102	4/4	0.76	0.21	32,35,40,49	0
4	EDO	C	102	4/4	0.77	0.20	37,38,40,43	0
7	SO4	A	310	5/5	0.77	0.17	44,52,55,58	5
4	EDO	A	301	4/4	0.78	0.17	46,46,48,51	0
4	EDO	D	305	4/4	0.80	0.22	39,41,41,45	0
5	ACY	D	301	4/4	0.81	0.17	40,44,49,53	0
4	EDO	E	102	4/4	0.82	0.13	53,56,60,61	0
5	ACY	D	304	4/4	0.83	0.16	36,41,42,44	0
4	EDO	C	101	4/4	0.83	0.23	39,40,44,45	0
4	EDO	D	306	4/4	0.84	0.12	35,42,43,43	0
7	SO4	A	309	5/5	0.85	0.13	35,41,43,47	5
5	ACY	A	305	4/4	0.85	0.14	34,41,45,46	0
4	EDO	A	307	4/4	0.86	0.18	42,48,50,51	0
4	EDO	D	307	4/4	0.86	0.16	44,44,51,51	0
9	CL	E	104	1/1	0.86	0.11	60,60,60,60	0
7	SO4	D	310	5/5	0.87	0.12	52,55,61,64	5
7	SO4	B	105	5/5	0.87	0.16	39,42,44,46	5

*Continued on next page...*

*Continued from previous page...*

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
4	EDO	A	306	4/4	0.88	0.17	37,37,39,44	0
4	EDO	D	303	4/4	0.88	0.10	37,38,48,51	0
4	EDO	A	302	4/4	0.90	0.10	31,33,37,44	0
4	EDO	B	101	4/4	0.90	0.14	29,31,36,39	0
9	CL	E	103	1/1	0.91	0.11	57,57,57,57	0
9	CL	B	104	1/1	0.93	0.14	53,53,53,53	0
8	ZN	D	308	1/1	0.96	0.05	47,47,47,47	0
8	ZN	B	103	1/1	0.96	0.05	42,42,42,42	0
6	NI	D	309	1/1	0.99	0.05	47,47,47,47	0
6	NI	A	308	1/1	0.99	0.03	32,32,32,32	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.