



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 11:08 AM UTC

PDB ID : 5C0B / pdb_00005c0b
Title : 1E6 TCR in complex with HLA-A02 carrying RQFGPDFPTI
Authors : Rizkallah, P.J.; Bulek, A.M.; Cole, D.K.; Sewell, A.K.
Deposited on : 2015-06-12
Resolution : 2.03 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

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

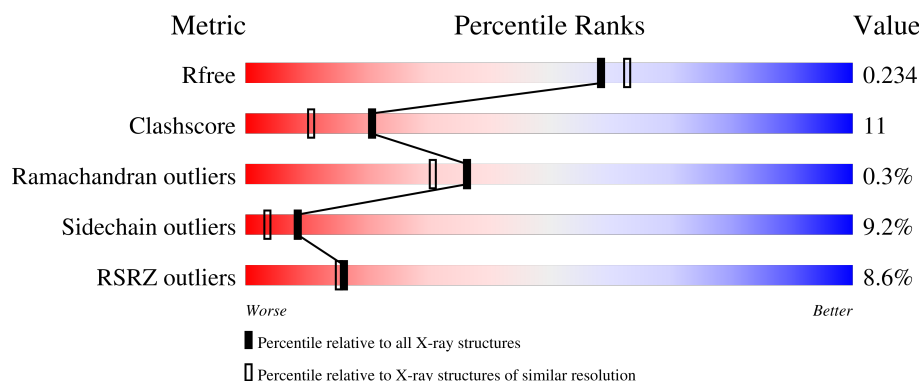
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.03 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	13299 (2.04-2.00)
Clashscore	190562	1022 (2.02-2.02)
Ramachandran outliers	187476	1014 (2.02-2.02)
Sidechain outliers	187428	1014 (2.02-2.02)
RSRZ outliers	180081	13314 (2.04-2.00)

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 ≥ 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	275	% 76% 21% ..
1	F	275	3% 79% 19% .
2	B	100	% 75% 23% .
2	G	100	2% 81% 15% .
3	C	10	90% 10%

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Mol	Chain	Length	Quality of chain
3	H	10	
4	D	199	
4	I	199	
5	E	247	
5	J	247	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
6	EDO	A	301	-	-	X	-
6	EDO	J	305	-	-	X	-
7	GOL	B	306	-	X	-	-
7	GOL	E	311	-	-	X	-
8	SO4	E	312	-	-	X	-
9	PG4	J	308	-	-	X	-

2 Entry composition [i](#)

There are 10 unique types of molecules in this entry. The entry contains 14197 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
1	A	275	Total	C	N	O	S	0	1	0
			2257	1409	413	426	9			
1	F	275	Total	C	N	O	S	0	0	0
			2246	1403	409	425	9			

- 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
			842	536	142	160	4			
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 Marker peptide.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
3	C	10	Total	C	N	O	0	0	0
			84	55	14	15			
3	H	10	Total	C	N	O	0	0	0
			84	55	14	15			

- Molecule 4 is a protein called 1E6 TCR Alpha Chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	D	197	Total	C	N	O	S	0	0	0
			1557	975	256	316	10			

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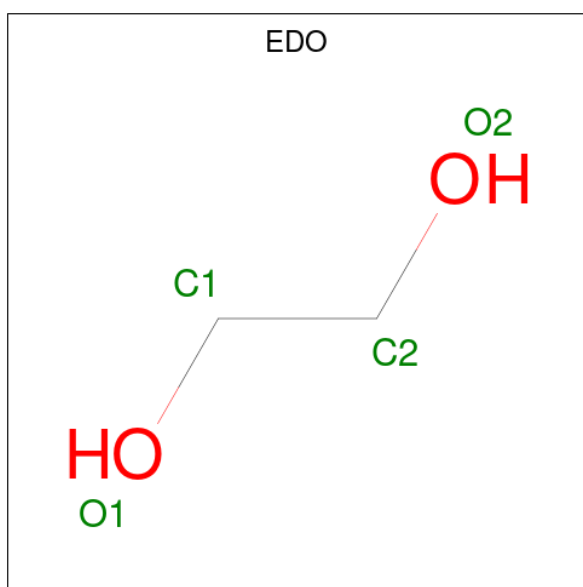
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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	I	199	Total	C	N	O	S	0	0	0
			1570	983	258	319	10			

- Molecule 5 is a protein called 1E6 TCR Beta Chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	E	247	Total	C	N	O	S	0	0	0
			1981	1254	342	374	11			
5	J	244	Total	C	N	O	S	0	0	0
			1961	1242	339	370	10			

- Molecule 6 is 1,2-ETHANEDIOL (CCD ID: EDO) (formula: C₂H₆O₂).



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

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

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	E	1	Total 4	C 2	O 2	0	0
6	E	1	Total 4	C 2	O 2	0	0
6	E	1	Total 4	C 2	O 2	0	0
6	F	1	Total 4	C 2	O 2	0	0
6	F	1	Total 4	C 2	O 2	0	0
6	F	1	Total 4	C 2	O 2	0	0
6	F	1	Total 4	C 2	O 2	0	0
6	F	1	Total 4	C 2	O 2	0	0
6	F	1	Total 4	C 2	O 2	0	0
6	F	1	Total 4	C 2	O 2	0	0
6	F	1	Total 4	C 2	O 2	0	0
6	G	1	Total 4	C 2	O 2	0	0
6	G	1	Total 4	C 2	O 2	0	0
6	G	1	Total 4	C 2	O 2	0	0
6	G	1	Total 4	C 2	O 2	0	0
6	H	1	Total 4	C 2	O 2	0	0
6	I	1	Total 4	C 2	O 2	0	0
6	I	1	Total 4	C 2	O 2	0	0
6	I	1	Total 4	C 2	O 2	0	0
6	I	1	Total 4	C 2	O 2	0	0
6	I	1	Total 4	C 2	O 2	0	0
6	I	1	Total 4	C 2	O 2	0	0

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

- Molecule 7 is GLYCEROL (CCD ID: GOL) (formula: $C_3H_8O_3$).



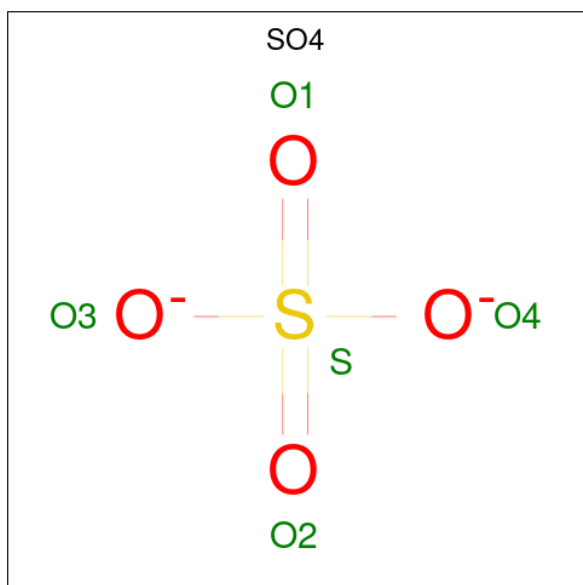
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	A	1	Total	C	O	0	0
			6	3	3		
7	B	1	Total	C	O	0	0
			6	3	3		
7	E	1	Total	C	O	0	0
			6	3	3		
7	F	1	Total	C	O	0	0
			6	3	3		

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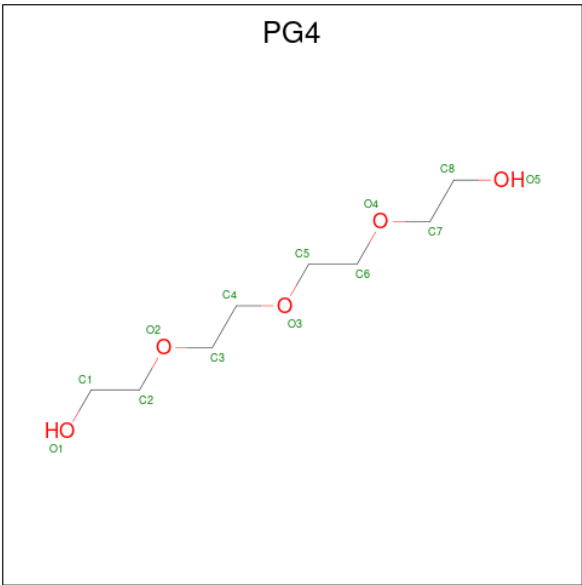
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	I	1	Total	C	O	0	0
			6	3	3		
7	J	1	Total	C	O	0	0
			6	3	3		

- Molecule 8 is SULFATE ION (CCD ID: SO4) (formula: O₄S).



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

- Molecule 9 is TETRAETHYLENE GLYCOL (CCD ID: PG4) (formula: C₈H₁₈O₅).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
9	J	1	Total	C	O	0	0
			10	6	4		

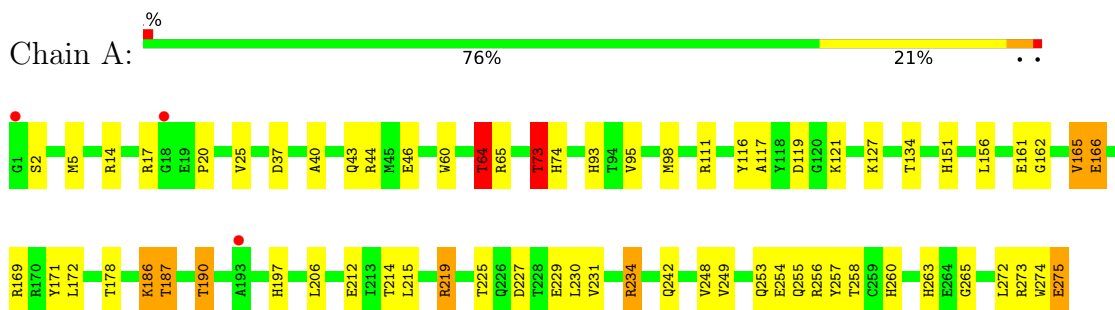
- Molecule 10 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
10	A	61	Total	O	0	0
			61	61		
10	B	52	Total	O	0	0
			52	52		
10	C	6	Total	O	0	0
			6	6		
10	D	39	Total	O	0	0
			39	39		
10	E	79	Total	O	0	0
			79	79		
10	F	100	Total	O	0	0
			100	100		
10	G	31	Total	O	0	0
			31	31		
10	H	8	Total	O	0	0
			8	8		
10	I	32	Total	O	0	0
			32	32		
10	J	64	Total	O	0	0
			64	64		

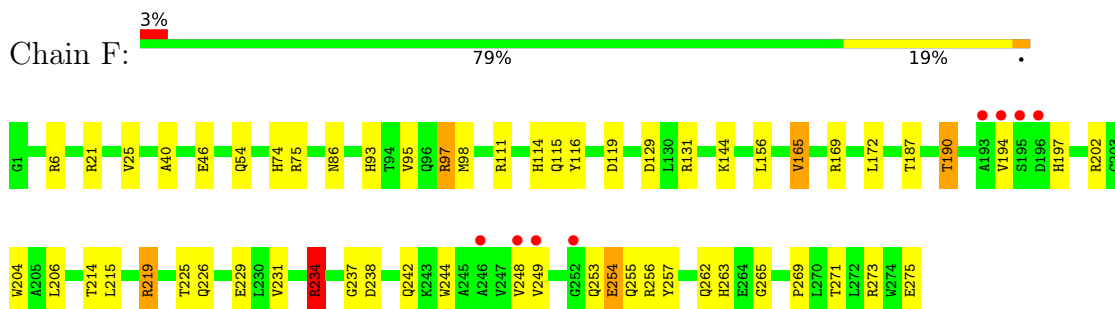
3 Residue-property plots

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.

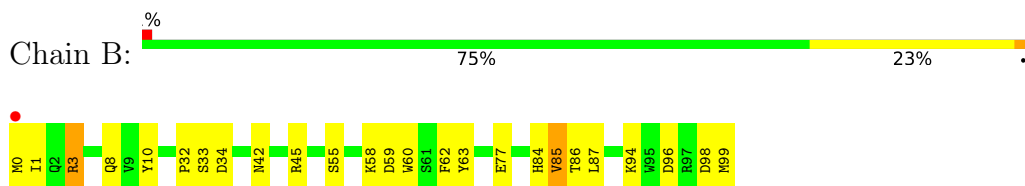
- Molecule 1: HLA class I histocompatibility antigen, A-2 alpha chain



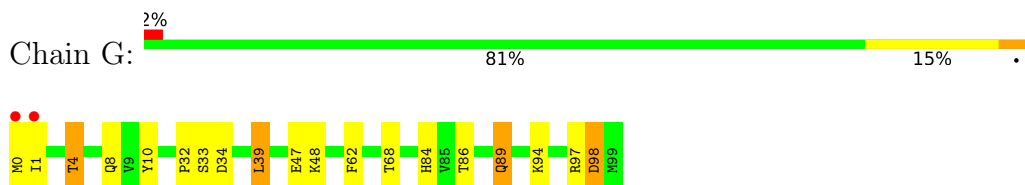
- Molecule 1: HLA class I histocompatibility antigen, A-2 alpha chain



- Molecule 2: Beta-2-microglobulin



- Molecule 2: Beta-2-microglobulin



- Molecule 3: Marker peptide

Chain C:  90% 10%



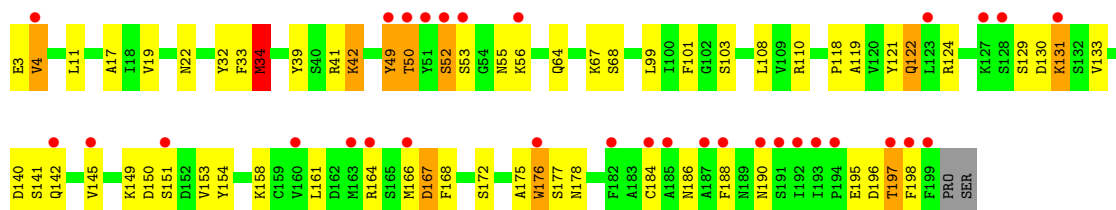
- Molecule 3: Marker peptide

Chain H:  90% 10%



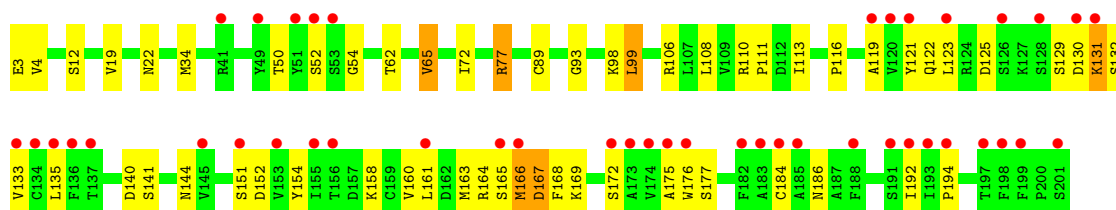
- Molecule 4: 1E6 TCR Alpha Chain

Chain D:  16% 67% 26% 5% ..



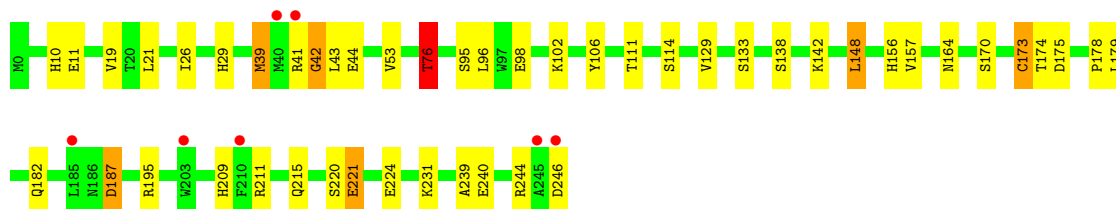
- Molecule 4: 1E6 TCR Alpha Chain

Chain I:  22% 71% 26% .



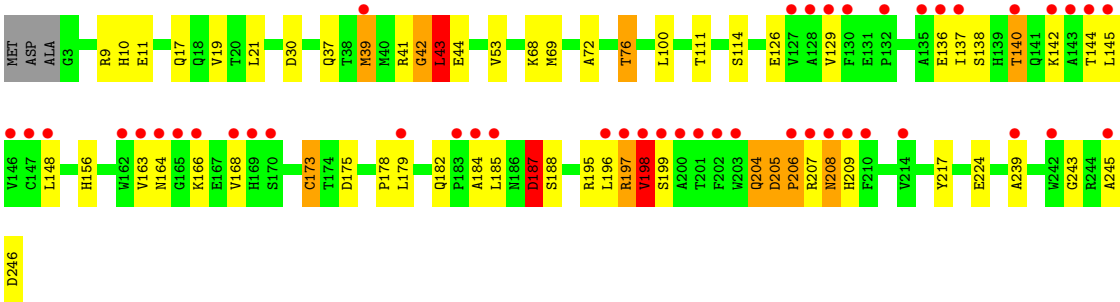
- Molecule 5: 1E6 TCR Beta Chain

Chain E:  3% 81% 17% .



- Molecule 5: 1E6 TCR Beta Chain

Chain J:  19% 74% 20% ..



4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	43.94Å 100.28Å 122.44Å 96.98° 98.05° 96.53°	Depositor
Resolution (Å)	42.76 – 2.03 42.76 – 2.03	Depositor EDS
% Data completeness (in resolution range)	97.5 (42.76-2.03) 97.6 (42.76-2.03)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.05	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.20 (at 2.03Å)	Xtriage
Refinement program	REFMAC 5.8.0073	Depositor
R, R_{free}	0.192 , 0.231 0.198 , 0.234	Depositor DCC
R_{free} test set	6446 reflections (5.02%)	wwPDB-VP
Wilson B-factor (Å ²)	36.7	Xtriage
Anisotropy	0.393	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 41.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	14197	wwPDB-VP
Average B, all atoms (Å ²)	53.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.51% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical 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

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: PG4, EDO, SO4, GOL

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	1.14	3/2322 (0.1%)	1.14	11/3151 (0.3%)
1	F	1.11	1/2311 (0.0%)	1.14	10/3137 (0.3%)
2	B	1.08	0/865	1.08	2/1170 (0.2%)
2	G	1.11	0/860	1.07	3/1162 (0.3%)
3	C	1.10	0/87	1.12	0/116
3	H	1.21	0/87	1.09	0/116
4	D	1.13	2/1592 (0.1%)	1.13	4/2154 (0.2%)
4	I	1.19	1/1606 (0.1%)	1.18	6/2174 (0.3%)
5	E	1.14	2/2036 (0.1%)	1.14	7/2769 (0.3%)
5	J	1.18	2/2016 (0.1%)	1.18	6/2741 (0.2%)
All	All	1.14	11/13782 (0.1%)	1.14	49/18690 (0.3%)

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
4	I	0	1
5	J	0	3
All	All	0	4

All (11) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	73	THR	CB-CG2	-9.48	1.21	1.52
5	J	43	LEU	CA-C	7.84	1.62	1.52
5	E	98	GLU	C-O	-7.17	1.14	1.24
4	D	68	SER	N-CA	6.68	1.54	1.46
1	F	25	VAL	C-O	6.41	1.30	1.23
5	E	95	SER	N-CA	-6.30	1.38	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	D	49	TYR	CA-C	6.28	1.60	1.52
5	J	206	PRO	CA-C	5.35	1.59	1.52
1	A	161	GLU	C-O	-5.23	1.17	1.24
1	A	25	VAL	CA-C	5.19	1.58	1.52
4	I	93	GLY	CA-C	-5.11	1.45	1.51

All (49) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	J	208	ASN	N-CA-C	11.92	127.03	108.79
1	F	234	ARG	NE-CZ-NH2	9.38	127.64	119.20
1	A	234	ARG	CB-CG-CD	9.08	132.19	111.30
2	B	85	VAL	CB-CA-C	-8.84	99.15	112.05
1	F	234	ARG	CB-CG-CD	8.71	131.34	111.30
4	D	176	TRP	N-CA-C	7.15	119.61	108.96
1	A	231	VAL	CB-CA-C	-7.03	103.86	111.59
2	G	47	GLU	CA-C-N	-7.01	108.15	121.54
2	G	47	GLU	C-N-CA	-7.01	108.15	121.54
2	G	47	GLU	N-CA-C	6.95	120.23	111.69
5	J	166	LYS	N-CA-C	6.89	119.65	109.24
1	A	73	THR	N-CA-CB	-6.69	100.26	110.16
1	F	234	ARG	NE-CZ-NH1	-6.67	114.83	121.50
1	F	238	ASP	CB-CA-C	-6.47	97.29	109.72
1	A	64	THR	N-CA-CB	6.47	119.73	110.16
4	D	34	MET	CG-SD-CE	-6.46	86.68	100.90
4	I	54	GLY	N-CA-C	6.32	121.02	112.17
5	J	42	GLY	CA-C-N	6.16	130.61	122.30
5	J	42	GLY	C-N-CA	6.16	130.61	122.30
4	I	131	LYS	N-CA-C	5.87	117.18	107.73
5	E	76	THR	N-CA-CB	-5.79	100.52	111.00
5	E	220	SER	CA-C-N	-5.79	110.37	121.94
5	E	220	SER	C-N-CA	-5.79	110.37	121.94
5	J	198	VAL	CB-CA-C	5.76	120.74	111.29
1	A	234	ARG	NE-CZ-NH2	-5.75	114.02	119.20
1	A	234	ARG	NE-CZ-NH1	5.67	127.17	121.50
4	I	77	ARG	CG-CD-NE	-5.57	99.74	112.00
4	I	22	ASN	N-CA-C	5.56	117.25	108.96
4	I	194	PRO	N-CA-C	5.55	119.73	111.41
1	F	97	ARG	NE-CZ-NH2	5.48	124.13	119.20
4	I	89	CYS	N-CA-C	-5.42	102.02	110.42
5	E	42	GLY	CA-C-N	5.41	129.61	122.30
5	E	42	GLY	C-N-CA	5.41	129.61	122.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	75	ARG	NE-CZ-NH2	5.41	124.07	119.20
1	A	73	THR	CB-CA-C	5.38	120.00	110.85
5	E	221	GLU	N-CA-CB	5.29	118.98	110.42
1	A	65	ARG	NE-CZ-NH2	5.28	123.95	119.20
5	E	240	GLU	N-CA-C	5.24	116.25	108.60
1	F	237	GLY	CA-C-N	5.24	131.80	122.06
1	F	237	GLY	C-N-CA	5.24	131.80	122.06
1	A	178	THR	CB-CA-C	5.20	117.40	109.34
1	F	46	GLU	CA-C-N	5.19	125.35	119.90
1	F	46	GLU	C-N-CA	5.19	125.35	119.90
2	B	85	VAL	N-CA-CB	5.18	118.67	110.54
4	D	4	VAL	CB-CA-C	5.16	118.31	110.62
4	D	22	ASN	N-CA-C	5.14	116.62	108.96
1	A	46	GLU	CA-C-N	5.06	124.82	119.76
1	A	46	GLU	C-N-CA	5.06	124.82	119.76
5	J	137	ILE	N-CA-C	5.04	115.76	110.62

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
4	I	129	SER	Peptide
5	J	187	ASP	Peptide
5	J	204	GLN	Peptide
5	J	205	ASP	Peptide

5.2 Too-close contacts ⓘ

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	2257	0	2108	54	0
1	F	2246	0	2096	37	0
2	B	842	0	807	19	0
2	G	837	0	803	14	1
3	C	84	0	80	1	0
3	H	84	0	80	1	0
4	D	1557	0	1469	47	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	I	1570	0	1481	40	0
5	E	1981	0	1896	46	1
5	J	1961	0	1875	58	0
6	A	36	0	54	8	0
6	B	20	0	30	3	0
6	D	24	0	36	8	0
6	E	40	0	60	3	0
6	F	28	0	42	7	0
6	G	16	0	24	1	0
6	H	4	0	6	0	0
6	I	28	0	42	5	0
6	J	24	0	36	6	0
7	A	6	0	8	0	0
7	B	6	0	7	1	0
7	E	6	0	8	11	0
7	F	6	0	8	2	0
7	I	6	0	8	1	0
7	J	6	0	8	0	0
8	A	10	0	0	0	0
8	B	5	0	0	0	0
8	E	10	0	0	3	0
8	F	15	0	0	0	0
9	J	10	0	13	14	0
10	A	61	0	0	4	0
10	B	52	0	0	1	1
10	C	6	0	0	0	0
10	D	39	0	0	1	0
10	E	79	0	0	5	0
10	F	100	0	0	2	0
10	G	31	0	0	0	0
10	H	8	0	0	0	0
10	I	32	0	0	2	0
10	J	64	0	0	6	1
All	All	14197	0	13085	297	2

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 11.

All (297) 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)
5:J:42:GLY:CA	9:J:308:PG4:H12	1.80	1.10
1:A:5:MET:HE1	1:A:171:TYR:HE2	1.13	1.08
5:J:164:ASN:HB2	5:J:208:ASN:HD21	1.20	1.06
5:E:42:GLY:HA2	7:E:311:GOL:H2	1.37	1.04
1:A:5:MET:CE	1:A:171:TYR:HE2	1.75	0.99
1:A:5:MET:HE1	1:A:171:TYR:CE2	1.96	0.99
5:E:42:GLY:HA2	7:E:311:GOL:C2	1.92	0.99
1:F:40:ALA:HB3	6:F:306:EDO:H22	1.45	0.96
4:D:101:PHE:CD1	5:E:43:LEU:HD12	2.10	0.87
1:A:5:MET:CE	1:A:171:TYR:CE2	2.55	0.86
1:F:6:ARG:HD2	7:F:308:GOL:H31	1.56	0.86
5:J:42:GLY:HA2	9:J:308:PG4:H12	1.57	0.86
1:A:187:THR:CG2	1:A:272:LEU:HD21	2.07	0.84
4:I:163:MET:HE3	5:J:197:ARG:HB3	1.59	0.83
4:D:101:PHE:CE1	5:E:43:LEU:HD12	2.13	0.83
4:I:133:VAL:HG12	4:I:176:TRP:HB3	1.61	0.83
4:I:62:THR:OG1	4:I:77:ARG:NH2	2.12	0.82
4:D:52:SER:O	4:D:67:LYS:HD2	1.80	0.82
5:J:42:GLY:HA3	9:J:308:PG4:H12	1.60	0.81
6:D:301:EDO:O2	10:D:401:HOH:O	1.98	0.81
5:E:114:SER:OG	5:E:156:HIS:HE1	1.64	0.80
1:A:190:THR:HG21	2:B:98:ASP:OD2	1.82	0.80
5:E:42:GLY:CA	7:E:311:GOL:H2	2.11	0.80
5:J:114:SER:OG	5:J:156:HIS:HE1	1.65	0.79
1:A:73:THR:HG22	10:A:446:HOH:O	1.83	0.79
1:A:60:TRP:O	1:A:64:THR:HG23	1.81	0.78
4:D:133:VAL:HG12	4:D:176:TRP:HB3	1.66	0.78
2:B:45:ARG:HD3	10:B:402:HOH:O	1.83	0.78
4:I:163:MET:HE2	5:J:198:VAL:HA	1.64	0.78
4:I:12:SER:O	7:I:308:GOL:O2	2.02	0.77
5:E:43:LEU:C	5:E:43:LEU:HD13	2.11	0.76
5:J:164:ASN:HB2	5:J:208:ASN:ND2	1.98	0.75
5:E:221:GLU:HG2	5:E:231:LYS:NZ	2.02	0.75
5:J:198:VAL:HG22	5:J:199:SER:H	1.52	0.73
4:D:50:THR:HG23	4:D:56:LYS:HG3	1.70	0.73
5:E:221:GLU:HA	5:E:231:LYS:HZ3	1.54	0.73
1:A:93:HIS:HD2	1:A:119:ASP:OD2	1.72	0.72
1:A:14:ARG:HD3	6:B:302:EDO:H21	1.72	0.71
4:D:42:LYS:N	6:D:304:EDO:H21	2.05	0.71
1:F:93:HIS:HD2	1:F:119:ASP:OD2	1.74	0.70
4:D:41:ARG:C	6:D:304:EDO:H21	2.17	0.70
1:F:54:GLN:HB3	6:F:307:EDO:H12	1.72	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:40:ALA:HB3	6:F:306:EDO:C2	2.19	0.70
5:J:198:VAL:CG2	5:J:199:SER:H	2.04	0.69
4:D:145:VAL:HA	4:D:190:ASN:HD22	1.59	0.68
1:F:202:ARG:NH2	2:G:98:ASP:O	2.26	0.68
1:A:227:ASP:HB3	1:A:248:VAL:HG12	1.77	0.67
4:I:113:ILE:HD11	4:I:140:ASP:HA	1.77	0.67
1:A:127:LYS:HE3	1:A:134:THR:HG22	1.76	0.66
5:E:42:GLY:HA3	7:E:311:GOL:H31	1.76	0.66
1:A:187:THR:HG23	1:A:272:LEU:HD21	1.77	0.66
5:E:43:LEU:HD13	5:E:44:GLU:N	2.11	0.66
2:B:3:ARG:NH1	2:B:59:ASP:OD2	2.28	0.66
1:A:40:ALA:HB3	6:A:301:EDO:C1	2.27	0.65
5:J:164:ASN:CB	5:J:208:ASN:HD21	2.03	0.65
1:A:73:THR:CG2	10:A:446:HOH:O	2.42	0.65
1:A:40:ALA:HB3	6:A:301:EDO:H11	1.77	0.65
4:I:131:LYS:NZ	4:I:177:SER:O	2.26	0.65
5:J:205:ASP:HB3	5:J:243:GLY:HA3	1.78	0.65
4:D:166:MET:O	4:D:168:PHE:N	2.30	0.64
5:J:76:THR:CG2	10:J:453:HOH:O	2.45	0.64
5:E:42:GLY:CA	7:E:311:GOL:C2	2.72	0.63
1:A:95:VAL:HG11	1:A:116:TYR:OH	1.98	0.63
5:J:208:ASN:HB2	10:J:461:HOH:O	1.98	0.63
5:J:76:THR:HG23	10:J:453:HOH:O	1.98	0.63
4:I:77:ARG:HD2	6:I:302:EDO:H11	1.81	0.62
5:E:244:ARG:NH2	5:E:246:ASP:O	2.32	0.62
1:A:234:ARG:HD2	1:A:242:GLN:HB2	1.81	0.62
1:A:187:THR:HG22	1:A:272:LEU:HD21	1.77	0.62
5:J:43:LEU:N	9:J:308:PG4:H12	2.14	0.62
5:E:76:THR:CG2	10:E:471:HOH:O	2.47	0.62
5:J:43:LEU:H	9:J:308:PG4:C1	2.13	0.61
5:J:136:GLU:OE1	5:J:140:THR:OG1	2.12	0.61
1:A:151:HIS:HB2	8:E:312:SO4:O1	1.99	0.61
1:A:17[B]:ARG:HD3	1:A:17[B]:ARG:N	2.16	0.61
4:D:129:SER:O	4:D:131:LYS:O	2.19	0.61
1:A:121:LYS:HE3	2:B:1:ILE:HG13	1.83	0.61
5:J:43:LEU:H	9:J:308:PG4:H12	1.66	0.60
5:J:208:ASN:CB	10:J:461:HOH:O	2.49	0.60
1:A:258:THR:HG23	1:A:260:HIS:NE2	2.16	0.60
1:F:234:ARG:HD3	1:F:242:GLN:OE1	2.01	0.60
4:I:166:MET:O	4:I:168:PHE:N	2.34	0.60
1:A:121:LYS:HE3	2:B:1:ILE:CG1	2.31	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:I:122:GLN:HG3	4:I:184:CYS:SG	2.42	0.60
5:J:129:VAL:HG23	5:J:239:ALA:HB3	1.83	0.60
4:D:118:PRO:HG2	4:D:195:GLU:HB2	1.84	0.60
1:F:263:HIS:CD2	1:F:265:GLY:H	2.19	0.59
4:D:101:PHE:CE1	5:E:43:LEU:CD1	2.85	0.59
1:F:93:HIS:HE1	10:F:413:HOH:O	1.85	0.59
4:D:17:ALA:HB1	6:D:303:EDO:H11	1.84	0.59
1:A:17[B]:ARG:N	1:A:17[B]:ARG:CD	2.66	0.58
5:J:42:GLY:C	9:J:308:PG4:H12	2.28	0.58
2:B:34:ASP:OD2	6:B:302:EDO:H11	2.03	0.58
5:J:42:GLY:HA3	9:J:308:PG4:C1	2.33	0.58
5:E:129:VAL:HG23	5:E:239:ALA:HB3	1.86	0.58
2:B:84:HIS:HD2	2:B:86:THR:OG1	1.87	0.58
5:E:42:GLY:HA2	7:E:311:GOL:C1	2.34	0.58
5:E:26:ILE:HD11	6:E:304:EDO:H11	1.86	0.58
4:D:122:GLN:HG3	4:D:184:CYS:SG	2.43	0.57
5:E:42:GLY:CA	7:E:311:GOL:C3	2.83	0.57
1:A:187:THR:HG21	1:A:272:LEU:HD11	1.87	0.57
1:A:263:HIS:CD2	1:A:265:GLY:H	2.22	0.56
4:D:176:TRP:CD2	5:E:148:LEU:HD21	2.40	0.56
5:E:42:GLY:CA	7:E:311:GOL:H31	2.35	0.56
1:F:234:ARG:HD2	1:F:242:GLN:HB2	1.87	0.56
5:J:126:GLU:OE1	5:J:126:GLU:HA	2.05	0.56
4:D:55:ASN:ND2	4:D:64:GLN:HE21	2.03	0.56
5:E:187:ASP:HB2	10:E:476:HOH:O	2.05	0.56
5:E:76:THR:HG23	10:E:471:HOH:O	2.06	0.56
4:D:154:TYR:O	4:D:175:ALA:HA	2.06	0.56
1:F:54:GLN:HB3	6:F:307:EDO:C1	2.36	0.56
4:I:154:TYR:O	4:I:175:ALA:HA	2.06	0.56
1:A:37:ASP:O	6:A:301:EDO:H11	2.06	0.55
5:J:198:VAL:HG22	5:J:199:SER:N	2.21	0.55
4:D:196:ASP:CG	4:D:197:THR:H	2.15	0.55
1:F:95:VAL:HG11	1:F:116:TYR:OH	2.07	0.55
5:J:207:ARG:CG	5:J:207:ARG:O	2.55	0.54
1:F:254:GLU:CD	1:F:254:GLU:H	2.12	0.54
1:F:249:VAL:CG2	1:F:257:TYR:CE1	2.91	0.54
2:G:32:PRO:O	2:G:84:HIS:HE1	1.90	0.54
4:I:163:MET:CE	5:J:198:VAL:HA	2.35	0.54
4:I:158:LYS:HA	4:I:172:SER:O	2.08	0.54
1:F:97:ARG:HE	1:F:114:HIS:HE1	1.56	0.53
5:E:43:LEU:C	5:E:43:LEU:CD1	2.81	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:221:GLU:HG2	5:E:231:LYS:HZ2	1.70	0.53
4:D:150:ASP:OD1	4:D:150:ASP:N	2.42	0.53
5:J:21:LEU:HD22	5:J:111:THR:HG21	1.91	0.53
1:A:234:ARG:HD3	2:B:10:TYR:CE2	2.43	0.53
1:A:234:ARG:HH21	2:B:8:GLN:NE2	2.07	0.53
4:D:158:LYS:HA	4:D:172:SER:O	2.09	0.52
4:D:17:ALA:CB	6:D:303:EDO:H11	2.39	0.52
2:B:32:PRO:O	2:B:84:HIS:HE1	1.92	0.52
4:D:110:ARG:HB3	4:D:141:SER:HB3	1.91	0.52
5:J:30:ASP:HA	6:J:305:EDO:H21	1.91	0.52
1:A:5:MET:HE3	1:A:171:TYR:CD2	2.44	0.52
5:J:37:GLN:HE21	9:J:308:PG4:H21	1.74	0.52
1:A:5:MET:HE3	1:A:171:TYR:CE2	2.40	0.52
1:A:186:LYS:HD3	1:A:186:LYS:N	2.25	0.52
2:G:84:HIS:HD2	2:G:86:THR:OG1	1.92	0.52
5:J:69:MET:HE2	6:J:305:EDO:H22	1.92	0.52
5:E:221:GLU:HG2	5:E:231:LYS:HZ3	1.74	0.52
1:F:253:GLN:OE1	1:F:256:ARG:NH1	2.43	0.52
3:H:10:ILE:HD12	3:H:10:ILE:C	2.35	0.51
4:I:110:ARG:HB3	4:I:141:SER:HB3	1.92	0.51
1:A:95:VAL:CG1	1:A:116:TYR:CZ	2.94	0.51
1:A:249:VAL:CG2	1:A:257:TYR:CE1	2.93	0.51
1:A:253:GLN:OE1	1:A:256:ARG:NH1	2.44	0.51
3:C:10:ILE:HD12	3:C:10:ILE:C	2.35	0.51
4:D:161:LEU:HB3	5:E:173:CYS:HB3	1.91	0.51
1:F:6:ARG:HD2	7:F:308:GOL:C3	2.33	0.51
4:I:119:ALA:HB1	4:I:121:TYR:CZ	2.45	0.51
5:E:96:LEU:HB3	6:E:310:EDO:H11	1.91	0.51
1:F:234:ARG:HG3	2:G:10:TYR:CZ	2.45	0.51
1:F:249:VAL:HG23	1:F:257:TYR:CE1	2.46	0.51
4:D:55:ASN:HD21	4:D:64:GLN:NE2	2.10	0.50
2:G:97:ARG:O	2:G:98:ASP:OD2	2.29	0.50
4:I:113:ILE:CD1	4:I:140:ASP:HA	2.42	0.50
1:A:95:VAL:HG13	1:A:116:TYR:CZ	2.46	0.50
1:F:234:ARG:CD	1:F:242:GLN:HB2	2.41	0.50
4:I:77:ARG:HD2	6:I:302:EDO:C1	2.41	0.50
1:F:97:ARG:HE	1:F:114:HIS:CE1	2.29	0.50
4:I:123:LEU:HD11	4:I:135:LEU:HB2	1.93	0.50
5:E:106:TYR:HB3	6:E:304:EDO:H12	1.94	0.50
1:F:202:ARG:HD2	1:F:244:TRP:CD2	2.47	0.50
1:A:74:HIS:HD2	10:A:446:HOH:O	1.95	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:21:LEU:HD22	5:E:111:THR:HG21	1.94	0.50
5:J:163:VAL:HG22	5:J:168:VAL:CG1	2.43	0.49
5:E:114:SER:OG	5:E:156:HIS:CE1	2.55	0.49
5:J:42:GLY:HA2	9:J:308:PG4:C1	2.37	0.49
1:A:249:VAL:HG23	1:A:257:TYR:CE1	2.47	0.49
6:F:301:EDO:O1	6:F:305:EDO:H22	2.12	0.49
5:J:37:GLN:HE21	9:J:308:PG4:C2	2.26	0.49
4:D:166:MET:O	4:D:167:ASP:C	2.54	0.49
1:F:95:VAL:HG13	1:F:116:TYR:CZ	2.48	0.49
2:G:4:THR:HG22	2:G:86:THR:HB	1.94	0.48
4:I:161:LEU:HB3	5:J:173:CYS:HB3	1.94	0.48
1:F:262:GLN:HG2	1:F:269:PRO:HB3	1.94	0.48
1:F:98:MET:CE	1:F:115:GLN:HE21	2.27	0.48
2:G:34:ASP:OD1	6:G:102:EDO:O1	2.30	0.48
4:D:42:LYS:O	6:D:304:EDO:H22	2.14	0.48
4:I:50:THR:HG21	4:I:65:VAL:HG13	1.96	0.48
1:A:162:GLY:O	1:A:166:GLU:HG2	2.15	0.47
5:J:175:ASP:OD1	5:J:195:ARG:NH1	2.47	0.47
1:A:274:TRP:O	1:A:275:GLU:C	2.57	0.47
2:B:55[B]:SER:HB2	2:B:63:TYR:CZ	2.49	0.47
4:I:166:MET:O	4:I:167:ASP:C	2.56	0.47
4:D:168:PHE:CZ	5:E:142:LYS:HE3	2.50	0.47
1:A:127:LYS:CE	1:A:134:THR:HG22	2.44	0.47
5:E:42:GLY:C	7:E:311:GOL:H2	2.40	0.47
4:I:62:THR:HG1	4:I:77:ARG:HH22	1.55	0.47
4:I:113:ILE:HG13	4:I:113:ILE:O	2.13	0.47
5:J:42:GLY:CA	9:J:308:PG4:C1	2.71	0.47
4:D:149:LYS:HA	4:D:149:LYS:HE2	1.97	0.47
1:F:190:THR:HG21	1:F:202:ARG:NH2	2.30	0.47
4:I:152:ASP:O	4:I:152:ASP:OD1	2.33	0.47
4:I:166:MET:O	4:I:166:MET:CG	2.62	0.47
5:J:10:HIS:ND1	5:J:156:HIS:HD2	2.13	0.47
4:I:125:ASP:OD2	4:I:130:ASP:HB3	2.15	0.47
5:E:221:GLU:HG3	10:E:477:HOH:O	2.15	0.46
4:D:33:PHE:C	4:D:34:MET:HE3	2.40	0.46
4:I:166:MET:O	4:I:166:MET:HG2	2.16	0.46
5:J:41:ARG:HB3	5:J:44:GLU:OE1	2.15	0.46
5:E:10:HIS:ND1	5:E:156:HIS:HD2	2.14	0.46
4:D:196:ASP:O	4:D:197:THR:OG1	2.24	0.46
1:F:165:VAL:HG13	1:F:169:ARG:NH1	2.30	0.46
5:J:9:ARG:HG3	6:J:306:EDO:H21	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:I:65:VAL:HB	4:I:72:ILE:HG22	1.98	0.46
4:D:52:SER:O	4:D:67:LYS:CD	2.57	0.46
1:F:234:ARG:HH11	2:G:8:GLN:NE2	2.14	0.46
5:J:114:SER:OG	5:J:156:HIS:CE1	2.56	0.46
4:I:98:LYS:NZ	10:I:402:HOH:O	2.38	0.45
2:B:34:ASP:OD1	7:B:306:GOL:O3	2.34	0.45
1:A:219:ARG:HD3	1:A:256:ARG:HH21	1.81	0.45
4:D:32:TYR:CE2	6:D:305:EDO:C1	3.00	0.45
4:D:39:TYR:HB2	4:D:42:LYS:HG3	1.98	0.45
1:F:249:VAL:HG21	1:F:257:TYR:CE1	2.52	0.45
6:F:301:EDO:O1	6:F:305:EDO:C2	2.64	0.45
1:A:20:PRO:HD2	6:A:303:EDO:H22	1.98	0.45
1:A:40:ALA:HB3	6:A:301:EDO:H12	1.98	0.45
1:A:93:HIS:HE1	10:A:407:HOH:O	1.99	0.45
1:F:129:ASP:O	1:F:131:ARG:NH1	2.49	0.45
5:E:175:ASP:OD1	5:E:195:ARG:NH1	2.50	0.45
2:G:97:ARG:O	2:G:98:ASP:CG	2.60	0.45
4:I:192:ILE:HG13	4:I:192:ILE:O	2.17	0.45
4:I:163:MET:HE3	5:J:197:ARG:C	2.42	0.45
5:E:102:LYS:CG	8:E:312:SO4:O2	2.65	0.44
5:E:42:GLY:HA3	7:E:311:GOL:C3	2.43	0.44
5:J:144:THR:OG1	5:J:197:ARG:HD2	2.17	0.44
4:D:119:ALA:HB1	4:D:121:TYR:CZ	2.51	0.44
1:A:117:ALA:HB2	2:B:60:TRP:CE2	2.52	0.44
1:F:95:VAL:CG1	1:F:116:TYR:CZ	3.00	0.44
1:F:219:ARG:HD3	1:F:256:ARG:HH21	1.83	0.44
5:J:144:THR:HA	5:J:197:ARG:HG3	2.00	0.44
4:D:55:ASN:ND2	4:D:64:GLN:NE2	2.64	0.44
1:A:43:GLN:HA	6:A:301:EDO:O1	2.18	0.44
4:D:129:SER:O	4:D:130:ASP:C	2.60	0.44
4:D:196:ASP:CG	4:D:197:THR:N	2.75	0.44
4:D:121:TYR:HB3	5:E:133:SER:CB	2.48	0.43
1:F:234:ARG:HH11	2:G:8:GLN:HE21	1.66	0.43
5:J:187:ASP:OD1	5:J:187:ASP:N	2.51	0.43
5:E:39:MET:N	5:E:39:MET:HE2	2.33	0.43
1:A:165:VAL:HG13	1:A:169:ARG:NH1	2.34	0.43
5:J:163:VAL:HG22	5:J:168:VAL:HG13	2.01	0.43
2:B:42:ASN:ND2	2:B:77:GLU:H	2.17	0.43
1:F:144:LYS:NZ	10:F:404:HOH:O	2.51	0.43
1:F:255:GLN:HA	1:F:255:GLN:NE2	2.33	0.43
5:J:204:GLN:HB3	5:J:245:ALA:HB2	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:J:224:GLU:HG3	10:J:436:HOH:O	2.19	0.43
2:B:33:SER:HB3	2:B:62:PHE:CE2	2.54	0.43
2:G:39:LEU:HD23	2:G:68:THR:HG22	2.01	0.42
1:A:44:ARG:O	6:A:301:EDO:H21	2.19	0.42
4:I:34:MET:HE3	4:I:99:LEU:HD11	2.01	0.42
4:I:77:ARG:CD	6:I:302:EDO:H11	2.49	0.42
4:I:123:LEU:CD1	4:I:135:LEU:HB2	2.49	0.42
5:E:102:LYS:HG2	8:E:312:SO4:O2	2.20	0.42
6:I:305:EDO:H12	10:I:426:HOH:O	2.19	0.42
5:J:156:HIS:HB3	5:J:217:TYR:HB2	2.01	0.42
2:B:96:ASP:CB	2:B:99:MET:HE2	2.50	0.42
5:J:129:VAL:CG1	5:J:145:LEU:HD12	2.49	0.42
1:A:249:VAL:HG21	1:A:257:TYR:CE1	2.55	0.42
4:I:113:ILE:HD11	4:I:116:PRO:HB3	2.00	0.42
4:I:131:LYS:CG	4:I:132:SER:N	2.83	0.42
5:J:30:ASP:HA	6:J:305:EDO:H12	2.02	0.42
1:F:187:THR:HA	1:F:204:TRP:O	2.20	0.42
2:G:33:SER:HB3	2:G:62:PHE:CE2	2.54	0.42
4:I:77:ARG:HG2	6:I:306:EDO:H21	2.01	0.42
5:J:30:ASP:HA	6:J:305:EDO:C2	2.49	0.42
4:D:52:SER:O	4:D:67:LYS:HG3	2.20	0.42
4:D:129:SER:C	4:D:131:LYS:N	2.78	0.42
4:D:164:ARG:HB2	4:D:164:ARG:HH21	1.83	0.42
5:J:163:VAL:O	5:J:164:ASN:HB3	2.20	0.42
4:I:167:ASP:O	4:I:167:ASP:CG	2.63	0.41
5:E:29:HIS:HE1	10:E:478:HOH:O	2.03	0.41
4:I:108:LEU:C	4:I:108:LEU:HD13	2.46	0.41
5:J:208:ASN:HB3	10:J:461:HOH:O	2.16	0.41
1:F:21:ARG:HG2	6:F:304:EDO:H12	2.02	0.41
5:E:157:VAL:HA	5:E:215:GLN:O	2.20	0.41
2:G:39:LEU:N	2:G:39:LEU:CD1	2.84	0.41
1:A:197:HIS:HB3	6:A:308:EDO:C1	2.50	0.41
1:A:121:LYS:HE3	2:B:1:ILE:HG12	2.03	0.41
4:D:56:LYS:HE3	4:D:56:LYS:HB3	1.94	0.41
2:G:4:THR:HG22	2:G:86:THR:CB	2.50	0.41
4:D:103:SER:HA	7:E:311:GOL:C3	2.50	0.41
4:D:108:LEU:HD13	4:D:108:LEU:C	2.46	0.41
5:E:187:ASP:OD1	5:E:187:ASP:N	2.54	0.41
5:J:39:MET:HE3	9:J:308:PG4:H61	2.02	0.41
5:J:72:ALA:HB1	6:J:305:EDO:H11	2.03	0.41
1:A:234:ARG:HD3	2:B:10:TYR:CD2	2.55	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:164:ASN:OD1	5:E:209:HIS:N	2.48	0.40
2:B:45:ARG:HH22	6:B:304:EDO:H21	1.86	0.40
4:D:32:TYR:CE2	6:D:305:EDO:H12	2.56	0.40
4:D:186:ASN:OD1	4:D:188:PHE:CZ	2.75	0.40
4:I:110:ARG:HA	4:I:111:PRO:HD3	1.89	0.40
5:J:182:GLN:C	5:J:184:ALA:N	2.79	0.40
5:E:174:THR:O	5:E:175:ASP:C	2.61	0.40
5:J:42:GLY:HA2	9:J:308:PG4:H42	2.03	0.40
4:D:52:SER:C	4:D:67:LYS:HD2	2.44	0.40

All (2) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:B:402:HOH:O	10:J:402:HOH:O[1_556]	1.48	0.72
5:E:211:ARG:NH1	2:G:89:GLN:OE1[1_556]	2.17	0.03

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	274/275 (100%)	272 (99%)	2 (1%)	0	100	100
1	F	273/275 (99%)	268 (98%)	5 (2%)	0	100	100
2	B	99/100 (99%)	96 (97%)	3 (3%)	0	100	100
2	G	98/100 (98%)	95 (97%)	3 (3%)	0	100	100
3	C	8/10 (80%)	8 (100%)	0	0	100	100
3	H	8/10 (80%)	8 (100%)	0	0	100	100
4	D	195/199 (98%)	184 (94%)	8 (4%)	3 (2%)	8	3
4	I	197/199 (99%)	184 (93%)	12 (6%)	1 (0%)	24	17

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
5	E	245/247 (99%)	242 (99%)	3 (1%)	0	100	100
5	J	242/247 (98%)	235 (97%)	6 (2%)	1 (0%)	30	22
All	All	1639/1662 (99%)	1592 (97%)	42 (3%)	5 (0%)	36	31

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
4	D	167	ASP
4	I	167	ASP
5	J	206	PRO
4	D	197	THR
4	D	52	SER

5.3.2 Protein sidechains ⓘ

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	232/231 (100%)	208 (90%)	24 (10%)	7	2
1	F	231/231 (100%)	208 (90%)	23 (10%)	7	2
2	B	96/95 (101%)	90 (94%)	6 (6%)	16	9
2	G	95/95 (100%)	87 (92%)	8 (8%)	10	5
3	C	9/9 (100%)	9 (100%)	0	100	100
3	H	9/9 (100%)	9 (100%)	0	100	100
4	D	178/180 (99%)	158 (89%)	20 (11%)	6	1
4	I	180/180 (100%)	165 (92%)	15 (8%)	10	5
5	E	217/217 (100%)	202 (93%)	15 (7%)	14	7
5	J	215/217 (99%)	191 (89%)	24 (11%)	6	1
All	All	1462/1464 (100%)	1327 (91%)	135 (9%)	8	3

All (135) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	2	SER
1	A	64	THR
1	A	73	THR
1	A	98	MET
1	A	111	ARG
1	A	156	LEU
1	A	165	VAL
1	A	166	GLU
1	A	172	LEU
1	A	186	LYS
1	A	187	THR
1	A	190	THR
1	A	206	LEU
1	A	212	GLU
1	A	214	THR
1	A	215	LEU
1	A	219	ARG
1	A	225	THR
1	A	229	GLU
1	A	230	LEU
1	A	254	GLU
1	A	255	GLN
1	A	273	ARG
1	A	275	GLU
2	B	0	MET
2	B	3	ARG
2	B	58	LYS
2	B	85	VAL
2	B	87	LEU
2	B	94	LYS
4	D	3	GLU
4	D	4	VAL
4	D	11	LEU
4	D	19	VAL
4	D	34	MET
4	D	42	LYS
4	D	49	TYR
4	D	50	THR
4	D	53	SER
4	D	99	LEU
4	D	122	GLN
4	D	124	ARG
4	D	131	LYS

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Mol	Chain	Res	Type
4	D	140	ASP
4	D	142	GLN
4	D	151	SER
4	D	153	VAL
4	D	177	SER
4	D	178	ASN
4	D	198	PHE
5	E	11	GLU
5	E	19	VAL
5	E	39	MET
5	E	41	ARG
5	E	53	VAL
5	E	76	THR
5	E	138	SER
5	E	148	LEU
5	E	170	SER
5	E	173	CYS
5	E	178	PRO
5	E	179	LEU
5	E	182	GLN
5	E	187	ASP
5	E	224	GLU
1	F	74	HIS
1	F	86	ASN
1	F	111	ARG
1	F	156	LEU
1	F	165	VAL
1	F	172	LEU
1	F	190	THR
1	F	194	VAL
1	F	197	HIS
1	F	206	LEU
1	F	214	THR
1	F	215	LEU
1	F	219	ARG
1	F	225	THR
1	F	226	GLN
1	F	229	GLU
1	F	231	VAL
1	F	234	ARG
1	F	248	VAL
1	F	254	GLU

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Mol	Chain	Res	Type
1	F	271	THR
1	F	273	ARG
1	F	275	GLU
2	G	0	MET
2	G	1	ILE
2	G	4	THR
2	G	39	LEU
2	G	48	LYS
2	G	89	GLN
2	G	94	LYS
2	G	98	ASP
4	I	3	GLU
4	I	4	VAL
4	I	19	VAL
4	I	52	SER
4	I	65	VAL
4	I	99	LEU
4	I	106	ARG
4	I	144	ASN
4	I	151	SER
4	I	160	VAL
4	I	164	ARG
4	I	165	SER
4	I	166	MET
4	I	169	LYS
4	I	186	ASN
5	J	11	GLU
5	J	17	GLN
5	J	19	VAL
5	J	39	MET
5	J	43	LEU
5	J	53	VAL
5	J	68	LYS
5	J	76	THR
5	J	100	LEU
5	J	138	SER
5	J	140	THR
5	J	142	LYS
5	J	148	LEU
5	J	173	CYS
5	J	178	PRO
5	J	179	LEU

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Mol	Chain	Res	Type
5	J	185	LEU
5	J	187	ASP
5	J	188	SER
5	J	196	LEU
5	J	197	ARG
5	J	198	VAL
5	J	209	HIS
5	J	246	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (49) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	74	HIS
1	A	87	GLN
1	A	93	HIS
1	A	141	GLN
1	A	151	HIS
1	A	180	GLN
1	A	188	HIS
1	A	191	HIS
1	A	262	GLN
1	A	263	HIS
2	B	8	GLN
2	B	42	ASN
2	B	84	HIS
4	D	6	GLN
4	D	55	ASN
4	D	64	GLN
4	D	186	ASN
4	D	189	ASN
5	E	18	GLN
5	E	29	HIS
5	E	50	ASN
5	E	51	ASN
5	E	156	HIS
5	E	186	ASN
5	E	215	GLN
1	F	43	GLN
1	F	93	HIS
1	F	114	HIS
1	F	115	GLN
1	F	180	GLN

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Mol	Chain	Res	Type
1	F	188	HIS
1	F	191	HIS
1	F	255	GLN
1	F	263	HIS
2	G	8	GLN
2	G	13	HIS
2	G	84	HIS
4	I	31	GLN
4	I	38	GLN
4	I	55	ASN
4	I	80	GLN
4	I	144	ASN
5	J	37	GLN
5	J	50	ASN
5	J	51	ASN
5	J	80	GLN
5	J	156	HIS
5	J	204	GLN
5	J	209	HIS

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

70 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	$\# Z > 2$
6	EDO	F	304	-	3,3,3	0.48	0	2,2,2	0.35	0
6	EDO	E	304	-	3,3,3	0.51	0	2,2,2	0.79	0
6	EDO	A	308	-	3,3,3	0.49	0	2,2,2	0.45	0
6	EDO	B	304	-	3,3,3	0.44	0	2,2,2	0.70	0
6	EDO	I	302	-	3,3,3	0.45	0	2,2,2	0.79	0
6	EDO	I	307	-	3,3,3	0.90	0	2,2,2	0.11	0
6	EDO	G	103	-	3,3,3	0.38	0	2,2,2	1.08	0
6	EDO	E	310	-	3,3,3	0.63	0	2,2,2	0.16	0
6	EDO	J	301	-	3,3,3	0.51	0	2,2,2	0.67	0
6	EDO	J	302	-	3,3,3	0.29	0	2,2,2	0.65	0
6	EDO	F	305	-	3,3,3	0.40	0	2,2,2	0.68	0
6	EDO	J	303	-	3,3,3	0.44	0	2,2,2	0.39	0
6	EDO	J	304	-	3,3,3	0.72	0	2,2,2	0.17	0
6	EDO	H	101	-	3,3,3	0.57	0	2,2,2	0.55	0
6	EDO	F	303	-	3,3,3	0.82	0	2,2,2	0.22	0
6	EDO	D	302	-	3,3,3	0.81	0	2,2,2	0.68	0
6	EDO	E	308	-	3,3,3	0.26	0	2,2,2	0.81	0
8	SO4	A	312	-	4,4,4	0.48	0	6,6,6	0.64	0
6	EDO	A	305	-	3,3,3	0.54	0	2,2,2	0.88	0
8	SO4	B	307	-	4,4,4	0.68	0	6,6,6	0.39	0
6	EDO	E	301	-	3,3,3	0.46	0	2,2,2	0.56	0
6	EDO	I	306	-	3,3,3	0.58	0	2,2,2	0.39	0
7	GOL	I	308	-	5,5,5	0.95	0	5,5,5	2.04	2 (40%)
6	EDO	A	307	-	3,3,3	0.50	0	2,2,2	0.47	0
6	EDO	D	303	-	3,3,3	0.99	0	2,2,2	0.77	0
6	EDO	F	302	-	3,3,3	0.17	0	2,2,2	0.42	0
6	EDO	I	304	-	3,3,3	0.55	0	2,2,2	0.26	0
8	SO4	E	313	-	4,4,4	0.74	0	6,6,6	0.43	0
8	SO4	F	311	-	4,4,4	0.53	0	6,6,6	0.47	0
8	SO4	A	311	-	4,4,4	0.95	0	6,6,6	0.70	0
6	EDO	B	302	-	3,3,3	0.59	0	2,2,2	0.61	0
7	GOL	B	306	-	5,5,5	1.17	1 (20%)	5,5,5	1.39	1 (20%)
7	GOL	F	308	-	5,5,5	0.99	0	5,5,5	2.06	2 (40%)
6	EDO	A	309	-	3,3,3	0.57	0	2,2,2	0.19	0
6	EDO	A	304	-	3,3,3	0.63	0	2,2,2	0.41	0
6	EDO	F	306	-	3,3,3	0.32	0	2,2,2	0.46	0
6	EDO	E	306	-	3,3,3	0.50	0	2,2,2	0.30	0
6	EDO	G	102	-	3,3,3	0.37	0	2,2,2	0.34	0
7	GOL	E	311	-	5,5,5	0.86	0	5,5,5	1.04	1 (20%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
6	EDO	B	303	-	3,3,3	0.72	0	2,2,2	0.42	0
8	SO4	F	310	-	4,4,4	0.63	0	6,6,6	0.57	0
6	EDO	E	309	-	3,3,3	0.45	0	2,2,2	0.43	0
6	EDO	D	306	-	3,3,3	0.65	0	2,2,2	0.25	0
6	EDO	E	307	-	3,3,3	0.78	0	2,2,2	0.08	0
6	EDO	D	305	-	3,3,3	0.45	0	2,2,2	0.36	0
8	SO4	E	312	-	4,4,4	0.43	0	6,6,6	0.63	0
6	EDO	I	303	-	3,3,3	0.35	0	2,2,2	0.52	0
6	EDO	J	306	-	3,3,3	0.66	0	2,2,2	0.07	0
6	EDO	E	303	-	3,3,3	0.58	0	2,2,2	0.21	0
6	EDO	I	301	-	3,3,3	0.88	0	2,2,2	0.56	0
6	EDO	F	307	-	3,3,3	0.49	0	2,2,2	0.59	0
6	EDO	A	302	-	3,3,3	0.40	0	2,2,2	0.67	0
6	EDO	A	303	-	3,3,3	0.40	0	2,2,2	0.84	0
6	EDO	D	304	-	3,3,3	0.77	0	2,2,2	0.86	0
6	EDO	E	305	-	3,3,3	0.26	0	2,2,2	0.85	0
6	EDO	J	305	-	3,3,3	0.52	0	2,2,2	1.50	1 (50%)
6	EDO	G	104	-	3,3,3	0.58	0	2,2,2	0.17	0
7	GOL	A	310	-	5,5,5	0.88	0	5,5,5	0.82	0
6	EDO	D	301	-	3,3,3	0.48	0	2,2,2	0.58	0
6	EDO	B	305	-	3,3,3	0.48	0	2,2,2	0.43	0
6	EDO	F	301	-	3,3,3	0.35	0	2,2,2	0.84	0
8	SO4	F	309	-	4,4,4	1.05	0	6,6,6	1.24	1 (16%)
6	EDO	E	302	-	3,3,3	0.43	0	2,2,2	0.26	0
6	EDO	A	301	-	3,3,3	0.27	0	2,2,2	0.74	0
6	EDO	B	301	-	3,3,3	0.48	0	2,2,2	0.60	0
6	EDO	G	101	-	3,3,3	0.47	0	2,2,2	0.64	0
6	EDO	I	305	-	3,3,3	0.54	0	2,2,2	0.40	0
7	GOL	J	307	-	5,5,5	0.55	0	5,5,5	0.85	0
9	PG4	J	308	-	9,9,12	0.65	0	8,8,11	1.19	1 (12%)
6	EDO	A	306	-	3,3,3	0.59	0	2,2,2	0.34	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	EDO	F	304	-	-	0/1/1/1	-
6	EDO	E	304	-	-	0/1/1/1	-
6	EDO	A	308	-	-	1/1/1/1	-
6	EDO	B	304	-	-	1/1/1/1	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	EDO	I	302	-	-	1/1/1/1	-
6	EDO	I	307	-	-	1/1/1/1	-
6	EDO	G	103	-	-	1/1/1/1	-
6	EDO	E	310	-	-	0/1/1/1	-
6	EDO	J	301	-	-	1/1/1/1	-
6	EDO	J	302	-	-	1/1/1/1	-
6	EDO	F	305	-	-	1/1/1/1	-
6	EDO	J	303	-	-	1/1/1/1	-
6	EDO	J	304	-	-	0/1/1/1	-
6	EDO	H	101	-	-	1/1/1/1	-
6	EDO	F	303	-	-	1/1/1/1	-
6	EDO	D	302	-	-	1/1/1/1	-
6	EDO	E	308	-	-	1/1/1/1	-
6	EDO	A	305	-	-	1/1/1/1	-
6	EDO	E	301	-	-	0/1/1/1	-
6	EDO	I	306	-	-	1/1/1/1	-
7	GOL	I	308	-	-	2/4/4/4	-
6	EDO	A	307	-	-	1/1/1/1	-
6	EDO	D	303	-	-	1/1/1/1	-
6	EDO	F	302	-	-	0/1/1/1	-
6	EDO	I	304	-	-	1/1/1/1	-
6	EDO	B	302	-	-	1/1/1/1	-
7	GOL	B	306	-	-	4/4/4/4	-
7	GOL	F	308	-	-	3/4/4/4	-
6	EDO	A	309	-	-	1/1/1/1	-
6	EDO	A	304	-	-	0/1/1/1	-
6	EDO	F	306	-	-	0/1/1/1	-
6	EDO	E	306	-	-	0/1/1/1	-
6	EDO	G	102	-	-	1/1/1/1	-
7	GOL	E	311	-	-	0/4/4/4	-
6	EDO	B	303	-	-	1/1/1/1	-
6	EDO	E	309	-	-	1/1/1/1	-
6	EDO	D	306	-	-	0/1/1/1	-
6	EDO	E	307	-	-	0/1/1/1	-
6	EDO	D	305	-	-	1/1/1/1	-
6	EDO	I	303	-	-	0/1/1/1	-
6	EDO	J	306	-	-	1/1/1/1	-
6	EDO	E	303	-	-	0/1/1/1	-
6	EDO	I	301	-	-	0/1/1/1	-
6	EDO	F	307	-	-	1/1/1/1	-
6	EDO	A	302	-	-	1/1/1/1	-
6	EDO	A	303	-	-	1/1/1/1	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	EDO	D	304	-	-	0/1/1/1	-
6	EDO	E	305	-	-	0/1/1/1	-
6	EDO	J	305	-	-	1/1/1/1	-
6	EDO	G	104	-	-	1/1/1/1	-
7	GOL	A	310	-	-	4/4/4/4	-
6	EDO	D	301	-	-	1/1/1/1	-
6	EDO	B	305	-	-	0/1/1/1	-
6	EDO	F	301	-	-	1/1/1/1	-
6	EDO	E	302	-	-	1/1/1/1	-
6	EDO	A	301	-	-	1/1/1/1	-
6	EDO	B	301	-	-	1/1/1/1	-
6	EDO	G	101	-	-	1/1/1/1	-
6	EDO	I	305	-	-	1/1/1/1	-
7	GOL	J	307	-	-	0/4/4/4	-
9	PG4	J	308	-	-	7/7/7/10	-
6	EDO	A	306	-	-	1/1/1/1	-

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	B	306	GOL	O2-C2	-2.39	1.36	1.43

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	I	308	GOL	O2-C2-C1	-3.32	95.44	109.18
9	J	308	PG4	O2-C2-C1	-2.89	97.37	110.11
7	F	308	GOL	O2-C2-C1	-2.87	97.29	109.18
7	F	308	GOL	O3-C3-C2	2.80	122.99	110.38
7	I	308	GOL	O3-C3-C2	2.71	122.60	110.38
8	F	309	SO4	O4-S-O1	2.55	122.86	109.56
7	B	306	GOL	O3-C3-C2	-2.20	100.48	110.38
6	J	305	EDO	O1-C1-C2	-2.09	96.44	112.39
7	E	311	GOL	O3-C3-C2	2.04	119.57	110.38

There are no chirality outliers.

All (58) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
7	A	310	GOL	C1-C2-C3-O3
7	B	306	GOL	O1-C1-C2-O2

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Mol	Chain	Res	Type	Atoms
7	B	306	GOL	O1-C1-C2-C3
7	F	308	GOL	C1-C2-C3-O3
7	I	308	GOL	O1-C1-C2-C3
7	F	308	GOL	O2-C2-C3-O3
9	J	308	PG4	O3-C5-C6-O4
7	B	306	GOL	C1-C2-C3-O3
7	I	308	GOL	O1-C1-C2-O2
9	J	308	PG4	O1-C1-C2-O2
6	B	303	EDO	O1-C1-C2-O2
6	G	103	EDO	O1-C1-C2-O2
6	I	305	EDO	O1-C1-C2-O2
6	J	302	EDO	O1-C1-C2-O2
7	B	306	GOL	O2-C2-C3-O3
6	A	301	EDO	O1-C1-C2-O2
6	B	302	EDO	O1-C1-C2-O2
6	B	304	EDO	O1-C1-C2-O2
6	J	306	EDO	O1-C1-C2-O2
9	J	308	PG4	O2-C3-C4-O3
7	A	310	GOL	O2-C2-C3-O3
6	A	302	EDO	O1-C1-C2-O2
6	A	307	EDO	O1-C1-C2-O2
6	F	301	EDO	O1-C1-C2-O2
6	F	303	EDO	O1-C1-C2-O2
7	F	308	GOL	O1-C1-C2-O2
9	J	308	PG4	C6-C5-O3-C4
6	A	306	EDO	O1-C1-C2-O2
6	E	308	EDO	O1-C1-C2-O2
6	I	302	EDO	O1-C1-C2-O2
6	I	306	EDO	O1-C1-C2-O2
9	J	308	PG4	C3-C4-O3-C5
9	J	308	PG4	C1-C2-O2-C3
6	A	309	EDO	O1-C1-C2-O2
6	B	301	EDO	O1-C1-C2-O2
6	H	101	EDO	O1-C1-C2-O2
6	J	305	EDO	O1-C1-C2-O2
6	A	308	EDO	O1-C1-C2-O2
6	D	303	EDO	O1-C1-C2-O2
6	F	307	EDO	O1-C1-C2-O2
7	A	310	GOL	O1-C1-C2-C3
6	A	303	EDO	O1-C1-C2-O2
6	D	305	EDO	O1-C1-C2-O2
6	E	309	EDO	O1-C1-C2-O2

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Mol	Chain	Res	Type	Atoms
6	G	102	EDO	O1-C1-C2-O2
6	I	307	EDO	O1-C1-C2-O2
6	J	303	EDO	O1-C1-C2-O2
7	A	310	GOL	O1-C1-C2-O2
6	A	305	EDO	O1-C1-C2-O2
6	D	301	EDO	O1-C1-C2-O2
6	E	302	EDO	O1-C1-C2-O2
6	G	104	EDO	O1-C1-C2-O2
6	I	304	EDO	O1-C1-C2-O2
6	D	302	EDO	O1-C1-C2-O2
6	F	305	EDO	O1-C1-C2-O2
6	G	101	EDO	O1-C1-C2-O2
6	J	301	EDO	O1-C1-C2-O2
9	J	308	PG4	C4-C3-O2-C2

There are no ring outliers.

28 monomers are involved in 73 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	F	304	EDO	1	0
6	E	304	EDO	2	0
6	A	308	EDO	1	0
6	B	304	EDO	1	0
6	I	302	EDO	3	0
6	E	310	EDO	1	0
6	F	305	EDO	2	0
6	I	306	EDO	1	0
7	I	308	GOL	1	0
6	D	303	EDO	2	0
6	B	302	EDO	2	0
7	B	306	GOL	1	0
7	F	308	GOL	2	0
6	F	306	EDO	2	0
6	G	102	EDO	1	0
7	E	311	GOL	11	0
6	D	305	EDO	2	0
8	E	312	SO4	3	0
6	J	306	EDO	1	0
6	F	307	EDO	2	0
6	A	303	EDO	1	0
6	D	304	EDO	3	0
6	J	305	EDO	5	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	D	301	EDO	1	0
6	F	301	EDO	2	0
6	A	301	EDO	6	0
6	I	305	EDO	1	0
9	J	308	PG4	14	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, 95th 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 ²)	Q < 0.9
1	A	275/275 (100%)	0.23	3 (1%) 78 78	22, 50, 82, 95	1 (0%)
1	F	275/275 (100%)	0.01	8 (2%) 53 53	22, 45, 86, 108	0
2	B	100/100 (100%)	-0.10	1 (1%) 79 80	17, 42, 62, 78	1 (1%)
2	G	100/100 (100%)	-0.05	2 (2%) 65 65	28, 40, 69, 83	0
3	C	10/10 (100%)	-0.60	0 100 100	32, 35, 42, 43	0
3	H	10/10 (100%)	-0.78	0 100 100	25, 28, 32, 35	0
4	D	197/199 (98%)	0.78	32 (16%) 4 4	29, 59, 113, 128	0
4	I	199/199 (100%)	0.82	44 (22%) 2 2	26, 56, 113, 131	0
5	E	247/247 (100%)	0.12	7 (2%) 55 54	22, 44, 87, 118	0
5	J	244/247 (98%)	0.65	46 (18%) 3 3	22, 49, 100, 124	0
All	All	1657/1662 (99%)	0.33	143 (8%) 16 15	17, 47, 99, 131	2 (0%)

All (143) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
5	J	198	VAL	5.2
4	D	192	ILE	5.1
4	I	198	PHE	4.8
4	I	192	ILE	4.8
4	D	198	PHE	4.7
4	D	193	ILE	4.7
5	J	135	ALA	4.6
4	D	199	PHE	4.6
4	I	135	LEU	4.1
4	I	123	LEU	4.1
4	D	194	PRO	4.1
5	J	143	ALA	3.9
5	J	184	ALA	3.9

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Mol	Chain	Res	Type	RSRZ
5	J	200	ALA	3.9
4	D	188	PHE	3.9
4	I	136	PHE	3.9
1	A	18	GLY	3.9
4	I	119	ALA	3.8
4	I	145	VAL	3.8
5	J	165	GLY	3.7
4	D	197	THR	3.7
4	I	176	TRP	3.7
5	J	144	THR	3.5
5	E	245	ALA	3.5
4	D	52	SER	3.4
4	I	52	SER	3.4
5	J	129	VAL	3.4
5	J	202	PHE	3.4
4	I	134	CYS	3.4
5	J	210	PHE	3.4
5	J	206	PRO	3.3
4	I	175	ALA	3.3
5	E	185	LEU	3.3
4	D	187	ALA	3.2
5	J	245	ALA	3.2
4	I	41	ARG	3.2
4	I	120	VAL	3.1
4	D	182	PHE	3.1
5	J	201	THR	3.1
4	D	185	ALA	3.1
5	J	127	VAL	3.1
4	I	174	VAL	3.1
4	I	153	VAL	3.0
5	J	145	LEU	3.0
5	J	179	LEU	3.0
5	J	170	SER	3.0
5	J	239	ALA	3.0
5	J	146	VAL	3.0
2	G	1	ILE	3.0
5	J	203	TRP	3.0
5	J	242	TRP	3.0
4	D	166	MET	3.0
5	J	185	LEU	2.9
5	J	168	VAL	2.9
4	I	201	SER	2.9

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Mol	Chain	Res	Type	RSRZ
4	I	182	PHE	2.9
4	I	184	CYS	2.8
5	J	199	SER	2.8
4	I	199	PHE	2.8
5	J	136	GLU	2.8
4	I	193	ILE	2.8
5	J	140	THR	2.8
5	J	163	VAL	2.8
4	D	190	ASN	2.7
4	I	165	SER	2.7
4	I	166	MET	2.7
4	D	50	THR	2.7
4	D	123	LEU	2.7
5	J	214	VAL	2.7
5	J	128	ALA	2.6
1	A	193	ALA	2.6
4	I	133	VAL	2.6
4	I	183	ALA	2.6
4	D	184	CYS	2.6
1	F	252	GLY	2.5
1	F	194	VAL	2.5
4	D	164	ARG	2.5
4	D	51	TYR	2.5
4	I	130	ASP	2.5
4	I	156	THR	2.5
4	I	194	PRO	2.5
5	J	197	ARG	2.5
1	F	196	ASP	2.4
4	I	53	SER	2.4
4	I	185	ALA	2.4
4	D	145	VAL	2.4
5	J	162	TRP	2.4
4	D	53	SER	2.4
4	D	160	VAL	2.4
4	D	128	SER	2.4
5	J	166	LYS	2.4
4	I	197	THR	2.4
4	I	121	TYR	2.3
4	D	142	GLN	2.3
1	A	1	GLY	2.3
5	J	207	ARG	2.3
5	J	183	PRO	2.3

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Mol	Chain	Res	Type	RSRZ
5	J	142	LYS	2.3
4	I	173	ALA	2.3
5	J	208	ASN	2.3
4	I	131	LYS	2.3
4	D	163	MET	2.3
4	D	49	TYR	2.3
1	F	248	VAL	2.2
5	E	246	ASP	2.2
4	I	161	LEU	2.2
5	J	148	LEU	2.2
4	D	151	SER	2.2
4	D	191	SER	2.2
4	I	126	SER	2.2
4	I	128	SER	2.2
5	E	210	PHE	2.2
4	I	155	ILE	2.2
4	I	137	THR	2.2
5	J	196	LEU	2.2
5	J	169	HIS	2.1
1	F	195	SER	2.1
4	I	151	SER	2.1
4	I	191	SER	2.1
4	D	56	LYS	2.1
2	G	0	MET	2.1
4	I	49	TYR	2.1
5	J	132	PRO	2.1
1	F	249	VAL	2.1
5	E	41	ARG	2.1
1	F	246	ALA	2.1
4	D	127	LYS	2.1
5	J	137	ILE	2.1
4	D	176	TRP	2.1
4	D	131	LYS	2.1
4	I	172	SER	2.1
5	E	40	MET	2.1
4	D	4	VAL	2.1
5	J	130	PHE	2.1
2	B	0	MET	2.0
5	J	39	MET	2.0
5	J	164	ASN	2.0
5	J	209	HIS	2.0
4	I	188	PHE	2.0

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Mol	Chain	Res	Type	RSRZ
1	F	193	ALA	2.0
5	E	203	TRP	2.0
5	J	147	CYS	2.0
4	I	51	TYR	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, 95th 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 ²)	Q<0.9
8	SO4	A	312	5/5	0.66	0.14	73,94,103,106	0
8	SO4	E	312	5/5	0.66	0.18	83,84,92,112	0
6	EDO	E	303	4/4	0.72	0.19	56,72,75,79	0
6	EDO	J	303	4/4	0.72	0.15	70,73,81,83	0
6	EDO	I	304	4/4	0.73	0.11	74,84,88,92	0
6	EDO	A	308	4/4	0.73	0.13	71,73,73,78	0
8	SO4	B	307	5/5	0.77	0.11	63,73,83,86	0
8	SO4	F	310	5/5	0.77	0.11	65,82,86,90	0
7	GOL	J	307	6/6	0.78	0.12	54,57,61,63	0
8	SO4	A	311	5/5	0.78	0.17	65,77,112,119	0
6	EDO	A	305	4/4	0.79	0.25	57,73,85,86	0
6	EDO	A	306	4/4	0.79	0.17	63,67,67,69	0
6	EDO	A	304	4/4	0.79	0.20	52,56,56,62	0
6	EDO	A	309	4/4	0.80	0.17	67,67,71,71	0
6	EDO	B	304	4/4	0.80	0.16	53,55,56,63	0
8	SO4	F	309	5/5	0.80	0.14	51,56,94,101	0
6	EDO	B	305	4/4	0.80	0.20	55,60,65,69	0
9	PG4	J	308	10/13	0.80	0.16	45,65,83,84	0
6	EDO	E	307	4/4	0.81	0.18	59,63,69,70	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
7	GOL	E	311	6/6	0.81	0.15	48,54,63,66	0
7	GOL	A	310	6/6	0.82	0.16	58,69,70,75	0
6	EDO	J	306	4/4	0.82	0.20	53,61,62,66	0
6	EDO	B	303	4/4	0.84	0.16	44,52,54,65	0
6	EDO	I	303	4/4	0.84	0.13	69,71,77,82	0
6	EDO	A	302	4/4	0.84	0.15	61,62,64,73	0
6	EDO	I	307	4/4	0.84	0.18	48,49,56,58	0
6	EDO	I	305	4/4	0.85	0.12	60,62,69,71	0
8	SO4	E	313	5/5	0.85	0.11	54,65,73,84	0
6	EDO	E	304	4/4	0.85	0.20	35,48,50,58	0
6	EDO	I	302	4/4	0.85	0.14	53,58,60,68	0
8	SO4	F	311	5/5	0.85	0.11	72,97,102,105	0
7	GOL	I	308	6/6	0.85	0.13	46,47,49,62	0
6	EDO	F	305	4/4	0.86	0.15	55,59,62,63	0
6	EDO	J	301	4/4	0.86	0.13	62,71,73,74	0
6	EDO	J	302	4/4	0.86	0.15	63,65,74,78	0
7	GOL	F	308	6/6	0.87	0.17	44,58,67,70	0
6	EDO	F	307	4/4	0.87	0.18	59,59,63,65	0
6	EDO	A	307	4/4	0.87	0.13	49,53,58,66	0
6	EDO	J	304	4/4	0.88	0.12	47,47,48,51	0
6	EDO	G	103	4/4	0.88	0.13	53,65,72,75	0
6	EDO	D	305	4/4	0.88	0.17	52,59,61,65	0
6	EDO	E	309	4/4	0.88	0.12	60,62,64,69	0
6	EDO	E	306	4/4	0.89	0.12	58,62,71,71	0
7	GOL	B	306	6/6	0.89	0.14	50,52,54,62	0
6	EDO	G	104	4/4	0.89	0.12	58,60,64,67	0
6	EDO	E	310	4/4	0.90	0.16	33,35,43,46	0
6	EDO	E	305	4/4	0.90	0.12	64,65,68,70	0
6	EDO	D	306	4/4	0.91	0.13	42,48,52,54	0
6	EDO	A	303	4/4	0.91	0.17	49,50,53,56	0
6	EDO	F	303	4/4	0.91	0.13	51,60,65,67	0
6	EDO	B	302	4/4	0.91	0.14	47,53,54,62	0
6	EDO	D	302	4/4	0.92	0.09	39,41,41,46	0
6	EDO	J	305	4/4	0.92	0.23	41,42,42,45	0
6	EDO	D	303	4/4	0.93	0.14	44,48,49,49	0
6	EDO	H	101	4/4	0.93	0.15	37,44,46,47	0
6	EDO	I	306	4/4	0.93	0.14	44,46,49,52	0
6	EDO	D	304	4/4	0.93	0.14	47,57,63,64	0
6	EDO	D	301	4/4	0.93	0.10	49,51,51,55	0
6	EDO	F	304	4/4	0.94	0.12	39,41,46,57	0
6	EDO	F	301	4/4	0.94	0.10	49,52,56,65	0
6	EDO	F	306	4/4	0.94	0.25	30,41,42,46	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
6	EDO	E	308	4/4	0.94	0.09	57,58,59,59	0
6	EDO	G	101	4/4	0.94	0.10	41,42,45,46	0
6	EDO	G	102	4/4	0.94	0.13	44,51,56,59	0
6	EDO	B	301	4/4	0.95	0.09	40,42,44,50	0
6	EDO	E	302	4/4	0.95	0.08	54,54,56,57	0
6	EDO	A	301	4/4	0.95	0.14	38,38,41,42	0
6	EDO	E	301	4/4	0.96	0.07	28,34,39,42	0
6	EDO	I	301	4/4	0.97	0.06	29,31,37,42	0
6	EDO	F	302	4/4	0.97	0.08	44,46,47,48	0

6.5 Other polymers [i](#)

There are no such residues in this entry.