



# Full wwPDB X-ray Structure Validation Report ⓘ

Mar 7, 2026 – 04:20 AM UTC

PDB ID : 5NMD / pdb\_00005nmd  
Title : 868 TCR Specific for HLA A02 presenting HIV Epitope SLYNTVATL  
Authors : Rizkallah, P.J.; Cole, D.K.; Fuller, A.; Sewell, A.K.  
Deposited on : 2017-04-05  
Resolution : 2.07 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 : 4-5-2 with Phenix2.0  
Mogul : 2022.3.0, CSD as543be (2022)  
Xtrriage (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

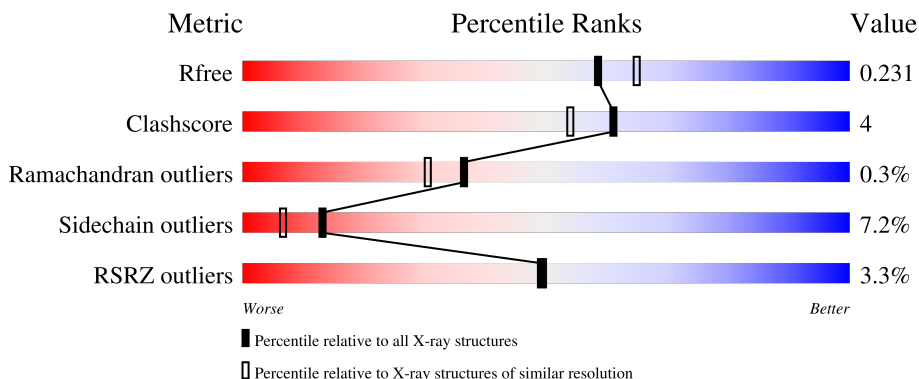
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*


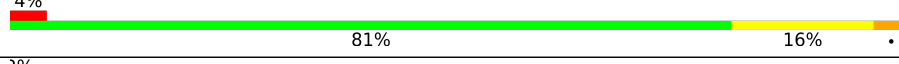

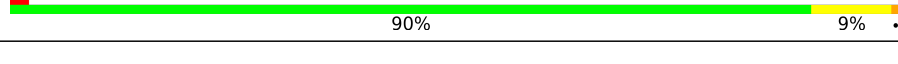
The reported resolution of this entry is 2.07 Å.

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	3774 (2.08-2.04)
Clashscore	190562	3883 (2.08-2.04)
Ramachandran outliers	187476	3860 (2.08-2.04)
Sidechain outliers	187428	3860 (2.08-2.04)
RSRZ outliers	180081	3775 (2.08-2.04)

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	200	 6% 78% 18%
1	C	200	 4% 81% 16%
2	B	242	 2% 87% 12%
2	D	242	 2% 90% 9%

## 2 Entry composition [i](#)

There are 5 unique types of molecules in this entry. The entry contains 7282 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.

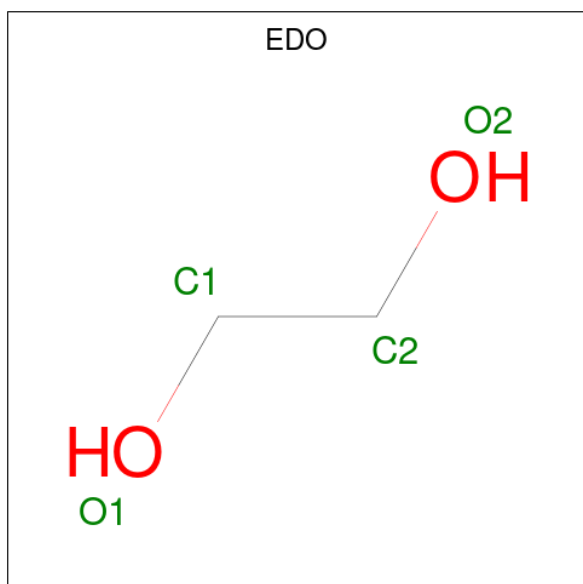
- Molecule 1 is a protein called human T-cell Receptor alpha chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	200	Total 1578	C 985	N 262	O 320	S 11	0	3	0
1	C	200	Total 1572	C 982	N 261	O 319	S 10	0	2	0

- Molecule 2 is a protein called Human T-cell Receptor, beta chain.

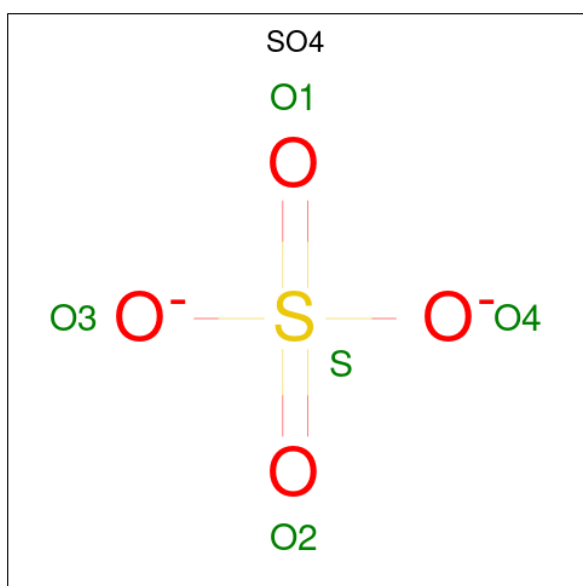
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	B	242	Total 1945	C 1222	N 338	O 379	S 6	0	1	0
2	D	242	Total 1939	C 1219	N 337	O 378	S 5	0	0	0

- Molecule 3 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
3	A	1	Total C O 4 2 2	0	0
3	B	1	Total C O 4 2 2	0	0
3	B	1	Total C O 4 2 2	0	0
3	C	1	Total C O 4 2 2	0	0

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



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

- Molecule 5 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	39	Total O 39 39	0	0

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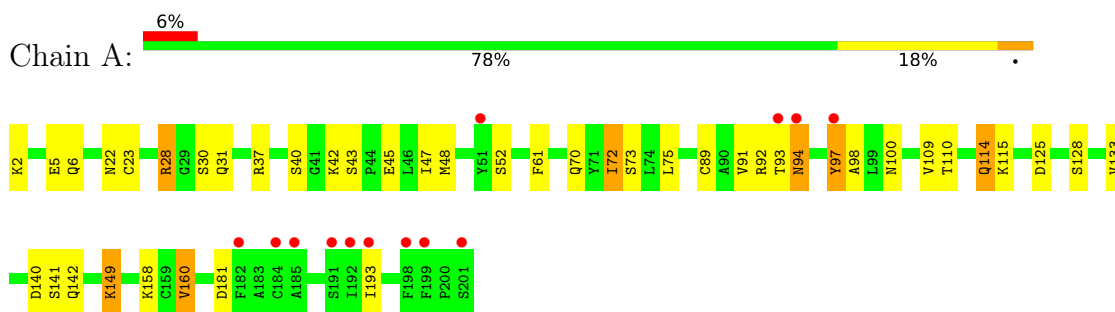
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<b>Mol</b>	<b>Chain</b>	<b>Residues</b>	<b>Atoms</b>		<b>ZeroOcc</b>	<b>AltConf</b>
5	B	101	Total 101	O 101	0	0
5	C	29	Total 29	O 29	0	0
5	D	38	Total 38	O 38	0	0

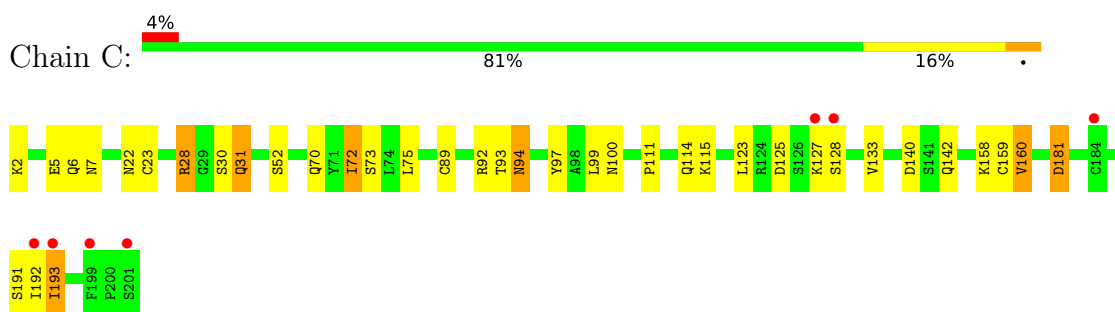
### 3 Residue-property plots [i](#)

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.

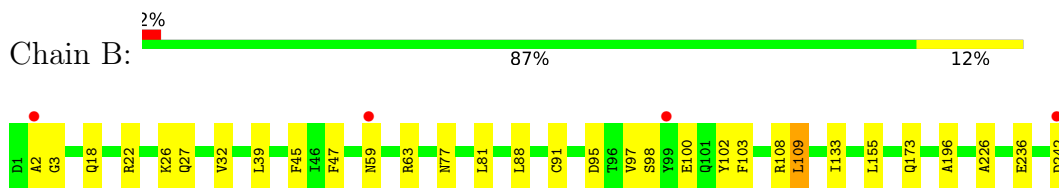
- Molecule 1: human T-cell Receptor alpha chain



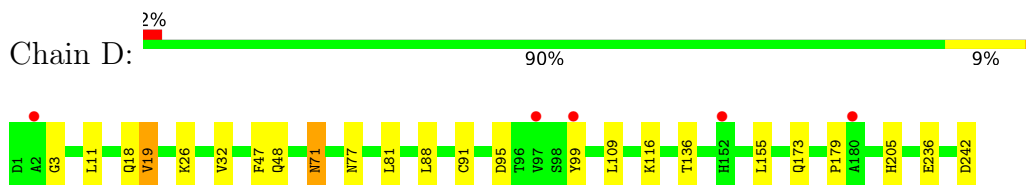
- Molecule 1: human T-cell Receptor alpha chain



- Molecule 2: Human T-cell Receptor, beta chain



- Molecule 2: Human T-cell Receptor, beta chain



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	87.47Å 50.62Å 114.31Å 90.00° 90.16° 90.00°	Depositor
Resolution (Å)	43.81 – 2.07 43.81 – 2.07	Depositor EDS
% Data completeness (in resolution range)	98.5 (43.81-2.07) 98.5 (43.81-2.07)	Depositor EDS
$R_{merge}$	0.05	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.60 (at 2.06Å)	Xtrriage
Refinement program	REFMAC 5.8.0158	Depositor
R, $R_{free}$	0.189 , 0.223 0.196 , 0.231	Depositor DCC
$R_{free}$ test set	3051 reflections (5.05%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	41.3	Xtrriage
Anisotropy	0.443	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.34 , 36.6	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.31$	Xtrriage
Estimated twinning fraction	0.025 for h,-k,-l	Xtrriage
$F_o, F_c$ correlation	0.96	EDS
Total number of atoms	7282	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	58.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.27% 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: SO4, EDO

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	1.25	6/1611 (0.4%)	1.10	3/2179 (0.1%)
1	C	1.15	1/1605 (0.1%)	1.08	1/2171 (0.0%)
2	B	1.35	8/2000 (0.4%)	1.15	7/2725 (0.3%)
2	D	1.10	1/1994 (0.1%)	1.06	2/2717 (0.1%)
All	All	1.22	16/7210 (0.2%)	1.10	13/9792 (0.1%)

All (16) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	37	ARG	CZ-NH2	9.27	1.45	1.33
2	B	226	ALA	CA-C	7.35	1.61	1.52
1	A	47	ILE	C-O	-7.16	1.17	1.24
2	B	3	GLY	N-CA	6.91	1.54	1.44
2	B	108	ARG	C-O	-6.79	1.15	1.24
2	B	103	PHE	C-O	-6.19	1.16	1.23
2	D	236	GLU	CD-OE2	6.07	1.36	1.25
1	A	160	VAL	C-O	-6.02	1.17	1.24
1	C	192	ILE	CA-CB	5.91	1.59	1.53
2	B	100	GLU	C-O	-5.79	1.17	1.23
2	B	236	GLU	CD-OE2	5.64	1.36	1.25
1	A	43	SER	CB-OG	-5.59	1.30	1.42
1	A	37	ARG	N-CA	-5.42	1.39	1.46
2	B	109	LEU	N-CA	-5.06	1.40	1.46
2	B	173	GLN	C-O	-5.05	1.17	1.24
1	A	109	VAL	N-CA	-5.05	1.40	1.46

All (13) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	71	ASN	N-CA-C	-10.16	94.14	110.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	100	GLU	CA-C-O	-6.94	113.08	120.09
2	B	97	VAL	N-CA-C	6.52	121.54	112.35
2	B	91	CYS	CA-CB-SG	-6.15	100.26	114.40
2	B	100	GLU	CB-CA-C	-5.92	104.08	111.43
2	B	97	VAL	CB-CA-C	-5.73	103.57	111.65
1	A	100	ASN	CB-CA-C	-5.66	100.40	109.75
2	D	91	CYS	CA-CB-SG	-5.49	101.78	114.40
1	A	92	ARG	NE-CZ-NH2	5.17	123.85	119.20
1	A	97	TYR	CA-CB-CG	5.10	123.07	113.90
2	B	22	ARG	NE-CZ-NH2	5.09	123.78	119.20
1	C	192	ILE	N-CA-CB	5.07	117.38	111.90
2	B	63	ARG	CG-CD-NE	-5.02	100.95	112.00

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	1578	0	1495	22	0
1	C	1572	0	1492	23	0
2	B	1945	0	1817	9	0
2	D	1939	0	1814	11	0
3	A	4	0	6	0	0
3	B	8	0	12	0	0
3	C	4	0	6	2	0
4	A	5	0	0	0	0
4	B	5	0	0	0	0
4	C	5	0	0	0	0
4	D	10	0	0	0	0
5	A	39	0	0	1	0
5	B	101	0	0	1	0
5	C	29	0	0	0	0
5	D	38	0	0	1	0
All	All	7282	0	6642	58	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 (58) 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:28:ARG:HD3	1:C:70:GLN:NE2	1.81	0.95
1:A:5:GLU:OE2	1:C:142:GLN:NE2	2.12	0.82
1:A:142:GLN:NE2	1:C:5:GLU:HG2	1.96	0.81
1:C:6:GLN:HB3	1:C:23[A]:CYS:SG	2.26	0.74
1:A:6:GLN:HB3	1:A:23[A]:CYS:SG	2.30	0.72
1:C:28:ARG:HD3	1:C:70:GLN:HE22	1.55	0.69
1:A:142:GLN:HE21	1:C:5:GLU:HG2	1.57	0.68
2:D:11:LEU:HD13	2:D:19:VAL:HG22	1.76	0.67
2:B:18:GLN:HE21	2:B:77:ASN:HD21	1.44	0.66
1:C:28:ARG:CD	1:C:70:GLN:NE2	2.59	0.65
2:D:11:LEU:HD13	2:D:19:VAL:CG2	2.27	0.64
2:D:71:ASN:O	2:D:71:ASN:OD1	2.17	0.63
1:A:28:ARG:CD	1:A:70:GLN:NE2	2.63	0.61
1:C:111:PRO:HG3	1:C:160:VAL:HG21	1.83	0.61
1:A:28:ARG:HD2	1:A:70:GLN:HE21	1.66	0.60
1:C:191:SER:HB2	1:C:193:ILE:CD1	2.31	0.60
1:A:28:ARG:HD3	1:A:70:GLN:NE2	2.17	0.59
2:B:59:ASN:HB3	5:B:493:HOH:O	2.03	0.58
1:C:97:TYR:HB3	2:D:48:GLN:OE1	2.04	0.58
1:C:28:ARG:HD3	1:C:70:GLN:HE21	1.64	0.57
2:D:71:ASN:OD1	2:D:71:ASN:C	2.47	0.57
1:C:28:ARG:CD	1:C:70:GLN:HE21	2.17	0.56
1:A:28:ARG:CD	1:A:70:GLN:HE21	2.19	0.56
2:B:18:GLN:NE2	2:B:77:ASN:HD21	2.06	0.53
1:C:92:ARG:NH1	2:D:99:TYR:O	2.41	0.53
1:C:7:ASN:HB3	3:C:301:EDO:C2	2.38	0.52
1:C:72:ILE:HD13	1:C:89[B]:CYS:SG	2.50	0.52
1:A:110:THR:CG2	1:A:141:SER:HB3	2.40	0.52
1:C:72:ILE:CD1	1:C:89[B]:CYS:SG	2.99	0.50
2:D:18:GLN:HE21	2:D:77:ASN:HD21	1.59	0.49
1:C:125:ASP:HB3	1:C:128:SER:O	2.12	0.49
1:C:7:ASN:HB3	3:C:301:EDO:H21	1.95	0.48
1:A:72:ILE:HD13	1:A:89[B]:CYS:SG	2.54	0.47
1:A:125:ASP:HB3	1:A:128:SER:O	2.13	0.47
2:B:26:LYS:HE3	2:B:102:TYR:CD2	2.50	0.47
1:A:28:ARG:CZ	1:C:114:GLN:HE22	2.28	0.47
2:B:95:ASP:C	2:B:95:ASP:OD1	2.58	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:205:HIS:HD2	5:D:404:HOH:O	1.98	0.45
1:A:98:ALA:CB	2:B:45:PHE:CE1	2.99	0.45
2:B:2:ALA:HA	2:B:27:GLN:HE21	1.82	0.45
1:A:22:ASN:ND2	1:A:73:SER:OG	2.50	0.45
2:B:155:LEU:C	2:B:155:LEU:HD23	2.43	0.44
1:A:93:THR:HG22	5:A:429:HOH:O	2.18	0.44
2:D:95:ASP:OD1	2:D:95:ASP:C	2.60	0.44
1:C:22:ASN:ND2	1:C:73:SER:OG	2.51	0.43
1:C:31:GLN:HE21	1:C:94:ASN:HB3	1.82	0.43
1:A:93:THR:HG23	1:A:97:TYR:CE2	2.53	0.43
1:C:30:SER:HA	1:C:93:THR:HA	1.99	0.43
1:A:48:MET:HE2	1:A:61:PHE:HB3	2.01	0.42
1:A:30:SER:HA	1:A:93:THR:HA	2.01	0.42
1:A:149:LYS:CD	1:A:149:LYS:C	2.93	0.42
2:D:155:LEU:C	2:D:155:LEU:HD23	2.45	0.42
1:A:149:LYS:HA	1:A:149:LYS:HE2	2.02	0.41
2:B:133:ILE:HG23	2:B:196:ALA:HB1	2.03	0.41
1:A:114:GLN:HE21	1:A:114:GLN:HB3	1.67	0.41
1:C:123:LEU:HD12	1:C:123:LEU:N	2.36	0.41
1:A:149:LYS:C	1:A:149:LYS:HD3	2.46	0.40
2:D:3:GLY:HA2	2:D:26:LYS:HG3	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	201/200 (100%)	190 (94%)	9 (4%)	2 (1%)	12	5
1	C	200/200 (100%)	190 (95%)	9 (4%)	1 (0%)	24	17
2	B	241/242 (100%)	236 (98%)	5 (2%)	0	100	100
2	D	240/242 (99%)	236 (98%)	4 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
All	All	882/884 (100%)	852 (97%)	27 (3%)	3 (0%)	36 30

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	181	ASP
1	C	181	ASP
1	A	94	ASN

### 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	181/178 (102%)	162 (90%)	19 (10%)	6 2
1	C	180/178 (101%)	162 (90%)	18 (10%)	7 3
2	B	212/211 (100%)	204 (96%)	8 (4%)	29 23
2	D	211/211 (100%)	200 (95%)	11 (5%)	21 14
All	All	784/778 (101%)	728 (93%)	56 (7%)	13 7

All (56) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	2	LYS
1	A	28	ARG
1	A	31	GLN
1	A	40	SER
1	A	42	LYS
1	A	45	GLU
1	A	52	SER
1	A	72	ILE
1	A	75	LEU
1	A	91	VAL
1	A	94	ASN
1	A	114	GLN

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	A	115	LYS
1	A	133	VAL
1	A	140	ASP
1	A	149	LYS
1	A	158	LYS
1	A	160	VAL
1	A	193	ILE
2	B	32	VAL
2	B	39	LEU
2	B	47	PHE
2	B	81	LEU
2	B	88	LEU
2	B	98	SER
2	B	109	LEU
2	B	242	ASP
1	C	2	LYS
1	C	28	ARG
1	C	31	GLN
1	C	52	SER
1	C	72	ILE
1	C	75	LEU
1	C	94	ASN
1	C	99	LEU
1	C	100	ASN
1	C	115	LYS
1	C	127	LYS
1	C	133	VAL
1	C	140	ASP
1	C	158	LYS
1	C	159	CYS
1	C	160	VAL
1	C	181	ASP
1	C	193	ILE
2	D	19	VAL
2	D	32	VAL
2	D	47	PHE
2	D	81	LEU
2	D	88	LEU
2	D	109	LEU
2	D	116	LYS
2	D	136	THR
2	D	173	GLN

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Mol	Chain	Res	Type
2	D	179	PRO
2	D	242	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (28) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	22	ASN
1	A	70	GLN
1	A	94	ASN
1	A	114	GLN
1	A	142	GLN
1	A	178	ASN
1	A	189	ASN
2	B	27	GLN
2	B	77	ASN
2	B	117	ASN
2	B	137	GLN
2	B	173	GLN
2	B	178	GLN
2	B	205	HIS
1	C	22	ASN
1	C	31	GLN
1	C	70	GLN
1	C	94	ASN
1	C	100	ASN
1	C	189	ASN
1	C	190	ASN
2	D	27	GLN
2	D	59	ASN
2	D	77	ASN
2	D	117	ASN
2	D	152	HIS
2	D	173	GLN
2	D	205	HIS

### 5.3.3 RNA

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](#)

9 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	$\# Z  > 2$
4	SO4	B	303	-	4,4,4	0.63	0	6,6,6	0.54	0
3	EDO	B	301	-	3,3,3	0.40	0	2,2,2	0.28	0
4	SO4	D	302	-	4,4,4	0.47	0	6,6,6	0.47	0
3	EDO	C	301	-	3,3,3	0.49	0	2,2,2	0.31	0
3	EDO	B	302	-	3,3,3	0.37	0	2,2,2	1.04	0
3	EDO	A	301	-	3,3,3	0.58	0	2,2,2	0.07	0
4	SO4	C	302	-	4,4,4	0.43	0	6,6,6	0.54	0
4	SO4	A	302	-	4,4,4	0.48	0	6,6,6	0.18	0
4	SO4	D	301	-	4,4,4	0.47	0	6,6,6	0.72	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	C	301	-	-	0/1/1/1	-
3	EDO	B	302	-	-	0/1/1/1	-
3	EDO	A	301	-	-	0/1/1/1	-
3	EDO	B	301	-	-	1/1/1/1	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	B	301	EDO	O1-C1-C2-O2

There are no ring outliers.

1 monomer is involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	C	301	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	200/200 (100%)	0.38	13 (6%) 25 24	19, 55, 103, 119	3 (1%)
1	C	200/200 (100%)	0.44	7 (3%) 47 48	21, 63, 109, 127	2 (1%)
2	B	242/242 (100%)	-0.19	4 (1%) 69 71	19, 42, 69, 106	1 (0%)
2	D	242/242 (100%)	0.24	5 (2%) 63 66	40, 59, 91, 110	0
All	All	884/884 (100%)	0.20	29 (3%) 49 49	19, 54, 100, 127	6 (0%)

All (29) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	192	ILE	4.7
1	C	192	ILE	4.5
2	B	99	TYR	3.3
2	D	97	VAL	3.3
2	B	2	ALA	3.2
2	D	99	TYR	3.0
1	A	201	SER	2.9
2	D	2	ALA	2.7
1	C	127	LYS	2.7
1	C	199	PHE	2.6
1	A	193	ILE	2.5
2	B	59	ASN	2.4
1	A	97	TYR	2.4
2	D	152	HIS	2.3
1	A	182	PHE	2.3
1	C	184	CYS	2.3
1	C	201	SER	2.3
1	C	193	ILE	2.3
1	A	184	CYS	2.3
1	A	93	THR	2.2
1	A	51	TYR	2.2

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Mol	Chain	Res	Type	RSRZ
2	D	180	ALA	2.2
1	A	199	PHE	2.1
1	A	185	ALA	2.1
2	B	242	ASP	2.1
1	A	198	PHE	2.1
1	C	128	SER	2.1
1	A	191	SER	2.0
1	A	94	ASN	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	SO4	B	303	5/5	0.73	0.16	98,101,122,129	0
4	SO4	A	302	5/5	0.77	0.08	97,105,109,120	0
3	EDO	C	301	4/4	0.88	0.13	60,63,64,67	0
4	SO4	C	302	5/5	0.88	0.07	73,83,85,93	0
4	SO4	D	302	5/5	0.89	0.09	84,87,92,100	0
3	EDO	B	302	4/4	0.91	0.14	49,53,53,56	0
3	EDO	B	301	4/4	0.93	0.08	48,53,62,64	0
3	EDO	A	301	4/4	0.96	0.08	49,52,57,57	0
4	SO4	D	301	5/5	0.98	0.06	41,42,44,45	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.