



Full wwPDB X-ray Structure Validation Report ⓘ

Jun 24, 2024 – 01:10 PM EDT

PDB ID : 6FR4
Title : 003 TCR Study of CDR Loop Flexibility
Authors : Rizkallah, P.J.; Cole, D.K.
Deposited on : 2018-02-15
Resolution : 1.28 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 : 4.02b-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

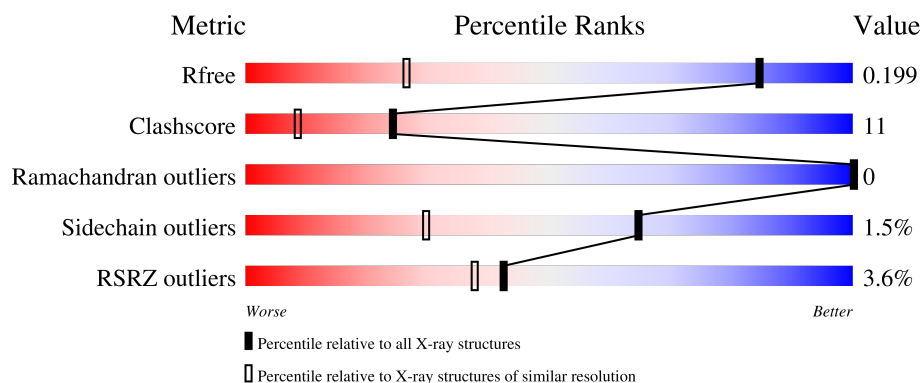
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.28 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	1850 (1.30-1.26)
Clashscore	141614	1926 (1.30-1.26)
Ramachandran outliers	138981	1860 (1.30-1.26)
Sidechain outliers	138945	1859 (1.30-1.26)
RSRZ outliers	127900	1807 (1.30-1.26)

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	202	<div> <div>4%</div> <div>81%</div> <div>16%</div> <div>.</div> </div>
2	B	244	<div> <div>3%</div> <div>87%</div> <div>12%</div> <div>.</div> </div>

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	GOL	A	302	-	-	X	-
4	EDO	B	306	-	-	X	-
5	ACT	A	312	-	-	X	-

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 4516 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 TCR 003 alpha chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	202	Total	C	N	O	S	0	22	0
			1721	1070	284	357	10			

There are 59 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1	MET	-	initiating methionine	UNP Q6NSA1
A	2	LYS	GLN	conflict	UNP Q6NSA1
A	3	GLN	LYS	conflict	UNP Q6NSA1
A	6	THR	GLU	conflict	UNP Q6NSA1
A	8	ILE	ASP	conflict	UNP Q6NSA1
A	10	ALA	GLY	conflict	UNP Q6NSA1
A	11	ALA	PRO	conflict	UNP Q6NSA1
A	19	GLU	ALA	conflict	UNP Q6NSA1
A	20	ASN	ILE	conflict	UNP Q6NSA1
A	21	LEU	VAL	conflict	UNP Q6NSA1
A	22	VAL	SER	conflict	UNP Q6NSA1
A	26	SER	THR	conflict	UNP Q6NSA1
A	27	PHE	TYR	conflict	UNP Q6NSA1
A	28	THR	SER	conflict	UNP Q6NSA1
A	29	ASP	ASN	conflict	UNP Q6NSA1
A	32	ILE	PHE	conflict	UNP Q6NSA1
A	33	TYR	GLN	conflict	UNP Q6NSA1
A	34	ASN	TYR	conflict	UNP Q6NSA1
A	35	LEU	PHE	conflict	UNP Q6NSA1
A	36	GLN	MET	conflict	UNP Q6NSA1
A	38	PHE	TYR	conflict	UNP Q6NSA1
A	41	ASP	TYR	conflict	UNP Q6NSA1
A	42	PRO	SER	conflict	UNP Q6NSA1
A	43	GLY	ARG	conflict	UNP Q6NSA1
A	46	LEU	-	insertion	UNP Q6NSA1
A	47	THR	PRO	conflict	UNP Q6NSA1
A	48	SER	GLU	conflict	UNP Q6NSA1

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Chain	Residue	Modelled	Actual	Comment	Reference
A	51	LEU	MET	conflict	UNP Q6NSA1
A	52	ILE	TYR	conflict	UNP Q6NSA1
A	53	GLN	THR	conflict	UNP Q6NSA1
A	54	SER	TYR	conflict	UNP Q6NSA1
A	56	GLN	SER	conflict	UNP Q6NSA1
A	57	ARG	GLY	conflict	UNP Q6NSA1
A	58	GLU	ASN	conflict	UNP Q6NSA1
A	59	GLN	LYS	conflict	UNP Q6NSA1
A	60	THR	GLU	conflict	UNP Q6NSA1
A	61	SER	ASP	conflict	UNP Q6NSA1
A	64	LEU	PHE	conflict	UNP Q6NSA1
A	65	ASN	THR	conflict	UNP Q6NSA1
A	67	SER	GLN	conflict	UNP Q6NSA1
A	68	LEU	VAL	conflict	UNP Q6NSA1
A	73	GLY	LYS	conflict	UNP Q6NSA1
A	74	ARG	TYR	conflict	UNP Q6NSA1
A	75	SER	ILE	conflict	UNP Q6NSA1
A	76	THR	SER	conflict	UNP Q6NSA1
A	78	TYR	PHE	conflict	UNP Q6NSA1
A	80	ALA	ARG	conflict	UNP Q6NSA1
A	81	ALA	ASP	conflict	UNP Q6NSA1
A	85	GLY	SER	conflict	UNP Q6NSA1
A	94	VAL	ALA	conflict	UNP Q6NSA1
A	95	THR	ARG	conflict	UNP Q6NSA1
A	96	ASN	THR	conflict	UNP Q6NSA1
A	97	PHE	GLY	conflict	UNP Q6NSA1
A	99	LYS	GLN	conflict	UNP Q6NSA1
A	104	SER	THR	conflict	UNP Q6NSA1
A	107	LYS	SER	conflict	UNP Q6NSA1
A	109	ASN	THR	conflict	UNP Q6NSA1
A	111	LYS	ILE	conflict	UNP Q6NSA1
A	160	CYS	THR	conflict	UNP Q6NSA1

- Molecule 2 is a protein called TCR 003 Beta Chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	244	Total	C	N	O	S	0	19	0
			2081	1301	373	399	8			

- Molecule 3 is GLYCEROL (three-letter code: GOL) (formula: C₃H₈O₃).



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

- Molecule 4 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: C₂H₆O₂).



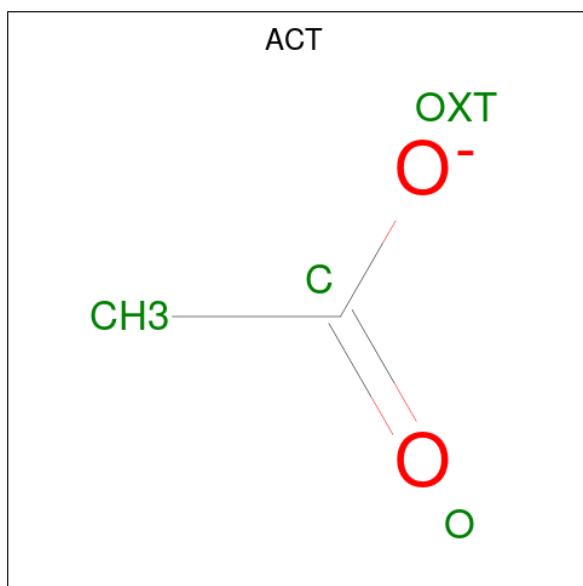
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			4	2	2		
4	A	1	Total	C	O	0	0
			4	2	2		
4	A	1	Total	C	O	0	0
			4	2	2		
4	A	1	Total	C	O	0	0
			4	2	2		
4	A	1	Total	C	O	0	0
			4	2	2		
4	A	1	Total	C	O	0	0
			4	2	2		
4	B	1	Total	C	O	0	0
			4	2	2		
4	B	1	Total	C	O	0	0
			4	2	2		
4	B	1	Total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

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

- Molecule 5 is ACETATE ION (three-letter code: ACT) (formula: $C_2H_3O_2$).



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

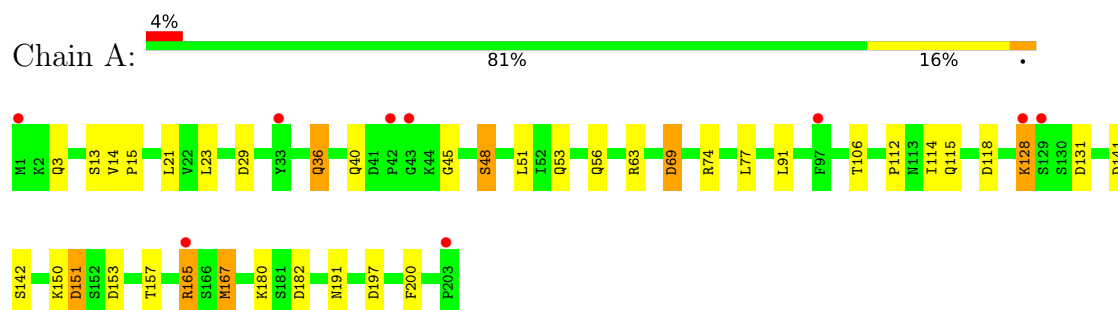
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	278	Total	O	0	0
			278	278		
6	B	336	Total	O	0	0
			336	336		

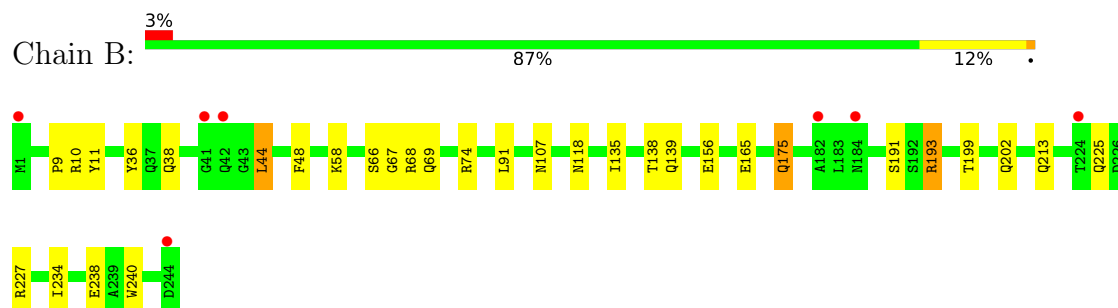
3 Residue-property plots

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: TCR 003 alpha chain



- Molecule 2: TCR 003 Beta Chain



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	43.28Å 81.29Å 65.09Å 90.00° 90.30° 90.00°	Depositor
Resolution (Å)	43.28 – 1.28 43.28 – 1.28	Depositor EDS
% Data completeness (in resolution range)	94.7 (43.28-1.28) 94.7 (43.28-1.28)	Depositor EDS
R_{merge}	0.04	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.24 (at 1.28Å)	Xtriage
Refinement program	REFMAC 5.8.0189	Depositor
R, R_{free}	0.168 , 0.190 0.175 , 0.199	Depositor DCC
R_{free} test set	5475 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	13.9	Xtriage
Anisotropy	0.163	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 38.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.026 for h,-k,-l	Xtriage
F_o, F_c correlation	0.97	EDS
Total number of atoms	4516	wwPDB-VP
Average B, all atoms (Å ²)	18.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.48% 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: ACT, EDO, 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	0.95	3/1764 (0.2%)	1.07	10/2393 (0.4%)
2	B	0.93	1/2170 (0.0%)	0.96	6/2944 (0.2%)
All	All	0.94	4/3934 (0.1%)	1.01	16/5337 (0.3%)

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	48	SER	CB-OG	7.05	1.51	1.42
2	B	165	GLU	CD-OE2	-6.47	1.18	1.25
1	A	36[A]	GLN	CD-OE1	5.74	1.36	1.24
1	A	36[B]	GLN	CD-OE1	5.74	1.36	1.24

All (16) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	69	ASP	CB-CG-OD1	9.57	126.92	118.30
2	B	193	ARG	NE-CZ-NH1	-8.87	115.86	120.30
1	A	167[A]	MET	CG-SD-CE	7.57	112.31	100.20
1	A	167[B]	MET	CG-SD-CE	7.57	112.31	100.20
1	A	74	ARG	NE-CZ-NH1	-7.28	116.66	120.30
2	B	74	ARG	NE-CZ-NH1	-6.26	117.17	120.30
1	A	63	ARG	NE-CZ-NH1	-6.15	117.22	120.30
2	B	44[A]	LEU	CB-CG-CD1	-5.58	101.51	111.00
2	B	44[B]	LEU	CB-CG-CD1	-5.58	101.51	111.00
2	B	74	ARG	NE-CZ-NH2	5.58	123.09	120.30
1	A	118	ASP	CB-CG-OD1	5.48	123.23	118.30
1	A	197	ASP	CB-CG-OD2	5.44	123.20	118.30
1	A	63	ARG	NE-CZ-NH2	5.31	122.95	120.30
1	A	151[A]	ASP	N-CA-CB	-5.18	101.27	110.60
1	A	151[B]	ASP	N-CA-CB	-5.18	101.27	110.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	227	ARG	NE-CZ-NH2	5.15	122.88	120.30

There are no chirality outliers.

There are no planarity outliers.

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	1721	0	1649	49	0
2	B	2081	0	1979	29	0
3	A	18	0	24	8	0
3	B	18	0	24	5	0
4	A	32	0	48	3	0
4	B	28	0	42	4	0
5	A	4	0	3	16	0
6	A	278	0	0	5	0
6	B	336	0	0	5	0
All	All	4516	0	3769	85	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 11.

All (85) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:36[B]:GLN:NE2	1:A:48:SER:OG	1.72	1.21
1:A:114:ILE:H	5:A:312:ACT:H1	1.16	1.11
1:A:180:LYS:HE2	1:A:182[B]:ASP:OD2	1.65	0.94
3:A:302:GOL:O2	5:A:312:ACT:C	2.23	0.87
2:B:68[C]:ARG:CA	2:B:69:GLN:N	2.40	0.84
2:B:67:GLY:C	2:B:68[C]:ARG:CA	2.52	0.77
5:A:312:ACT:O	6:A:401:HOH:O	2.03	0.77
2:B:240[B]:TRP:CZ3	6:B:601:HOH:O	2.38	0.77
1:A:40:GLN:HE22	2:B:38:GLN:HE22	1.31	0.76
1:A:3:GLN:HE22	1:A:29:ASP:H	1.37	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:21[B]:LEU:HD12	1:A:23[B]:LEU:CD1	2.22	0.69
1:A:21[B]:LEU:CD1	1:A:23[B]:LEU:CD1	2.73	0.67
1:A:131[A]:ASP:HB3	4:A:304:EDO:H12	1.75	0.67
1:A:114:ILE:N	5:A:312:ACT:H1	2.00	0.66
1:A:45:GLY:H	2:B:107:ASN:HD22	1.44	0.64
2:B:68[A]:ARG:N	2:B:68[A]:ARG:C	2.52	0.63
2:B:238:GLU:O	3:B:301:GOL:O2	2.16	0.62
1:A:131[A]:ASP:HB3	4:A:304:EDO:C1	2.30	0.60
2:B:135:ILE:HD13	4:B:306:EDO:H11	1.83	0.60
1:A:150[A]:LYS:HE3	1:A:191:ASN:HB2	1.83	0.60
1:A:151[A]:ASP:OD1	1:A:153:ASP:OD1	2.20	0.60
1:A:157[A]:THR:HG21	2:B:191:SER:OG	2.03	0.58
2:B:202:GLN:HE21	4:B:306:EDO:H12	1.68	0.58
1:A:21[B]:LEU:CD1	1:A:23[B]:LEU:HD11	2.35	0.57
2:B:66[B]:SER:HA	3:B:303:GOL:H11	1.87	0.57
1:A:115[A]:GLN:H	1:A:115[A]:GLN:CD	2.08	0.57
1:A:115[A]:GLN:NE2	6:A:405:HOH:O	2.38	0.56
1:A:167[A]:MET:HE3	6:B:706:HOH:O	2.04	0.56
3:A:302:GOL:O2	5:A:312:ACT:O	2.24	0.56
2:B:199[B]:THR:OG1	3:B:302:GOL:H31	2.06	0.56
2:B:10[C]:ARG:NH2	2:B:156:GLU:OE2	2.39	0.55
1:A:128:LYS:HA	1:A:128:LYS:HE3	1.88	0.55
1:A:200:PHE:CG	3:A:303:GOL:H11	2.41	0.55
1:A:141[B]:ASP:OD2	5:A:312:ACT:O	2.25	0.54
1:A:14[B]:VAL:O	1:A:14[B]:VAL:HG13	2.07	0.54
2:B:38:GLN:HB2	2:B:44[B]:LEU:HD23	1.89	0.54
1:A:91[B]:LEU:HD22	6:A:600:HOH:O	2.08	0.54
1:A:3:GLN:NE2	1:A:29:ASP:H	2.03	0.53
2:B:66[A]:SER:HA	3:B:303:GOL:H11	1.89	0.53
2:B:10[B]:ARG:CA	2:B:11:TYR:N	2.72	0.52
2:B:240[B]:TRP:CH2	6:B:601:HOH:O	2.61	0.52
2:B:44[B]:LEU:HD21	2:B:91:LEU:HD12	1.91	0.51
3:B:303:GOL:H31	6:B:447:HOH:O	2.10	0.51
1:A:141[B]:ASP:OD1	5:A:312:ACT:H2	2.11	0.50
1:A:151[A]:ASP:OD2	1:A:180:LYS:NZ	2.43	0.50
2:B:58:LYS:NZ	2:B:58:LYS:HB3	2.27	0.50
1:A:142:SER:HB2	5:A:312:ACT:H3	1.94	0.49
1:A:15:PRO:HB3	3:A:302:GOL:H2	1.95	0.49
2:B:135:ILE:HD13	4:B:306:EDO:C1	2.42	0.49
1:A:200:PHE:CD2	3:A:303:GOL:H11	2.48	0.49
5:A:312:ACT:C	6:A:401:HOH:O	2.54	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:23[A]:LEU:HD12	1:A:77:LEU:HD23	1.94	0.48
1:A:23[A]:LEU:CD2	1:A:106:THR:HG21	2.43	0.48
2:B:213:GLN:HG2	2:B:234:ILE:HG12	1.95	0.48
1:A:53[A]:GLN:H	1:A:56:GLN:NE2	2.10	0.48
1:A:53[B]:GLN:H	1:A:56:GLN:NE2	2.10	0.48
1:A:36[B]:GLN:HG2	1:A:51:LEU:HA	1.97	0.47
2:B:240[B]:TRP:HZ3	6:B:601:HOH:O	1.90	0.47
1:A:141[A]:ASP:HB2	5:A:312:ACT:H2	1.96	0.47
2:B:202:GLN:HE21	4:B:306:EDO:C1	2.27	0.47
6:A:600:HOH:O	2:B:44[B]:LEU:HB2	2.16	0.47
1:A:21[B]:LEU:HD12	1:A:23[B]:LEU:HD13	1.95	0.46
2:B:9:PRO:C	2:B:10[B]:ARG:CA	2.85	0.45
3:A:302:GOL:O2	5:A:312:ACT:OXT	2.35	0.45
1:A:21[B]:LEU:HD13	1:A:23[B]:LEU:HD11	1.98	0.45
2:B:36:TYR:HB3	2:B:44[B]:LEU:HD22	1.99	0.44
1:A:69:ASP:HB2	4:A:307:EDO:H22	1.99	0.44
1:A:14[A]:VAL:HG21	1:A:21[A]:LEU:HD21	2.00	0.44
1:A:114:ILE:H	5:A:312:ACT:CH3	2.06	0.44
2:B:118[B]:ASN:ND2	2:B:225:GLN:OE1	2.50	0.44
1:A:53[A]:GLN:H	1:A:56:GLN:HE21	1.67	0.43
1:A:23[A]:LEU:HD22	1:A:106:THR:HG21	2.00	0.42
1:A:53[B]:GLN:H	1:A:56:GLN:HE21	1.66	0.42
1:A:112:PRO:O	3:A:302:GOL:H12	2.19	0.42
2:B:138:THR:O	2:B:139[B]:GLN:HB2	2.19	0.42
1:A:15:PRO:HG3	3:A:302:GOL:H31	2.01	0.42
1:A:36[B]:GLN:NE2	1:A:48:SER:HG	2.04	0.42
2:B:175[A]:GLN:HE21	2:B:175[A]:GLN:HB3	1.49	0.41
1:A:14[B]:VAL:O	1:A:14[B]:VAL:CG1	2.67	0.41
1:A:165:ARG:H	1:A:165:ARG:HD2	1.86	0.41
1:A:14[A]:VAL:HG21	1:A:21[A]:LEU:CD2	2.51	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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	222/202 (110%)	220 (99%)	2 (1%)	0	100	100
2	B	263/244 (108%)	258 (98%)	5 (2%)	0	100	100
All	All	485/446 (109%)	478 (99%)	7 (1%)	0	100	100

There are no Ramachandran outliers to report.

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	202/180 (112%)	198 (98%)	4 (2%)	55	17
2	B	235/214 (110%)	231 (98%)	4 (2%)	60	24
All	All	437/394 (111%)	429 (98%)	8 (2%)	65	22

All (8) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	13[A]	SER
1	A	13[B]	SER
1	A	128	LYS
1	A	165	ARG
2	B	48	PHE
2	B	175[A]	GLN
2	B	175[B]	GLN
2	B	193	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (11) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	3	GLN
1	A	40	GLN

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Mol	Chain	Res	Type
1	A	56	GLN
1	A	65	ASN
1	A	143	GLN
1	A	148	GLN
2	B	45	GLN
2	B	57	ASN
2	B	107	ASN
2	B	202	GLN
2	B	213	GLN

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 monosaccharides in this entry.

5.6 Ligand geometry ⓘ

22 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	GOL	B	303	-	5,5,5	0.56	0	5,5,5	1.67	1 (20%)
4	EDO	A	310	-	3,3,3	0.53	0	2,2,2	0.06	0
4	EDO	B	304	-	3,3,3	0.33	0	2,2,2	0.75	0
4	EDO	A	308	-	3,3,3	0.53	0	2,2,2	0.43	0
3	GOL	A	303	-	5,5,5	0.57	0	5,5,5	1.19	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	EDO	B	305	-	3,3,3	0.34	0	2,2,2	0.47	0
4	EDO	B	310	-	3,3,3	0.42	0	2,2,2	0.08	0
4	EDO	B	308	-	3,3,3	0.37	0	2,2,2	0.24	0
4	EDO	B	306	-	3,3,3	0.47	0	2,2,2	0.57	0
3	GOL	A	302	-	5,5,5	0.65	0	5,5,5	0.69	0
4	EDO	A	309	-	3,3,3	0.36	0	2,2,2	0.61	0
4	EDO	A	311	-	3,3,3	0.37	0	2,2,2	0.10	0
4	EDO	A	304	-	3,3,3	0.58	0	2,2,2	0.38	0
4	EDO	A	306	-	3,3,3	0.53	0	2,2,2	0.17	0
5	ACT	A	312	-	3,3,3	1.08	0	3,3,3	1.74	1 (33%)
3	GOL	A	301	-	5,5,5	0.44	0	5,5,5	0.85	0
3	GOL	B	301	-	5,5,5	0.63	0	5,5,5	1.69	2 (40%)
4	EDO	A	305	-	3,3,3	0.43	0	2,2,2	0.42	0
4	EDO	A	307	-	3,3,3	0.66	0	2,2,2	0.34	0
3	GOL	B	302	-	5,5,5	0.66	0	5,5,5	1.26	1 (20%)
4	EDO	B	309	-	3,3,3	0.50	0	2,2,2	0.16	0
4	EDO	B	307	-	3,3,3	0.44	0	2,2,2	0.36	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	GOL	B	303	-	-	0/4/4/4	-
4	EDO	A	310	-	-	0/1/1/1	-
4	EDO	B	304	-	-	0/1/1/1	-
4	EDO	A	308	-	-	1/1/1/1	-
3	GOL	A	303	-	-	2/4/4/4	-
4	EDO	B	305	-	-	1/1/1/1	-
4	EDO	B	310	-	-	0/1/1/1	-
4	EDO	B	308	-	-	0/1/1/1	-
4	EDO	B	306	-	-	1/1/1/1	-
3	GOL	A	302	-	-	4/4/4/4	-
4	EDO	A	309	-	-	0/1/1/1	-
4	EDO	A	311	-	-	1/1/1/1	-
4	EDO	A	304	-	-	1/1/1/1	-
4	EDO	A	306	-	-	1/1/1/1	-
3	GOL	A	301	-	-	2/4/4/4	-
3	GOL	B	301	-	-	2/4/4/4	-
4	EDO	A	305	-	-	1/1/1/1	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	EDO	A	307	-	-	0/1/1/1	-
3	GOL	B	302	-	-	4/4/4/4	-
4	EDO	B	309	-	-	1/1/1/1	-
4	EDO	B	307	-	-	0/1/1/1	-

There are no bond length outliers.

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	301	GOL	O3-C3-C2	2.98	124.47	110.20
3	B	302	GOL	O3-C3-C2	2.63	122.79	110.20
5	A	312	ACT	O-C-CH3	-2.22	113.70	122.33
3	B	303	GOL	O3-C3-C2	2.21	120.79	110.20
3	B	301	GOL	O2-C2-C3	2.01	117.97	109.12

There are no chirality outliers.

All (22) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	301	GOL	C1-C2-C3-O3
3	A	302	GOL	O1-C1-C2-C3
3	A	302	GOL	C1-C2-C3-O3
3	A	303	GOL	C1-C2-C3-O3
3	B	301	GOL	C1-C2-C3-O3
3	B	302	GOL	O1-C1-C2-C3
3	A	302	GOL	O1-C1-C2-O2
3	A	303	GOL	O2-C2-C3-O3
3	B	301	GOL	O2-C2-C3-O3
4	A	305	EDO	O1-C1-C2-O2
3	B	302	GOL	C1-C2-C3-O3
3	A	301	GOL	O2-C2-C3-O3
3	A	302	GOL	O2-C2-C3-O3
3	B	302	GOL	O1-C1-C2-O2
4	A	304	EDO	O1-C1-C2-O2
4	B	305	EDO	O1-C1-C2-O2
3	B	302	GOL	O2-C2-C3-O3
4	A	311	EDO	O1-C1-C2-O2
4	A	306	EDO	O1-C1-C2-O2
4	B	306	EDO	O1-C1-C2-O2
4	A	308	EDO	O1-C1-C2-O2
4	B	309	EDO	O1-C1-C2-O2

There are no ring outliers.

9 monomers are involved in 33 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	303	GOL	3	0
3	A	303	GOL	2	0
4	B	306	EDO	4	0
3	A	302	GOL	6	0
4	A	304	EDO	2	0
5	A	312	ACT	16	0
3	B	301	GOL	1	0
4	A	307	EDO	1	0
3	B	302	GOL	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%)	0.11	9 (4%) 33 29	10, 16, 29, 43	0
2	B	244/244 (100%)	-0.05	7 (2%) 51 47	9, 15, 33, 53	0
All	All	446/446 (100%)	0.02	16 (3%) 42 38	9, 15, 31, 53	0

All (16) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	244	ASP	5.6
1	A	97	PHE	5.4
1	A	1	MET	4.1
1	A	33	TYR	3.7
1	A	203	PRO	3.6
2	B	184	ASN	3.6
2	B	224	THR	3.3
1	A	42	PRO	3.2
1	A	129	SER	2.5
2	B	1	MET	2.5
1	A	43	GLY	2.4
1	A	165	ARG	2.4
2	B	182	ALA	2.3
1	A	128	LYS	2.2
2	B	41	GLY	2.1
2	B	42	GLN	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(\AA^2)	Q<0.9
4	EDO	A	310	4/4	0.33	0.25	43,44,44,45	0
4	EDO	A	307	4/4	0.54	0.21	27,28,30,34	0
5	ACT	A	312	4/4	0.57	0.34	15,22,27,27	0
4	EDO	B	310	4/4	0.65	0.24	37,38,39,40	0
3	GOL	A	303	6/6	0.68	0.29	32,36,37,39	0
4	EDO	B	306	4/4	0.68	0.26	36,36,36,40	0
4	EDO	B	305	4/4	0.71	0.19	26,27,29,35	0
4	EDO	A	309	4/4	0.74	0.36	32,34,35,36	0
4	EDO	B	309	4/4	0.74	0.35	50,52,52,53	0
4	EDO	A	306	4/4	0.76	0.22	31,31,34,36	0
4	EDO	B	308	4/4	0.77	0.22	26,32,32,41	0
3	GOL	B	302	6/6	0.78	0.33	24,33,36,39	0
3	GOL	A	302	6/6	0.83	0.14	22,23,27,29	0
4	EDO	A	304	4/4	0.83	0.15	31,32,32,33	0
4	EDO	B	304	4/4	0.84	0.24	25,30,31,31	0
4	EDO	A	305	4/4	0.85	0.09	24,25,25,26	0
4	EDO	B	307	4/4	0.85	0.27	23,31,32,36	0
4	EDO	A	311	4/4	0.87	0.32	28,32,33,35	0
4	EDO	A	308	4/4	0.88	0.10	26,30,31,34	0
3	GOL	A	301	6/6	0.88	0.20	22,30,31,36	0
3	GOL	B	303	6/6	0.89	0.29	14,23,28,33	0
3	GOL	B	301	6/6	0.92	0.20	16,24,28,35	0

6.5 Other polymers [i](#)

There are no such residues in this entry.