Full wwPDB X-ray Structure Validation Report (i)

Jun 24, 2024 – 06:16 PM EDT

PDB ID	:	6FUR
Title	:	F11 T-Cell Receptor Recognising PKYVKQNTLKLAT Peptide Presented by HLA-DR*0101
Authors	:	Rizkallah, P.J.; Cole, D.K.
Deposited on	:	2018-02-27
Resolution	:	1.73 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 (i) 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 (i)) were used in the production of this report:

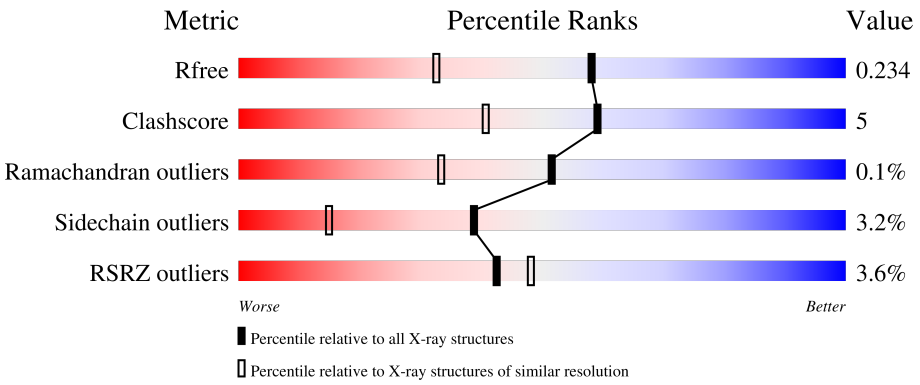
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.37.1
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.37.1

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 1.73 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}	130704	3764 (1.76-1.72)
Clashscore	141614	3923 (1.76-1.72)
Ramachandran outliers	138981	3878 (1.76-1.72)
Sidechain outliers	138945	3878 (1.76-1.72)
RSRZ outliers	127900	3705 (1.76-1.72)

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 <=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	202	5% 87% 11% •
1	C	202	4% 86% 12% •
2	B	240	2% 90% 9% •
2	D	240	3% 88% 12%

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
3	EDO	A	302	-	-	-	X
3	EDO	D	302	-	-	-	X
3	EDO	D	307	-	-	-	X
3	EDO	D	308	-	-	X	-

2 Entry composition (i)

There are 6 unique types of molecules in this entry. The entry contains 7912 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.

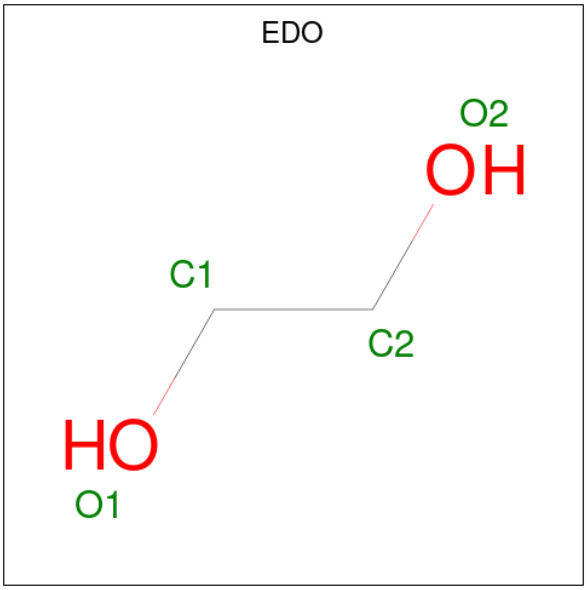
- Molecule 1 is a protein called Human F11 T-Cell Receptor alpha chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	202	1604	1014	261	318	11	0	4	0
1	C	202	1606	1014	262	321	9	0	4	0

- Molecule 2 is a protein called Human F11 T-Cell Receptor.

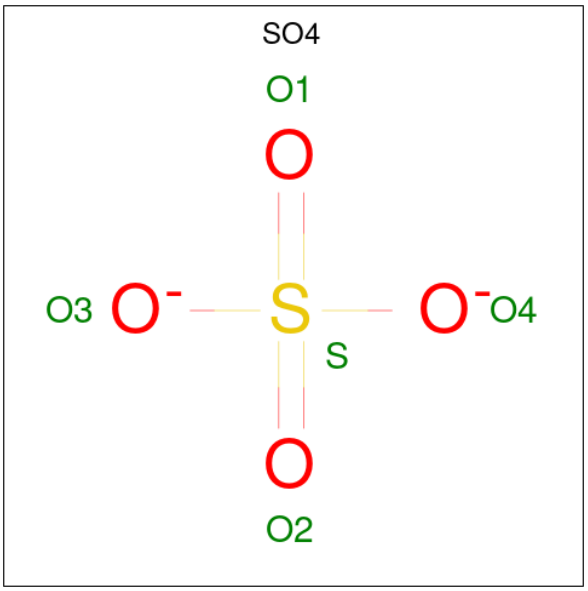
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	B	240	1962	1227	341	384	10	0	7	0
2	D	240	1930	1210	336	375	9	0	3	0

- Molecule 3 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: $C_2H_6O_2$).



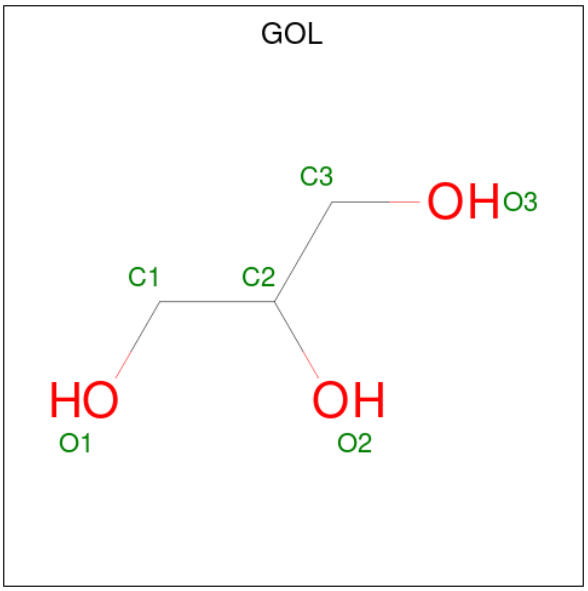
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	C	O		
3	A	1	4	2	2	0	0
			Total	C	O		
3	A	1	4	2	2	0	0
			Total	C	O		
3	B	1	4	2	2	0	0
			Total	C	O		
3	B	1	4	2	2	0	0
			Total	C	O		
3	C	1	4	2	2	0	0
			Total	C	O		
3	C	1	4	2	2	0	0
			Total	C	O		
3	C	1	4	2	2	0	0
			Total	C	O		
3	D	1	4	2	2	0	0
			Total	C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

- Molecule 4 is SULFATE ION (three-letter code: SO4) (formula: O_4S).



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

- Molecule 5 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	C	O		
5	A	1	6	3	3	0	0
			Total	C	O		
5	A	1	6	3	3	0	0
			Total	C	O		
5	B	1	6	3	3	0	0
			Total	C	O		
5	B	1	6	3	3	0	0
			Total	C	O		
5	B	1	6	3	3	0	0
			Total	C	O		
5	C	1	6	3	3	0	0
			Total	C	O		
5	C	1	6	3	3	0	0
			Total	C	O		
5	C	1	6	3	3	0	0
			Total	C	O		
5	D	1	6	3	3	0	0
			Total	C	O		
5	D	1	6	3	3	0	0

- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
6	A	158	158	158	0	0
			Total	O		
6	B	174	174	174	0	0

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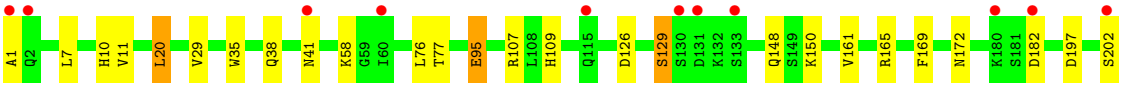
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
6	C	144	144	144	0	0
			Total	O		
6	D	161	161	161	0	0

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.

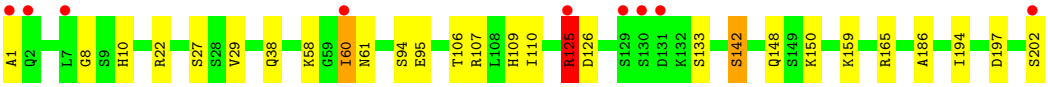
• Molecule 1: Human F11 T-Cell Receptor alpha chain

Chain A:



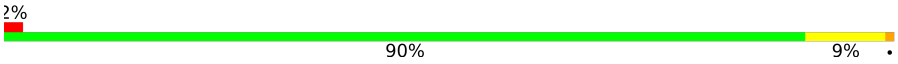
• Molecule 1: Human F11 T-Cell Receptor alpha chain

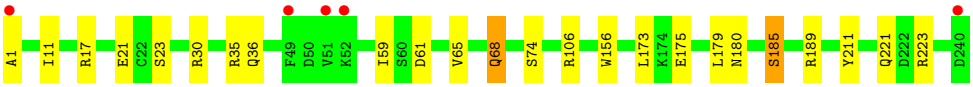
Chain C:



• Molecule 2: Human F11 T-Cell Receptor

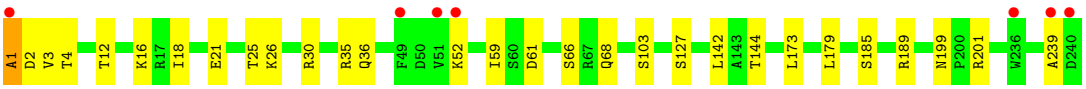
Chain B:





• Molecule 2: Human F11 T-Cell Receptor

Chain D:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	50.65Å 114.86Å 85.33Å 90.00° 91.01° 90.00°	Depositor
Resolution (Å)	46.34 – 1.73 46.34 – 1.73	Depositor EDS
% Data completeness (in resolution range)	94.8 (46.34-1.73) 90.1 (46.34-1.73)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.26 (at 1.73Å)	Xtriage
Refinement program	REFMAC 5.8.0189	Depositor
R, R_{free}	0.189 , 0.226 0.197 , 0.234	Depositor DCC
R_{free} test set	4819 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å^2)	21.0	Xtriage
Anisotropy	0.248	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.33 , 25.4	EDS
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.30$	Xtriage
Estimated twinning fraction	0.317 for h,-k,-l	Xtriage
F_o,F_c correlation	0.96	EDS
Total number of atoms	7912	wwPDB-VP
Average B, all atoms (Å^2)	27.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.70% of the height of the origin peak. No significant pseudotranslation is detected.*

[1]Intensities estimated from amplitudes.

[2]Theoretical values of $< |L| >$, $< L^2 >$ 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	0.90	0/1647	0.99	6/2234 (0.3%)
1	C	0.92	1/1646 (0.1%)	1.04	10/2232 (0.4%)
2	B	0.89	0/2016	0.97	10/2737 (0.4%)
2	D	0.91	1/1984 (0.1%)	0.94	4/2695 (0.1%)
All	All	0.90	2/7293 (0.0%)	0.98	30/9898 (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
1	A	0	1
2	B	0	1
2	D	0	2
All	All	0	4

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	142	SER	CB-OG	7.61	1.52	1.42
2	D	66	SER	CB-OG	-5.99	1.34	1.42

All (30) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	125	ARG	NE-CZ-NH1	13.28	126.94	120.30
2	D	2	ASP	N-CA-C	-8.53	87.97	111.00
1	C	22	ARG	NE-CZ-NH1	8.03	124.31	120.30
1	C	125	ARG	NE-CZ-NH2	-7.83	116.38	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	197	ASP	CB-CG-OD1	7.83	125.35	118.30
1	C	197	ASP	CB-CG-OD1	7.51	125.06	118.30
2	B	106	ARG	NE-CZ-NH1	-7.26	116.67	120.30
1	C	22	ARG	NE-CZ-NH2	-6.72	116.94	120.30
2	B	223	ARG	NE-CZ-NH2	6.58	123.59	120.30
2	B	106	ARG	NE-CZ-NH2	6.54	123.57	120.30
2	B	30	ARG	NE-CZ-NH2	6.54	123.57	120.30
1	A	20	LEU	CB-CG-CD1	6.37	121.84	111.00
1	C	126	ASP	CB-CG-OD1	6.23	123.90	118.30
2	D	30	ARG	NE-CZ-NH2	6.17	123.39	120.30
2	B	17	ARG	NE-CZ-NH2	-6.13	117.23	120.30
2	D	61	ASP	CB-CG-OD1	6.12	123.81	118.30
1	A	197	ASP	CB-CG-OD2	-6.11	112.80	118.30
1	A	126	ASP	CB-CG-OD1	6.04	123.74	118.30
1	A	165	ARG	NE-CZ-NH2	-6.02	117.29	120.30
2	B	61	ASP	CB-CG-OD1	5.92	123.63	118.30
1	A	107	ARG	NE-CZ-NH2	-5.76	117.42	120.30
1	C	107	ARG	NE-CZ-NH2	-5.57	117.52	120.30
2	B	61	ASP	CB-CG-OD2	-5.54	113.32	118.30
2	B	223	ARG	NE-CZ-NH1	-5.49	117.56	120.30
1	C	125	ARG	CD-NE-CZ	5.34	131.07	123.60
2	D	61	ASP	CB-CG-OD2	-5.22	113.60	118.30
2	B	17	ARG	CG-CD-NE	-5.19	100.89	111.80
1	C	165	ARG	NE-CZ-NH2	5.16	122.88	120.30
2	B	17	ARG	NE-CZ-NH1	5.08	122.84	120.30
1	C	142	SER	CB-CA-C	5.07	119.74	110.10

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	129	SER	Peptide
2	B	1	ALA	Peptide
2	D	1	ALA	Peptide
2	D	239	ALA	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	1604	0	1540	16	0
1	C	1606	0	1536	20	0
2	B	1962	0	1865	16	0
2	D	1930	0	1847	24	0
3	A	8	0	12	1	0
3	B	8	0	12	3	0
3	C	12	0	18	1	0
3	D	40	0	60	5	0
4	A	5	0	0	0	0
4	B	15	0	0	0	0
4	C	5	0	0	0	0
4	D	20	0	0	0	0
5	A	12	0	16	0	0
5	B	18	0	24	0	0
5	C	18	0	24	2	0
5	D	12	0	16	0	0
6	A	158	0	0	2	0
6	B	174	0	0	1	0
6	C	144	0	0	2	0
6	D	161	0	0	3	0
All	All	7912	0	6970	67	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 5.

All (67) 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:D:12[A]:THR:HG21	2:D:18:ILE:HD11	1.48	0.93
1:C:38:GLN:HE22	2:D:36:GLN:HE22	1.16	0.93
1:A:20:LEU:CD2	1:A:77:THR:HG22	2.02	0.88
2:D:1:ALA:HB1	6:D:458:HOH:O	1.77	0.84
2:D:1:ALA:HB3	2:D:26:LYS:HG2	1.66	0.78
1:A:20:LEU:HD23	1:A:77:THR:HG22	1.63	0.77
1:A:38:GLN:HE22	2:B:36:GLN:HE22	1.32	0.77
2:D:4:THR:HA	3:D:308:EDO:C2	2.23	0.69
2:D:4:THR:HA	3:D:308:EDO:H21	1.77	0.67
1:C:125:ARG:HH11	1:C:125:ARG:HG3	1.61	0.66
2:D:144:THR:HG22	2:D:185:SER:OG	1.97	0.65
2:B:11:ILE:HD11	2:B:211:TYR:O	1.98	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1:ALA:O	1:A:95:GLU:HG3	1.99	0.61
2:D:1:ALA:HB2	6:D:418:HOH:O	2.01	0.61
1:A:20:LEU:HD22	1:A:77:THR:HG22	1.82	0.61
2:D:12[A]:THR:CG2	2:D:18:ILE:HD11	2.28	0.61
1:A:129:SER:HA	6:A:404:HOH:O	2.02	0.59
1:C:1:ALA:CB	1:C:94:SER:O	2.52	0.57
3:C:301:EDO:O1	5:C:307:GOL:H11	2.05	0.56
2:D:35:ARG:HD3	2:D:59:ILE:HD12	1.88	0.56
2:B:11:ILE:CD1	2:B:211:TYR:O	2.55	0.55
2:D:1:ALA:HB3	2:D:26:LYS:CG	2.37	0.55
2:D:4:THR:HA	3:D:308:EDO:H22	1.88	0.54
2:D:103:SER:OG	3:D:308:EDO:C1	2.56	0.54
1:C:1:ALA:HA	1:C:27:SER:HB2	1.90	0.54
2:D:35:ARG:HD3	2:D:59:ILE:CD1	2.37	0.54
2:B:65:VAL:C	3:B:302:EDO:H21	2.30	0.52
1:C:38:GLN:HE22	2:D:36:GLN:NE2	1.98	0.51
1:A:38:GLN:HE22	2:B:36:GLN:NE2	2.06	0.51
2:B:35:ARG:HD3	2:B:59:ILE:HD12	1.93	0.51
1:C:10:HIS:ND1	1:C:109:HIS:HE1	2.09	0.51
1:A:38:GLN:NE2	2:B:36:GLN:HE22	2.07	0.50
1:C:1:ALA:HB2	1:C:94:SER:O	2.11	0.49
1:C:1:ALA:HB3	1:C:94:SER:O	2.12	0.49
1:A:10:HIS:ND1	1:A:109:HIS:HE1	2.10	0.49
1:C:60:ILE:H	1:C:60:ILE:HD13	1.78	0.49
1:A:7:LEU:HD22	1:C:186:ALA:HB1	1.96	0.48
2:B:175:GLU:OE2	2:B:185[B]:SER:OG	2.32	0.47
2:D:199:ASN:HD21	2:D:201:ARG:NH2	2.12	0.47
2:B:221:GLN:NE2	6:B:405:HOH:O	2.47	0.46
1:C:38:GLN:NE2	2:D:36:GLN:HE22	1.97	0.46
2:D:199:ASN:HD21	2:D:201:ARG:CZ	2.28	0.46
1:C:159:LYS:NZ	6:C:404:HOH:O	2.42	0.46
2:B:35:ARG:HG2	2:B:59:ILE:HD11	1.98	0.45
6:A:446:HOH:O	1:C:142:SER:HB2	2.17	0.45
1:A:148:GLN:OE1	1:C:148:GLN:NE2	2.50	0.44
2:D:173:LEU:C	2:D:173:LEU:HD12	2.38	0.44
2:B:35:ARG:HD3	2:B:59:ILE:CD1	2.48	0.44
1:C:125:ARG:NH2	2:D:127:SER:HA	2.32	0.44
2:B:21[A]:GLU:OE1	2:B:23:SER:OG	2.36	0.43
2:B:156:TRP:CH2	3:B:301:EDO:H12	2.53	0.43
1:A:161[B]:VAL:HG22	1:A:172:ASN:OD1	2.18	0.43
1:C:133:SER:O	6:C:401:HOH:O	2.21	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:68:GLN:HG3	6:D:456:HOH:O	2.20	0.42
2:D:103:SER:OG	3:D:308:EDO:H12	2.20	0.42
1:A:169:PHE:CZ	3:A:301:EDO:H21	2.54	0.42
1:A:35:TRP:CE2	1:A:76:LEU:HB2	2.55	0.41
2:B:68[A]:GLN:OE1	2:B:74:SER:OG	2.31	0.41
2:B:156:TRP:CZ3	3:B:301:EDO:H12	2.56	0.41
1:C:110:ILE:H	5:C:307:GOL:C3	2.33	0.41
1:A:11:VAL:HA	1:C:194:ILE:O	2.21	0.41
1:A:20:LEU:HD23	1:A:77:THR:CG2	2.42	0.41
2:D:1:ALA:HA	2:D:3:VAL:HG23	2.03	0.41
2:B:173:LEU:HD12	2:B:173:LEU:C	2.41	0.41
1:C:1:ALA:HA	1:C:27:SER:CB	2.51	0.40
2:D:1:ALA:N	2:D:25:THR:H	2.18	0.40
1:C:8:GLY:O	1:C:106:THR:HG23	2.21	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	205/202 (102%)	195 (95%)	10 (5%)	0	100	100
1	C	204/202 (101%)	195 (96%)	9 (4%)	0	100	100
2	B	245/240 (102%)	239 (98%)	6 (2%)	0	100	100
2	D	241/240 (100%)	236 (98%)	4 (2%)	1 (0%)	34	17
All	All	895/884 (101%)	865 (97%)	29 (3%)	1 (0%)	51	33

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	D	52	LYS

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	185/180 (103%)	178 (96%)	7 (4%)	33	11
1	C	184/180 (102%)	175 (95%)	9 (5%)	25	6
2	B	217/210 (103%)	210 (97%)	7 (3%)	39	15
2	D	213/210 (101%)	208 (98%)	5 (2%)	50	27
All	All	799/780 (102%)	771 (96%)	28 (4%)	39	12

All (28) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	29	VAL
1	A	41	ASN
1	A	58	LYS
1	A	95	GLU
1	A	150	LYS
1	A	182	ASP
1	A	202	SER
2	B	68[A]	GLN
2	B	68[B]	GLN
2	B	179	LEU
2	B	180	ASN
2	B	185[A]	SER
2	B	185[B]	SER
2	B	189	ARG
1	C	29	VAL
1	C	58	LYS
1	C	60	ILE
1	C	61	ASN
1	C	95[A]	GLU
1	C	95[B]	GLU
1	C	125	ARG
1	C	150	LYS
1	C	202	SER
2	D	16	LYS

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Mol	Chain	Res	Type
2	D	21	GLU
2	D	142	LEU
2	D	179	LEU
2	D	189	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (15) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	2	GLN
1	A	38	GLN
1	A	61	ASN
1	A	109	HIS
1	A	190	ASN
2	B	180	ASN
2	B	221	GLN
1	C	38	GLN
1	C	96	GLN
1	C	109	HIS
1	C	145	ASN
1	C	190	ASN
1	C	191	ASN
2	D	171	GLN
2	D	221	GLN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

36 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	$\#\|Z\| > 2$
3	EDO	A	302	-	3,3,3	0.57	0	2,2,2	0.08	0
3	EDO	C	302	-	3,3,3	0.44	0	2,2,2	0.18	0
3	EDO	D	306	-	3,3,3	0.43	0	2,2,2	0.44	0
5	GOL	A	304	-	5,5,5	0.43	0	5,5,5	0.55	0
3	EDO	D	304	-	3,3,3	0.49	0	2,2,2	0.29	0
4	SO4	B	303	-	4,4,4	0.38	0	6,6,6	0.47	0
4	SO4	C	304	-	4,4,4	0.35	0	6,6,6	0.09	0
4	SO4	B	304	-	4,4,4	0.43	0	6,6,6	0.22	0
3	EDO	D	307	-	3,3,3	0.57	0	2,2,2	0.20	0
4	SO4	D	314	-	4,4,4	0.40	0	6,6,6	0.35	0
5	GOL	C	306	-	5,5,5	0.33	0	5,5,5	0.56	0
3	EDO	D	308	-	3,3,3	0.38	0	2,2,2	0.77	0
3	EDO	D	302	-	3,3,3	0.45	0	2,2,2	0.35	0
5	GOL	B	307	-	5,5,5	0.59	0	5,5,5	0.63	0
5	GOL	D	315	-	5,5,5	0.49	0	5,5,5	1.26	0
5	GOL	A	305	-	5,5,5	0.50	0	5,5,5	0.95	0
3	EDO	D	303	-	3,3,3	0.39	0	2,2,2	0.20	0
4	SO4	B	305	-	4,4,4	0.32	0	6,6,6	0.19	0
3	EDO	C	301	-	3,3,3	0.40	0	2,2,2	0.47	0
3	EDO	B	301	-	3,3,3	0.48	0	2,2,2	0.46	0
5	GOL	C	305	-	5,5,5	0.69	0	5,5,5	0.41	0
3	EDO	A	301	-	3,3,3	0.39	0	2,2,2	0.34	0
4	SO4	D	311	-	4,4,4	0.35	0	6,6,6	0.21	0
3	EDO	D	301	-	3,3,3	0.55	0	2,2,2	0.07	0
5	GOL	C	307	-	5,5,5	0.33	0	5,5,5	0.83	0
3	EDO	D	309	-	3,3,3	0.38	0	2,2,2	0.52	0
4	SO4	A	303	-	4,4,4	0.32	0	6,6,6	0.13	0
5	GOL	B	306	-	5,5,5	0.39	0	5,5,5	0.43	0
5	GOL	D	316	-	5,5,5	0.56	0	5,5,5	0.48	0
3	EDO	D	305	-	3,3,3	0.56	0	2,2,2	0.17	0
5	GOL	B	308	-	5,5,5	0.50	0	5,5,5	0.72	0
4	SO4	D	312	-	4,4,4	0.34	0	6,6,6	0.40	0
4	SO4	D	313	-	4,4,4	0.36	0	6,6,6	0.23	0
3	EDO	B	302	-	3,3,3	0.38	0	2,2,2	0.36	0
3	EDO	D	310	-	3,3,3	0.35	0	2,2,2	0.54	0
3	EDO	C	303	-	3,3,3	0.64	0	2,2,2	0.13	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	A	302	-	-	0/1/1/1	-
3	EDO	C	302	-	-	1/1/1/1	-
3	EDO	D	306	-	-	1/1/1/1	-
5	GOL	A	304	-	-	3/4/4/4	-
3	EDO	D	304	-	-	0/1/1/1	-
3	EDO	D	307	-	-	1/1/1/1	-
5	GOL	C	306	-	-	2/4/4/4	-
3	EDO	D	308	-	-	0/1/1/1	-
3	EDO	D	302	-	-	1/1/1/1	-
5	GOL	B	307	-	-	2/4/4/4	-
5	GOL	D	315	-	-	2/4/4/4	-
5	GOL	A	305	-	-	3/4/4/4	-
3	EDO	D	303	-	-	1/1/1/1	-
3	EDO	C	301	-	-	1/1/1/1	-
3	EDO	B	301	-	-	1/1/1/1	-
5	GOL	C	305	-	-	4/4/4/4	-
3	EDO	A	301	-	-	0/1/1/1	-
3	EDO	D	301	-	-	0/1/1/1	-
5	GOL	C	307	-	-	0/4/4/4	-
3	EDO	D	309	-	-	0/1/1/1	-
5	GOL	B	306	-	-	4/4/4/4	-
5	GOL	D	316	-	-	4/4/4/4	-
3	EDO	D	305	-	-	1/1/1/1	-
5	GOL	B	308	-	-	4/4/4/4	-
3	EDO	B	302	-	-	1/1/1/1	-
3	EDO	D	310	-	-	0/1/1/1	-
3	EDO	C	303	-	-	1/1/1/1	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (38) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	A	304	GOL	O1-C1-C2-C3

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Mol	Chain	Res	Type	Atoms
5	A	305	GOL	O1-C1-C2-O2
5	A	305	GOL	O1-C1-C2-C3
5	B	306	GOL	O1-C1-C2-C3
5	B	308	GOL	O1-C1-C2-C3
5	C	305	GOL	O1-C1-C2-O2
5	C	305	GOL	O1-C1-C2-C3
5	C	305	GOL	C1-C2-C3-O3
5	C	306	GOL	C1-C2-C3-O3
5	D	315	GOL	C1-C2-C3-O3
5	D	316	GOL	O1-C1-C2-C3
5	D	316	GOL	C1-C2-C3-O3
5	B	308	GOL	O1-C1-C2-O2
5	B	306	GOL	C1-C2-C3-O3
5	B	307	GOL	C1-C2-C3-O3
5	B	308	GOL	C1-C2-C3-O3
5	A	304	GOL	O1-C1-C2-O2
5	B	308	GOL	O2-C2-C3-O3
5	D	316	GOL	O1-C1-C2-O2
5	D	316	GOL	O2-C2-C3-O3
3	C	303	EDO	O1-C1-C2-O2
3	D	305	EDO	O1-C1-C2-O2
5	B	306	GOL	O1-C1-C2-O2
5	C	305	GOL	O2-C2-C3-O3
5	C	306	GOL	O2-C2-C3-O3
5	D	315	GOL	O2-C2-C3-O3
3	B	301	EDO	O1-C1-C2-O2
3	C	301	EDO	O1-C1-C2-O2
3	D	307	EDO	O1-C1-C2-O2
3	C	302	EDO	O1-C1-C2-O2
5	B	307	GOL	O2-C2-C3-O3
3	D	306	EDO	O1-C1-C2-O2
5	A	304	GOL	C1-C2-C3-O3
3	B	302	EDO	O1-C1-C2-O2
3	D	302	EDO	O1-C1-C2-O2
3	D	303	EDO	O1-C1-C2-O2
5	B	306	GOL	O2-C2-C3-O3
5	A	305	GOL	C1-C2-C3-O3

There are no ring outliers.

6 monomers are involved in 11 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	D	308	EDO	5	0
3	C	301	EDO	1	0
3	B	301	EDO	2	0
3	A	301	EDO	1	0
5	C	307	GOL	2	0
3	B	302	EDO	1	0

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data (i)

6.1 Protein, DNA and RNA chains (i)

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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	202/202 (100%)	0.18	11 (5%)	25	30	14, 23, 54, 79	0
1	C	202/202 (100%)	0.11	9 (4%)	33	38	15, 24, 52, 76	0
2	B	240/240 (100%)	-0.04	5 (2%)	63	70	14, 23, 43, 78	0
2	D	240/240 (100%)	-0.05	7 (2%)	51	57	14, 23, 40, 73	0
All	All	884/884 (100%)	0.04	32 (3%)	42	48	14, 23, 48, 79	0

All (32) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	1	ALA	9.4
1	A	130	SER	7.9
2	B	240	ASP	7.0
1	C	1	ALA	6.1
1	C	129	SER	6.0
2	D	240	ASP	4.9
1	A	2	GLN	4.5
1	C	2	GLN	4.4
2	B	49	PHE	4.2
1	A	131	ASP	4.2
2	D	49	PHE	3.7
1	A	41	ASN	3.4
1	C	130	SER	3.3
2	B	52	LYS	3.1
2	D	52	LYS	3.1
1	C	202	SER	2.9
1	A	202	SER	2.7
2	B	1	ALA	2.7
1	C	125	ARG	2.7
2	D	236	TRP	2.7
1	C	7	LEU	2.7

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Mol	Chain	Res	Type	RSRZ
2	B	51	VAL	2.7
2	D	1	ALA	2.6
1	C	131	ASP	2.5
1	C	60	ILE	2.5
1	A	182	ASP	2.4
1	A	180	LYS	2.3
2	D	51	VAL	2.3
1	A	60	ILE	2.2
1	A	115	GLN	2.1
1	A	133	SER	2.1
2	D	239	ALA	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 monosaccharides 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
3	EDO	A	302	4/4	0.02	0.41	71,72,73,73	0
5	GOL	A	305	6/6	0.51	0.19	50,53,53,54	0
3	EDO	D	305	4/4	0.52	0.24	54,54,54,56	0
3	EDO	D	302	4/4	0.56	0.42	71,72,72,72	0
3	EDO	B	302	4/4	0.66	0.19	46,47,47,54	0
5	GOL	C	305	6/6	0.70	0.17	35,44,47,50	0
3	EDO	C	303	4/4	0.72	0.21	40,42,44,49	0
4	SO4	D	314	5/5	0.72	0.24	61,65,66,74	0
3	EDO	D	307	4/4	0.75	0.43	51,56,56,57	0
5	GOL	A	304	6/6	0.75	0.29	37,46,51,55	0
3	EDO	C	302	4/4	0.76	0.23	52,52,53,54	0
3	EDO	D	309	4/4	0.79	0.12	44,47,47,49	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
4	SO4	C	304	5/5	0.79	0.26	89,90,93,96	0
5	GOL	D	315	6/6	0.81	0.18	35,37,38,40	0
5	GOL	D	316	6/6	0.81	0.34	39,42,44,47	0
3	EDO	D	303	4/4	0.82	0.21	37,39,40,49	0
3	EDO	D	308	4/4	0.82	0.18	40,40,40,40	0
3	EDO	D	301	4/4	0.83	0.16	42,44,46,46	0
3	EDO	D	306	4/4	0.84	0.18	47,47,49,52	0
3	EDO	B	301	4/4	0.84	0.29	39,43,45,47	0
5	GOL	B	307	6/6	0.84	0.16	27,33,36,36	0
5	GOL	C	306	6/6	0.85	0.15	40,42,46,46	0
5	GOL	B	308	6/6	0.85	0.28	29,41,44,46	0
5	GOL	B	306	6/6	0.85	0.12	41,43,45,45	0
3	EDO	C	301	4/4	0.86	0.21	40,44,45,47	0
4	SO4	D	312	5/5	0.86	0.36	91,92,95,99	0
4	SO4	B	305	5/5	0.86	0.26	82,85,88,90	0
5	GOL	C	307	6/6	0.88	0.26	28,33,35,35	0
3	EDO	D	304	4/4	0.89	0.14	36,39,39,41	0
4	SO4	D	313	5/5	0.90	0.36	67,68,75,76	0
3	EDO	D	310	4/4	0.92	0.17	38,39,41,41	0
4	SO4	A	303	5/5	0.93	0.31	83,84,86,86	0
3	EDO	A	301	4/4	0.93	0.19	30,31,33,34	0
4	SO4	D	311	5/5	0.94	0.13	63,66,68,68	0
4	SO4	B	303	5/5	0.94	0.17	44,50,51,53	0
4	SO4	B	304	5/5	0.97	0.11	46,49,50,51	0

6.5 Other polymers (i)

There are no such residues in this entry.