



# Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 01:48 AM UTC

PDB ID : 5NMF / pdb\_00005nmf  
Title : 868 TCR in complex with HLA A02 presenting SLYNTIATL  
Authors : Rizkallah, P.J.; Cole, D.K.; Fuller, A.; Sewell, A.K.  
Deposited on : 2017-04-05  
Resolution : 2.89 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

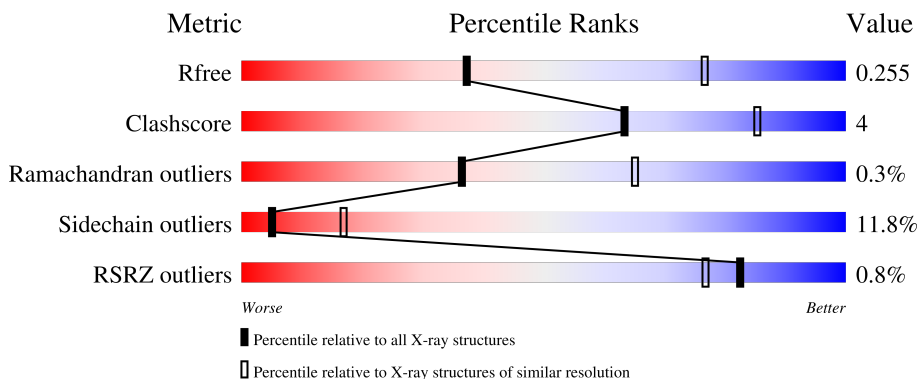
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.89 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	276	 5% (poor fit), 83% (0-1 outliers), 14% (2-3 outliers)
1	F	276	 82% (0-1 outliers), 14% (2-3 outliers)
2	B	100	 5% (poor fit), 71% (0-1 outliers), 23% (2-3 outliers)
2	G	100	 76% (0-1 outliers), 20% (2-3 outliers)
3	C	9	 78% (0-1 outliers), 22% (2-3 outliers)

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Mol	Chain	Length	Quality of chain
3	H	9	 67% 22% 11%
4	D	200	 82% 16% .
5	E	240	 % 83% 15% .
5	J	240	 85% 14% .
6	I	201	 % 81% 17% .

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
9	SO4	E	307	-	-	X	-

## 2 Entry composition i

There are 10 unique types of molecules in this entry. The entry contains 13511 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, A-2 alpha chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	276	Total	C	N	O	S	0	0	0
			2254	1408	410	427	9			
1	F	276	Total	C	N	O	S	0	0	0
			2254	1408	410	427	9			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	B	99	Total	C	N	O	S	0	0	0
			829	528	140	158	3			
2	G	100	Total	C	N	O	S	0	0	0
			837	533	141	159	4			

There are 2 discrepancies between the modelled and reference sequences:

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

- Molecule 3 is a protein called Gag protein.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
3	C	9	Total	C	N	O	0	0	0
			70	45	10	15			
3	H	9	Total	C	N	O	0	0	0
			70	45	10	15			

- Molecule 4 is a protein called HUman T-cell receptor Alpha chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
4	D	200	Total	C	N	O	S	0	0	0
			1560	976	259	317	8			

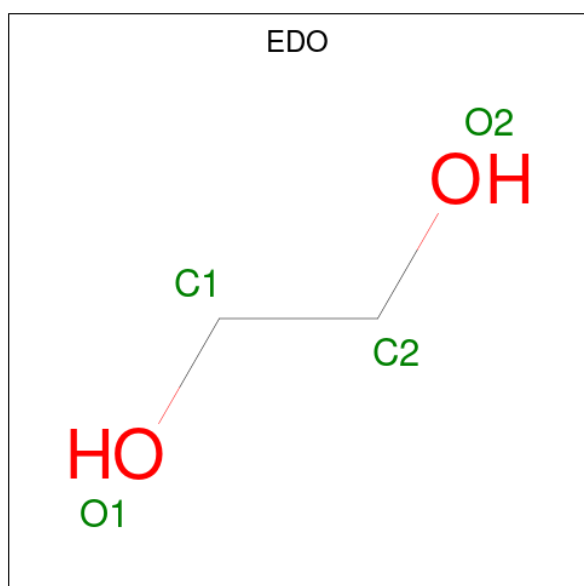
- Molecule 5 is a protein called Human T-cell receptor Beta chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
5	E	239	Total	C	N	O	S	0	0	0
			1917	1208	334	370	5			
5	J	240	Total	C	N	O	S	0	0	0
			1922	1211	335	371	5			

- Molecule 6 is a protein called HUman T-cell receptor Alpha chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
6	I	201	Total	C	N	O	S	0	0	0
			1567	981	260	318	8			

- Molecule 7 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
			Total	C	O		
7	A	1	Total	C	O	0	0
			4	2	2		
7	D	1	Total	C	O	0	0
			4	2	2		
7	E	1	Total	C	O	0	0
			4	2	2		
7	E	1	Total	C	O	0	0
			4	2	2		
7	E	1	Total	C	O	0	0
			4	2	2		
7	F	1	Total	C	O	0	0
			4	2	2		

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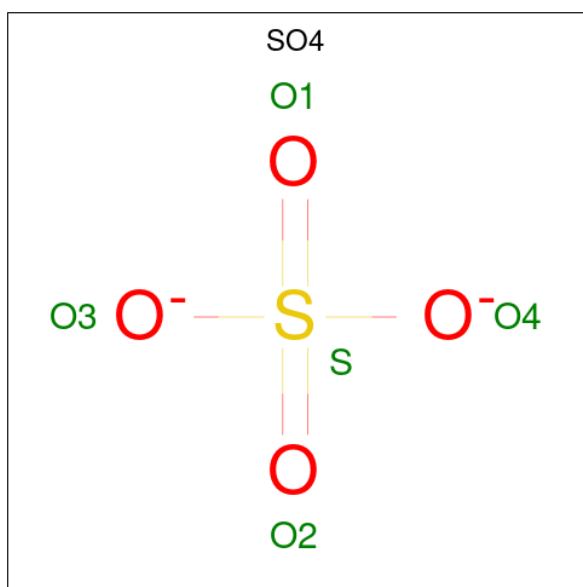
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	F	1	Total	C	O	0	0
			4	2	2		
7	F	1	Total	C	O	0	0
			4	2	2		
7	F	1	Total	C	O	0	0
			4	2	2		
7	F	1	Total	C	O	0	0
			4	2	2		
7	I	1	Total	C	O	0	0
			4	2	2		
7	I	1	Total	C	O	0	0
			4	2	2		
7	J	1	Total	C	O	0	0
			4	2	2		
7	J	1	Total	C	O	0	0
			4	2	2		
7	J	1	Total	C	O	0	0
			4	2	2		
7	J	1	Total	C	O	0	0
			4	2	2		
7	J	1	Total	C	O	0	0
			4	2	2		

- Molecule 8 is GLYCEROL (CCD ID: GOL) (formula: C<sub>3</sub>H<sub>8</sub>O<sub>3</sub>).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
8	A	1	Total C O 6 3 3	0	0
8	D	1	Total C O 6 3 3	0	0
8	I	1	Total C O 6 3 3	0	0

- Molecule 9 is SULFATE ION (CCD ID: SO4) (formula: O<sub>4</sub>S).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
9	A	1	Total O S 5 4 1	0	0

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
9	A	1	Total	O	S	0	0
			5	4	1		
9	A	1	Total	O	S	0	0
			5	4	1		
9	A	1	Total	O	S	0	0
			5	4	1		
9	E	1	Total	O	S	0	0
			5	4	1		
9	E	1	Total	O	S	0	0
			5	4	1		
9	E	1	Total	O	S	0	0
			5	4	1		
9	E	1	Total	O	S	0	0
			5	4	1		
9	F	1	Total	O	S	0	0
			5	4	1		
9	F	1	Total	O	S	0	0
			5	4	1		
9	J	1	Total	O	S	0	0
			5	4	1		
9	J	1	Total	O	S	0	0
			5	4	1		

- Molecule 10 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
10	A	3	Total	O	0	0
			3	3		
10	B	3	Total	O	0	0
			3	3		
10	D	9	Total	O	0	0
			9	9		
10	E	7	Total	O	0	0
			7	7		
10	F	19	Total	O	0	0
			19	19		
10	G	5	Total	O	0	0
			5	5		
10	H	1	Total	O	0	0
			1	1		
10	I	10	Total	O	0	0
			10	10		

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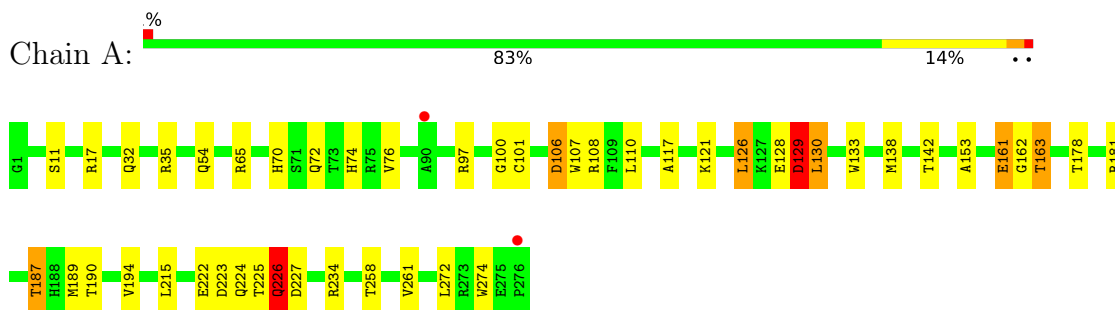
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<b>Mol</b>	<b>Chain</b>	<b>Residues</b>	<b>Atoms</b>		<b>ZeroOcc</b>	<b>AltConf</b>
10	J	20	Total	O	0	0
			20	20		

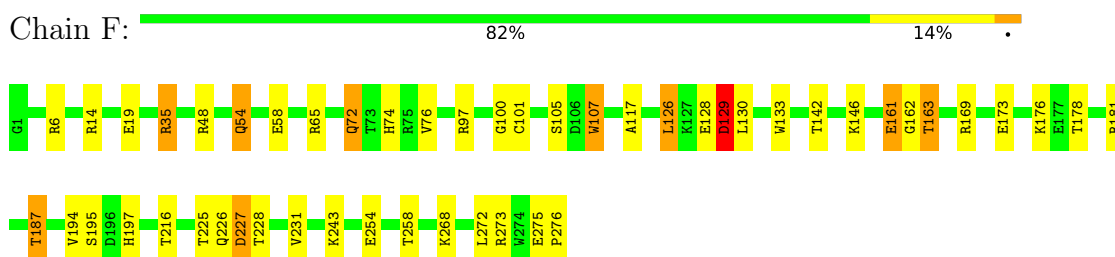
### 3 Residue-property plots [i](#)

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.

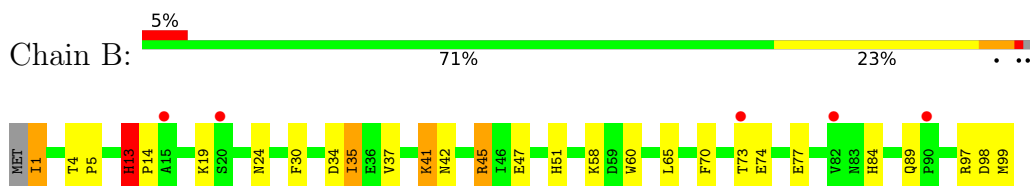
- Molecule 1: HLA class I histocompatibility antigen, A-2 alpha chain



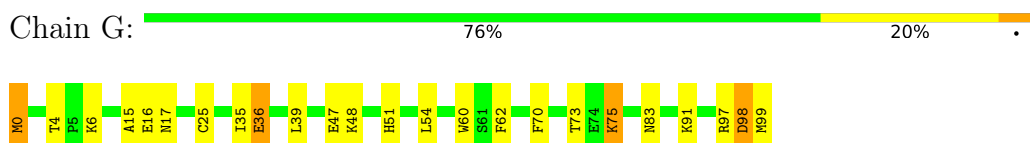
- Molecule 1: HLA class I histocompatibility antigen, A-2 alpha chain



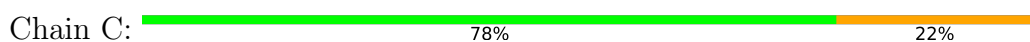
- Molecule 2: Beta-2-microglobulin

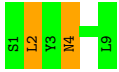


- Molecule 2: Beta-2-microglobulin

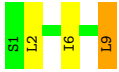


- Molecule 3: Gag protein

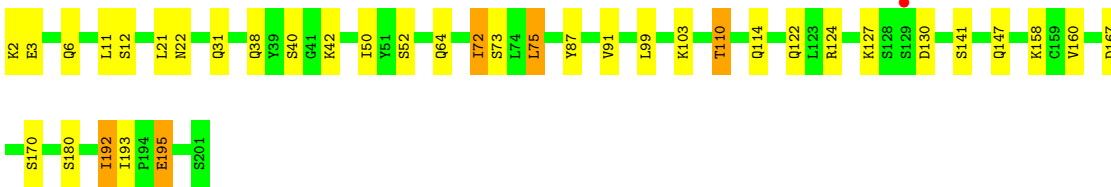
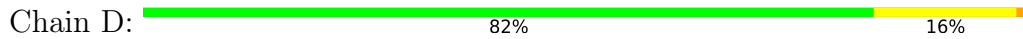




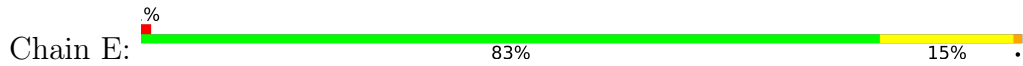
- Molecule 3: Gag protein



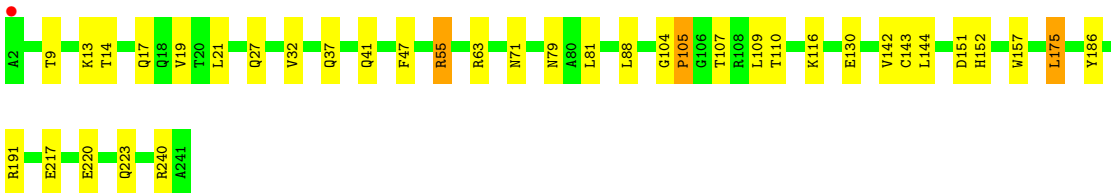
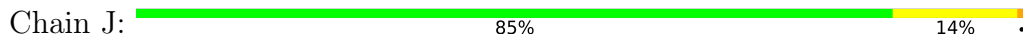
- Molecule 4: HUMAN T-cell receptor Alpha chain



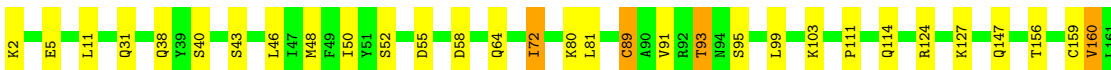
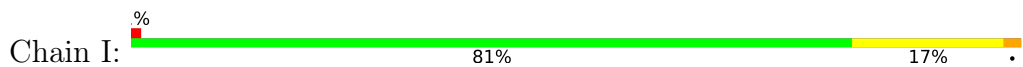
- Molecule 5: Human T-cell receptor Beta chain



- Molecule 5: Human T-cell receptor Beta chain



- Molecule 6: HUMAN T-cell receptor Alpha chain





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	207.59Å 84.71Å 112.12Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	112.12 – 2.89 112.12 – 2.89	Depositor EDS
% Data completeness (in resolution range)	99.9 (112.12-2.89) 99.9 (112.12-2.89)	Depositor EDS
$R_{merge}$	0.15	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.90 (at 2.91Å)	Xtrriage
Refinement program	REFMAC 5.8.0158	Depositor
R, $R_{free}$	0.193 , 0.255 0.196 , 0.255	Depositor DCC
$R_{free}$ test set	2277 reflections (5.04%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	51.6	Xtrriage
Anisotropy	0.251	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.33 , 46.6	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.47$ , $\langle L^2 \rangle = 0.29$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
$F_o, F_c$ correlation	0.93	EDS
Total number of atoms	13511	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	59.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.97% 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: GOL, 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	0.93	0/2320	1.07	8/3149 (0.3%)
1	F	1.07	0/2320	1.14	10/3149 (0.3%)
2	B	0.94	0/852	1.13	4/1152 (0.3%)
2	G	1.03	1/860 (0.1%)	1.11	2/1162 (0.2%)
3	C	0.97	0/70	1.26	0/94
3	H	1.26	0/70	1.44	0/94
4	D	1.06	0/1593	1.09	2/2155 (0.1%)
5	E	1.00	1/1972 (0.1%)	1.11	4/2688 (0.1%)
5	J	1.06	0/1977	1.15	6/2695 (0.2%)
6	I	1.09	1/1601 (0.1%)	1.08	1/2167 (0.0%)
All	All	1.03	3/13635 (0.0%)	1.11	37/18505 (0.2%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
2	G	0	1
4	D	0	2
6	I	0	1
All	All	0	4

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	E	60	PHE	CA-C	-5.90	1.47	1.52
2	G	15	ALA	C-O	-5.04	1.17	1.23
6	I	46	LEU	C-O	-5.03	1.18	1.24

All (37) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	E	71	ASN	N-CA-C	-9.16	98.44	110.53
5	J	71	ASN	N-CA-C	-9.14	98.47	110.53
1	F	162	GLY	N-CA-C	8.29	119.30	111.67
1	A	162	GLY	N-CA-C	8.03	119.05	111.67
1	F	161	GLU	N-CA-C	-7.72	99.61	110.50
1	F	107	TRP	CA-CB-CG	7.23	127.34	113.60
1	A	161	GLU	N-CA-C	-6.77	100.95	110.50
2	B	35	ILE	N-CA-C	6.74	117.25	108.35
2	B	13	HIS	CB-CA-C	6.68	119.14	108.91
4	D	180	SER	N-CA-C	-6.54	100.36	110.10
2	G	51	HIS	N-CA-C	6.25	118.68	109.24
2	B	41	LYS	N-CA-C	6.24	121.17	113.50
1	F	100	GLY	N-CA-C	6.23	118.97	110.69
1	A	106	ASP	N-CA-C	-6.18	99.09	108.67
5	J	55	ARG	CG-CD-NE	-6.12	98.53	112.00
5	J	71	ASN	CA-C-N	-5.86	112.92	122.65
5	J	71	ASN	C-N-CA	-5.86	112.92	122.65
1	A	100	GLY	N-CA-C	5.76	118.87	110.63
1	F	129	ASP	CA-C-N	-5.75	112.98	123.34
1	F	129	ASP	C-N-CA	-5.75	112.98	123.34
1	F	226	GLN	N-CA-C	-5.60	105.08	111.07
5	E	71	ASN	CA-C-N	-5.55	113.43	122.65
5	E	71	ASN	C-N-CA	-5.55	113.43	122.65
5	J	191	ARG	CG-CD-NE	5.54	124.19	112.00
1	F	227	ASP	N-CA-C	5.50	119.61	113.01
1	F	54	GLN	N-CA-C	5.39	118.64	111.75
5	J	105	PRO	N-CA-C	-5.38	101.38	112.47
2	B	51	HIS	N-CA-C	5.38	117.24	109.07
5	E	105	PRO	N-CA-C	-5.37	101.41	112.47
2	G	75	LYS	N-CA-C	5.29	117.05	111.28
4	D	72	ILE	CB-CA-C	-5.17	103.45	110.42
1	F	101	CYS	CB-CA-C	-5.15	100.80	109.50
1	A	129	ASP	CA-C-N	-5.09	114.17	123.34
1	A	129	ASP	C-N-CA	-5.09	114.17	123.34
1	A	101	CYS	CB-CA-C	-5.08	100.92	109.50
1	A	226	GLN	N-CA-C	-5.05	105.05	111.11
6	I	89	CYS	N-CA-CB	-5.04	102.58	110.69

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
4	D	130	ASP	Peptide

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Mol	Chain	Res	Type	Group
4	D	195	GLU	Peptide
2	G	0	MET	Peptide
6	I	201	SER	Peptide

## 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	2254	0	2103	23	0
1	F	2254	0	2103	19	0
2	B	829	0	794	15	0
2	G	837	0	803	7	0
3	C	70	0	74	3	0
3	H	70	0	74	3	0
4	D	1560	0	1486	13	0
5	E	1917	0	1798	16	0
5	J	1922	0	1803	13	0
6	I	1567	0	1493	17	0
7	A	4	0	6	0	0
7	D	4	0	6	0	0
7	E	12	0	18	0	0
7	F	24	0	36	0	0
7	I	8	0	12	0	0
7	J	24	0	36	2	0
8	A	6	0	8	0	0
8	D	6	0	8	0	0
8	I	6	0	8	0	0
9	A	20	0	0	1	0
9	E	20	0	0	2	0
9	F	10	0	0	0	0
9	J	10	0	0	0	0
10	A	3	0	0	0	0
10	B	3	0	0	0	0
10	D	9	0	0	0	0
10	E	7	0	0	0	0
10	F	19	0	0	0	0
10	G	5	0	0	0	0
10	H	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
10	I	10	0	0	0	0
10	J	20	0	0	0	0
All	All	13511	0	12669	104	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 (104) 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)
2:B:35:ILE:HD11	2:B:84:HIS:CD2	1.87	1.09
4:D:38:GLN:HE22	5:E:37:GLN:HE22	1.11	0.95
6:I:38:GLN:HE22	5:J:37:GLN:HE22	0.96	0.91
1:A:234:ARG:NH1	2:B:99:MET:SD	2.55	0.78
6:I:38:GLN:HE22	5:J:37:GLN:NE2	1.80	0.72
6:I:38:GLN:NE2	5:J:37:GLN:HE22	1.80	0.71
1:F:163:THR:CG2	6:I:31:GLN:HE21	2.02	0.71
1:A:74:HIS:HE1	1:A:97:ARG:HE	1.40	0.69
1:F:74:HIS:HE1	1:F:97:ARG:HE	1.41	0.68
1:F:163:THR:HG21	6:I:31:GLN:HE21	1.58	0.68
5:E:18:GLN:NE2	5:E:77:ASN:HD21	1.91	0.68
1:A:163:THR:CG2	4:D:31:GLN:HE21	2.09	0.66
5:J:151:ASP:HB3	5:J:186:TYR:CE2	2.34	0.63
4:D:110:THR:HG23	4:D:141:SER:CB	2.29	0.62
1:A:72:GLN:NE2	5:E:51:GLU:OE2	2.33	0.61
2:B:35:ILE:HG22	2:B:37:VAL:HG23	1.83	0.61
6:I:156:THR:HG22	5:J:175:LEU:HD21	1.82	0.60
5:E:15:ARG:NH2	9:E:307:SO4:O1	2.36	0.59
1:A:70:HIS:CE1	3:C:2:LEU:HD23	2.38	0.59
2:B:13:HIS:CG	2:B:14:PRO:HD2	2.39	0.58
5:J:21:LEU:HD22	5:J:107:THR:HG21	1.86	0.57
1:A:129:ASP:C	1:A:130:LEU:HG	2.29	0.57
5:J:13:LYS:HD2	5:J:17:GLN:NE2	2.20	0.57
4:D:38:GLN:NE2	5:E:37:GLN:HE22	1.93	0.56
1:F:163:THR:HG21	6:I:31:GLN:NE2	2.20	0.56
1:F:35:ARG:HD2	1:F:48:ARG:CZ	2.35	0.56
1:A:163:THR:HG21	4:D:31:GLN:HE21	1.70	0.55
4:D:110:THR:HG23	4:D:141:SER:HB3	1.88	0.55
5:E:173:GLN:HE21	5:E:173:GLN:HA	1.71	0.55
1:A:189:MET:HE1	1:A:274:TRP:HB2	1.89	0.54
1:A:70:HIS:CE1	3:C:2:LEU:CD2	2.91	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:129:ASP:C	1:F:130:LEU:HG	2.33	0.53
1:F:231:VAL:O	1:F:243:LYS:NZ	2.37	0.53
6:I:48:MET:HE3	6:I:58:ASP:HB3	1.88	0.53
1:F:117:ALA:HB2	2:G:60:TRP:CE2	2.43	0.53
4:D:38:GLN:HE22	5:E:37:GLN:NE2	1.94	0.53
5:J:223:GLN:HE21	7:J:303:EDO:H11	1.75	0.52
1:A:187:THR:HB	1:A:272:LEU:HD21	1.91	0.52
6:I:55:ASP:OD1	6:I:64:GLN:HG3	2.11	0.51
5:E:21:LEU:HD22	5:E:107:THR:HG21	1.93	0.51
1:F:272:LEU:N	1:F:272:LEU:HD12	2.25	0.50
5:E:30:ASP:OD2	5:E:50:TYR:HE1	1.92	0.50
5:J:104:GLY:C	5:J:105:PRO:O	2.53	0.50
4:D:21:LEU:HD22	4:D:87:TYR:HB2	1.93	0.50
1:F:128:GLU:C	1:F:129:ASP:O	2.50	0.50
1:F:146:LYS:HE3	3:H:9:LEU:OXT	2.12	0.49
1:F:72:GLN:HG3	7:J:306:EDO:O2	2.12	0.49
6:I:162:ASP:HB3	6:I:164:ARG:HE	1.76	0.49
1:A:226:GLN:HE21	1:A:226:GLN:HA	1.77	0.49
3:H:6:ILE:HG23	3:H:6:ILE:O	2.13	0.48
1:A:106:ASP:O	1:A:106:ASP:CG	2.54	0.48
5:E:104:GLY:C	5:E:105:PRO:O	2.53	0.48
1:A:121:LYS:HD3	2:B:1:ILE:HG21	1.96	0.48
1:F:163:THR:HG23	6:I:31:GLN:HE21	1.75	0.48
5:J:151:ASP:HB3	5:J:186:TYR:CD2	2.49	0.48
1:A:128:GLU:C	1:A:129:ASP:O	2.53	0.48
2:B:34:ASP:O	2:B:35:ILE:HD13	2.14	0.48
2:G:36:GLU:HG2	2:G:83:ASN:HB3	1.96	0.47
1:F:126:LEU:HD13	1:F:133:TRP:CZ3	2.50	0.47
2:B:5:PRO:HD3	2:B:84:HIS:CD2	2.50	0.47
2:B:41:LYS:O	2:B:42:ASN:ND2	2.48	0.46
1:A:153:ALA:HB3	9:A:305:SO4:O3	2.15	0.46
4:D:22:ASN:ND2	4:D:73:SER:OG	2.49	0.46
1:F:187:THR:HB	1:F:272:LEU:HD21	1.98	0.46
6:I:43:SER:OG	5:J:104:GLY:O	2.25	0.46
4:D:6:GLN:O	4:D:103:LYS:HE2	2.15	0.45
1:A:190:THR:HG21	2:B:98:ASP:OD1	2.16	0.45
1:A:215:LEU:HD12	1:A:261:VAL:HG22	1.97	0.45
2:B:35:ILE:CD1	2:B:84:HIS:CD2	2.79	0.45
6:I:81:LEU:HD21	6:I:111:PRO:HB3	1.99	0.45
1:A:163:THR:HG23	4:D:31:GLN:HE21	1.79	0.45
6:I:93:THR:HG22	6:I:95:SER:H	1.81	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:126:LEU:HD13	1:A:133:TRP:CZ3	2.52	0.44
5:E:143:CYS:HB2	5:E:157:TRP:CZ2	2.53	0.44
2:G:17:ASN:OD1	2:G:97:ARG:NH1	2.49	0.44
2:B:45:ARG:NH1	2:B:47:GLU:OE1	2.50	0.44
2:G:35:ILE:O	2:G:35:ILE:HG23	2.17	0.44
5:E:133:ILE:HG23	5:E:196:ALA:HB1	1.99	0.43
4:D:192:ILE:HD13	4:D:192:ILE:O	2.19	0.43
5:E:151:ASP:CG	5:E:151:ASP:O	2.62	0.43
6:I:111:PRO:HG3	6:I:160:VAL:HG21	2.01	0.43
1:A:215:LEU:CD1	1:A:261:VAL:HG22	2.48	0.43
1:A:126:LEU:HD23	1:A:130:LEU:HD22	2.00	0.43
1:F:275:GLU:O	1:F:276:PRO:C	2.62	0.43
2:B:24:ASN:HB3	2:B:65:LEU:HD11	1.99	0.42
6:I:103:LYS:HG2	5:J:41:GLN:HE22	1.84	0.42
2:B:35:ILE:HD11	2:B:84:HIS:CG	2.46	0.42
1:A:106:ASP:O	1:A:106:ASP:OD1	2.37	0.42
1:F:126:LEU:HD23	1:F:130:LEU:HD22	2.00	0.42
3:C:4:ASN:H	3:C:4:ASN:HD22	1.66	0.42
5:J:143:CYS:HB2	5:J:157:TRP:CZ2	2.55	0.42
4:D:75:LEU:HD22	4:D:75:LEU:N	2.35	0.41
5:E:15:ARG:NH2	9:E:307:SO4:S	2.94	0.41
3:H:6:ILE:O	3:H:6:ILE:CG2	2.68	0.41
6:I:72:ILE:HD13	6:I:89:CYS:SG	2.61	0.41
2:G:54:LEU:HD11	2:G:62:PHE:HB3	2.02	0.41
1:F:194:VAL:HG12	1:F:195:SER:N	2.36	0.41
2:B:30:PHE:HB2	2:B:84:HIS:NE2	2.36	0.41
1:F:169:ARG:O	1:F:173:GLU:HG3	2.21	0.41
2:G:25:CYS:HB2	2:G:39:LEU:HD21	2.02	0.41
1:A:117:ALA:HB2	2:B:60:TRP:CE2	2.56	0.40
2:G:98:ASP:O	2:G:99:MET:HG2	2.21	0.40
5:E:18:GLN:HE21	5:E:18:GLN:HB2	1.67	0.40
5:E:170:THR:O	5:E:171:ASP:C	2.65	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	274/276 (99%)	257 (94%)	15 (6%)	2 (1%)	18	48
1	F	274/276 (99%)	260 (95%)	13 (5%)	1 (0%)	30	59
2	B	97/100 (97%)	91 (94%)	6 (6%)	0	100	100
2	G	98/100 (98%)	94 (96%)	4 (4%)	0	100	100
3	C	7/9 (78%)	6 (86%)	1 (14%)	0	100	100
3	H	7/9 (78%)	6 (86%)	1 (14%)	0	100	100
4	D	198/200 (99%)	185 (93%)	12 (6%)	1 (0%)	24	54
5	E	237/240 (99%)	229 (97%)	8 (3%)	0	100	100
5	J	238/240 (99%)	230 (97%)	7 (3%)	1 (0%)	30	59
6	I	199/201 (99%)	182 (92%)	17 (8%)	0	100	100
All	All	1629/1651 (99%)	1540 (94%)	84 (5%)	5 (0%)	36	65

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
4	D	167	ASP
1	A	107	TRP
1	A	129	ASP
1	F	129	ASP
5	J	63	ARG

### 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	232/232 (100%)	206 (89%)	26 (11%)	6	19
1	F	232/232 (100%)	204 (88%)	28 (12%)	5	16
2	B	94/95 (99%)	82 (87%)	12 (13%)	4	14

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	G	95/95 (100%)	83 (87%)	12 (13%)	4	14
3	C	8/8 (100%)	6 (75%)	2 (25%)	0	2
3	H	8/8 (100%)	6 (75%)	2 (25%)	0	2
4	D	178/178 (100%)	153 (86%)	25 (14%)	3	11
5	E	209/209 (100%)	188 (90%)	21 (10%)	7	24
5	J	209/209 (100%)	188 (90%)	21 (10%)	7	24
6	I	179/179 (100%)	158 (88%)	21 (12%)	5	17
All	All	1444/1445 (100%)	1274 (88%)	170 (12%)	5	17

All (170) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	11	SER
1	A	17	ARG
1	A	32	GLN
1	A	35	ARG
1	A	54	GLN
1	A	65	ARG
1	A	76	VAL
1	A	108	ARG
1	A	110	LEU
1	A	126	LEU
1	A	130	LEU
1	A	138	MET
1	A	142	THR
1	A	161	GLU
1	A	163	THR
1	A	178	THR
1	A	181	ARG
1	A	187	THR
1	A	194	VAL
1	A	222	GLU
1	A	223	ASP
1	A	224	GLN
1	A	225	THR
1	A	226	GLN
1	A	227	ASP
1	A	258	THR
2	B	1	ILE
2	B	4	THR

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
2	B	13	HIS
2	B	19	LYS
2	B	45	ARG
2	B	58	LYS
2	B	70	PHE
2	B	73	THR
2	B	74	GLU
2	B	77	GLU
2	B	89	GLN
2	B	97	ARG
3	C	2	LEU
3	C	4	ASN
4	D	2	LYS
4	D	3	GLU
4	D	11	LEU
4	D	12	SER
4	D	40	SER
4	D	42	LYS
4	D	50	ILE
4	D	52	SER
4	D	64	GLN
4	D	72	ILE
4	D	75	LEU
4	D	91	VAL
4	D	99	LEU
4	D	110	THR
4	D	114	GLN
4	D	122	GLN
4	D	124	ARG
4	D	127	LYS
4	D	147	GLN
4	D	158	LYS
4	D	160	VAL
4	D	170	SER
4	D	192	ILE
4	D	193	ILE
4	D	195	GLU
5	E	14	THR
5	E	18	GLN
5	E	19	VAL
5	E	32	VAL
5	E	47	PHE

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
5	E	79	ASN
5	E	81	LEU
5	E	83	LEU
5	E	88	LEU
5	E	109	LEU
5	E	110	THR
5	E	116	LYS
5	E	127	GLU
5	E	142	VAL
5	E	159	VAL
5	E	169	CYS
5	E	173	GLN
5	E	178	GLN
5	E	203	ARG
5	E	223	GLN
5	E	240	ARG
1	F	6	ARG
1	F	14	ARG
1	F	19	GLU
1	F	35	ARG
1	F	54	GLN
1	F	58	GLU
1	F	65	ARG
1	F	72	GLN
1	F	76	VAL
1	F	105	SER
1	F	107	TRP
1	F	126	LEU
1	F	142	THR
1	F	161	GLU
1	F	163	THR
1	F	176	LYS
1	F	178	THR
1	F	181	ARG
1	F	187	THR
1	F	197	HIS
1	F	216	THR
1	F	225	THR
1	F	227	ASP
1	F	228	THR
1	F	254	GLU
1	F	258	THR

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	F	268	LYS
1	F	273	ARG
2	G	0	MET
2	G	4	THR
2	G	6	LYS
2	G	16	GLU
2	G	36	GLU
2	G	47	GLU
2	G	48	LYS
2	G	70	PHE
2	G	73	THR
2	G	75	LYS
2	G	91	LYS
2	G	98	ASP
3	H	2	LEU
3	H	9	LEU
6	I	2	LYS
6	I	5	GLU
6	I	11	LEU
6	I	40	SER
6	I	50	ILE
6	I	52	SER
6	I	72	ILE
6	I	80	LYS
6	I	91	VAL
6	I	93	THR
6	I	99	LEU
6	I	114	GLN
6	I	124	ARG
6	I	127	LYS
6	I	147	GLN
6	I	159	CYS
6	I	160	VAL
6	I	165	SER
6	I	169	LYS
6	I	170	SER
6	I	195	GLU
5	J	9	THR
5	J	14	THR
5	J	19	VAL
5	J	27	GLN
5	J	32	VAL

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Mol	Chain	Res	Type
5	J	47	PHE
5	J	55	ARG
5	J	79	ASN
5	J	81	LEU
5	J	88	LEU
5	J	109	LEU
5	J	110	THR
5	J	116	LYS
5	J	130	GLU
5	J	142	VAL
5	J	144	LEU
5	J	152	HIS
5	J	175	LEU
5	J	217	GLU
5	J	220	GLU
5	J	240	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (44) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	74	HIS
1	A	86	ASN
1	A	93	HIS
1	A	115	GLN
1	A	155	GLN
1	A	174	ASN
1	A	226	GLN
1	A	262	GLN
1	A	263	HIS
2	B	42	ASN
2	B	89	GLN
3	C	4	ASN
4	D	6	GLN
4	D	22	ASN
4	D	31	GLN
4	D	100	ASN
4	D	122	GLN
4	D	142	GLN
4	D	189	ASN
5	E	10	HIS
5	E	18	GLN
5	E	36	GLN

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Mol	Chain	Res	Type
5	E	37	GLN
5	E	117	ASN
5	E	173	GLN
5	E	205	HIS
5	E	218	ASN
1	F	43	GLN
1	F	72	GLN
1	F	74	HIS
1	F	93	HIS
1	F	115	GLN
1	F	174	ASN
1	F	253	GLN
1	F	263	HIS
6	I	6	GLN
6	I	31	GLN
6	I	70	GLN
5	J	36	GLN
5	J	37	GLN
5	J	41	GLN
5	J	59	ASN
5	J	117	ASN
5	J	218	ASN

### 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](#)

34 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
7	EDO	F	304	-	3,3,3	0.40	0	2,2,2	0.48	0
7	EDO	E	301	-	3,3,3	0.45	0	2,2,2	0.54	0
7	EDO	J	305	-	3,3,3	0.53	0	2,2,2	0.22	0
9	SO4	A	304	-	4,4,4	0.45	0	6,6,6	0.21	0
7	EDO	A	301	-	3,3,3	0.58	0	2,2,2	0.16	0
9	SO4	E	304	-	4,4,4	0.51	0	6,6,6	0.15	0
7	EDO	F	303	-	3,3,3	0.53	0	2,2,2	0.19	0
9	SO4	A	306	-	4,4,4	0.45	0	6,6,6	0.18	0
7	EDO	J	303	-	3,3,3	0.61	0	2,2,2	0.11	0
9	SO4	J	307	-	4,4,4	0.49	0	6,6,6	0.20	0
7	EDO	D	301	-	3,3,3	0.54	0	2,2,2	0.31	0
7	EDO	J	306	-	3,3,3	0.48	0	2,2,2	0.40	0
9	SO4	F	308	-	4,4,4	0.52	0	6,6,6	0.30	0
7	EDO	F	301	-	3,3,3	0.36	0	2,2,2	0.56	0
7	EDO	F	305	-	3,3,3	0.49	0	2,2,2	0.36	0
7	EDO	J	304	-	3,3,3	0.54	0	2,2,2	0.30	0
7	EDO	F	302	-	3,3,3	0.42	0	2,2,2	0.42	0
9	SO4	A	305	-	4,4,4	0.50	0	6,6,6	0.21	0
8	GOL	D	302	-	5,5,5	0.56	0	5,5,5	0.24	0
8	GOL	A	302	-	5,5,5	0.57	0	5,5,5	0.56	0
9	SO4	E	305	-	4,4,4	0.48	0	6,6,6	0.20	0
9	SO4	E	307	-	4,4,4	0.37	0	6,6,6	0.44	0
7	EDO	I	302	-	3,3,3	0.42	0	2,2,2	0.33	0
7	EDO	E	302	-	3,3,3	0.40	0	2,2,2	0.41	0
7	EDO	J	302	-	3,3,3	0.39	0	2,2,2	0.45	0
7	EDO	I	301	-	3,3,3	0.49	0	2,2,2	0.32	0
9	SO4	J	308	-	4,4,4	0.41	0	6,6,6	0.50	0
8	GOL	I	303	-	5,5,5	0.48	0	5,5,5	0.64	0
7	EDO	J	301	-	3,3,3	0.45	0	2,2,2	0.40	0
9	SO4	A	303	-	4,4,4	0.42	0	6,6,6	0.38	0
9	SO4	E	306	-	4,4,4	0.48	0	6,6,6	0.31	0
7	EDO	F	306	-	3,3,3	0.51	0	2,2,2	0.31	0
7	EDO	E	303	-	3,3,3	0.46	0	2,2,2	0.28	0
9	SO4	F	307	-	4,4,4	0.62	0	6,6,6	0.42	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
7	EDO	F	304	-	-	0/1/1/1	-
7	EDO	E	301	-	-	1/1/1/1	-
7	EDO	J	305	-	-	0/1/1/1	-
7	EDO	A	301	-	-	0/1/1/1	-
7	EDO	F	303	-	-	0/1/1/1	-
7	EDO	J	303	-	-	1/1/1/1	-
7	EDO	D	301	-	-	0/1/1/1	-
7	EDO	J	306	-	-	1/1/1/1	-
7	EDO	F	301	-	-	0/1/1/1	-
7	EDO	F	305	-	-	1/1/1/1	-
7	EDO	J	304	-	-	1/1/1/1	-
7	EDO	F	302	-	-	1/1/1/1	-
8	GOL	D	302	-	-	3/4/4/4	-
8	GOL	A	302	-	-	2/4/4/4	-
7	EDO	I	302	-	-	1/1/1/1	-
7	EDO	E	302	-	-	0/1/1/1	-
7	EDO	J	302	-	-	0/1/1/1	-
7	EDO	I	301	-	-	1/1/1/1	-
8	GOL	I	303	-	-	2/4/4/4	-
7	EDO	J	301	-	-	0/1/1/1	-
7	EDO	F	306	-	-	1/1/1/1	-
7	EDO	E	303	-	-	1/1/1/1	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (17) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
8	D	302	GOL	O1-C1-C2-O2
8	D	302	GOL	O1-C1-C2-C3
8	I	303	GOL	O1-C1-C2-C3
8	A	302	GOL	C1-C2-C3-O3
8	D	302	GOL	C1-C2-C3-O3
8	A	302	GOL	O2-C2-C3-O3
8	I	303	GOL	O1-C1-C2-O2
7	I	301	EDO	O1-C1-C2-O2
7	I	302	EDO	O1-C1-C2-O2
7	J	304	EDO	O1-C1-C2-O2

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Mol	Chain	Res	Type	Atoms
7	J	306	EDO	O1-C1-C2-O2
7	E	301	EDO	O1-C1-C2-O2
7	F	302	EDO	O1-C1-C2-O2
7	F	306	EDO	O1-C1-C2-O2
7	J	303	EDO	O1-C1-C2-O2
7	F	305	EDO	O1-C1-C2-O2
7	E	303	EDO	O1-C1-C2-O2

There are no ring outliers.

4 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	J	303	EDO	1	0
7	J	306	EDO	1	0
9	A	305	SO4	1	0
9	E	307	SO4	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 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	276/276 (100%)	0.05	2 (0%) 84 79	43, 70, 107, 143	0
1	F	276/276 (100%)	-0.32	0 100 100	26, 47, 86, 125	0
2	B	99/100 (99%)	0.60	5 (5%) 33 26	63, 95, 123, 128	0
2	G	100/100 (100%)	-0.36	0 100 100	28, 48, 73, 82	0
3	C	9/9 (100%)	-0.35	0 100 100	45, 50, 62, 71	0
3	H	9/9 (100%)	-0.69	0 100 100	28, 30, 35, 41	0
4	D	200/200 (100%)	-0.10	1 (0%) 87 83	33, 53, 106, 137	0
5	E	239/240 (99%)	-0.31	2 (0%) 82 77	31, 50, 76, 109	0
5	J	240/240 (100%)	-0.40	1 (0%) 88 85	26, 43, 71, 102	0
6	I	201/201 (100%)	-0.15	2 (0%) 79 73	27, 51, 102, 119	0
All	All	1649/1651 (99%)	-0.17	13 (0%) 82 77	26, 54, 102, 143	0

All (13) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	15	ALA	2.8
6	I	165	SER	2.7
1	A	90	ALA	2.5
5	J	2	ALA	2.3
5	E	238	TRP	2.3
2	B	90	PRO	2.2
6	I	202	PRO	2.2
2	B	73	THR	2.2
2	B	82	VAL	2.1
1	A	276	PRO	2.1
4	D	129	SER	2.1
5	E	198	PHE	2.1
2	B	20	SER	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
8	GOL	D	302	6/6	0.56	0.20	87,93,97,97	0
9	SO4	A	304	5/5	0.74	0.13	98,104,110,113	0
7	EDO	J	301	4/4	0.77	0.14	63,67,70,72	0
7	EDO	I	302	4/4	0.82	0.13	72,80,80,81	0
7	EDO	F	303	4/4	0.83	0.17	57,58,59,61	0
8	GOL	A	302	6/6	0.83	0.12	63,67,69,69	0
9	SO4	A	305	5/5	0.83	0.16	95,95,101,102	0
7	EDO	F	305	4/4	0.84	0.13	51,57,60,60	0
7	EDO	F	302	4/4	0.84	0.11	57,60,62,64	0
7	EDO	A	301	4/4	0.84	0.12	61,63,65,65	0
7	EDO	J	305	4/4	0.84	0.14	57,60,62,63	0
7	EDO	J	303	4/4	0.85	0.21	41,49,55,61	0
7	EDO	F	304	4/4	0.85	0.21	69,75,77,78	0
7	EDO	E	303	4/4	0.85	0.17	65,66,67,69	0
8	GOL	I	303	6/6	0.86	0.12	55,59,62,64	0
7	EDO	E	301	4/4	0.86	0.20	52,54,55,55	0
7	EDO	F	301	4/4	0.86	0.12	46,46,47,49	0
7	EDO	J	302	4/4	0.87	0.10	53,53,54,55	0
7	EDO	J	304	4/4	0.87	0.09	54,54,56,56	0
9	SO4	J	307	5/5	0.87	0.18	87,88,92,93	0
7	EDO	E	302	4/4	0.89	0.14	38,42,46,46	0
9	SO4	A	306	5/5	0.89	0.16	109,109,112,116	0
9	SO4	E	304	5/5	0.89	0.15	80,81,84,85	0
9	SO4	E	305	5/5	0.89	0.13	100,100,101,107	0
7	EDO	F	306	4/4	0.89	0.16	57,58,58,60	0
7	EDO	D	301	4/4	0.90	0.13	39,42,44,44	0
9	SO4	F	307	5/5	0.91	0.11	58,58,65,70	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
7	EDO	J	306	4/4	0.91	0.18	48,53,54,55	0
7	EDO	I	301	4/4	0.92	0.12	50,51,52,52	0
9	SO4	A	303	5/5	0.93	0.12	66,72,76,78	0
9	SO4	J	308	5/5	0.93	0.07	61,64,66,71	0
9	SO4	F	308	5/5	0.94	0.12	57,63,65,66	0
9	SO4	E	307	5/5	0.97	0.06	37,37,39,40	5
9	SO4	E	306	5/5	0.98	0.06	52,54,57,60	0

## 6.5 Other polymers [\(i\)](#)

There are no such residues in this entry.