



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 11:55 AM GMT

PDB ID : 3QEU
Title : The crystal structure of TCR DMF5
Authors : Borbulevych, O.Y.; Santhanagopalan, S.M.; Baker, B.M.
Deposited on : 2011-01-20
Resolution : 2.09 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
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix) : 1.9-1692
EDS : rb-20026688
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac : 5.8.0135
CCP4 : 6.5.0
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : trunk26865

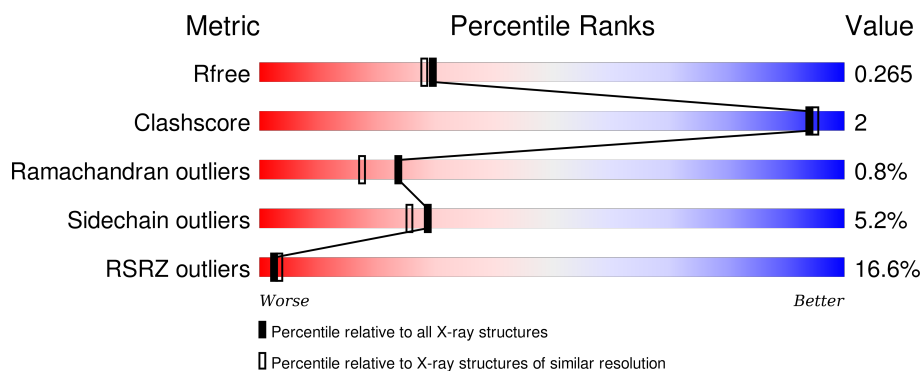
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.09 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}	91344	3939 (2.10-2.10)
Clashscore	102246	4460 (2.10-2.10)
Ramachandran outliers	100387	4413 (2.10-2.10)
Sidechain outliers	100360	4414 (2.10-2.10)
RSRZ outliers	91569	3948 (2.10-2.10)

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 on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. 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>31%</div> <div>84%</div> <div>11%</div> <div>..</div> </div>
1	D	202	<div> <div>5%</div> <div>94%</div> <div>..</div> </div>
2	B	243	<div> <div>25%</div> <div>87%</div> <div>11%</div> <div>.</div> </div>
2	E	243	<div> <div>5%</div> <div>93%</div> <div>7%</div> </div>

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 7373 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 DMF5 alpha chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	D	202	Total	C	N	O	S	0	2	0
			1573	982	258	325	8			
1	A	195	Total	C	N	O	S	0	1	0
			1516	947	249	312	8			

- Molecule 2 is a protein called DMF5 beta chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	E	243	Total	C	N	O	S	0	0	0
			1905	1196	334	366	9			
2	B	238	Total	C	N	O	S	0	0	0
			1868	1176	326	358	8			

- Molecule 3 is LITHIUM ION (three-letter code: LI) (formula: Li).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	D	1	Total	Li	0	0
			1	1		

- Molecule 4 is GLYCEROL (three-letter code: GOL) (formula: C₃H₈O₃).



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

- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	D	144	Total	O	0	0
			144	144		
5	E	208	Total	O	0	0
			208	208		
5	A	72	Total	O	0	0
			72	72		
5	B	74	Total	O	0	0
			74	74		

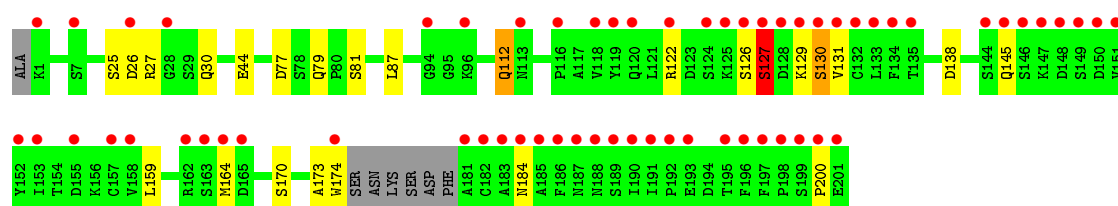
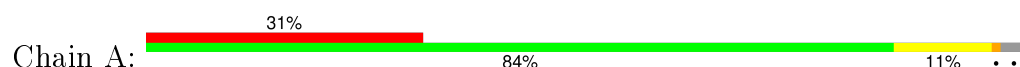
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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.

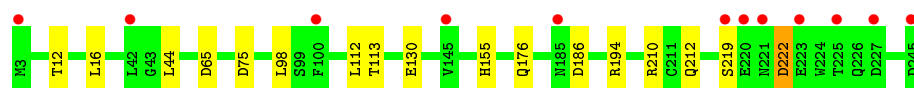
- Molecule 1: DMF5 alpha chain



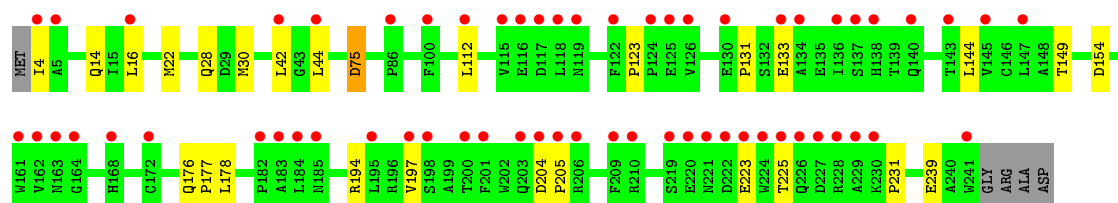
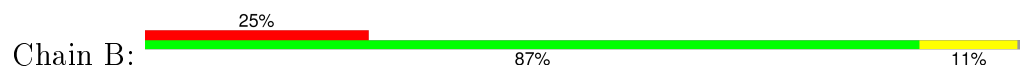
- Molecule 1: DMF5 alpha chain



- Molecule 2: DMF5 beta chain



- Molecule 2: DMF5 beta chain



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	184.16Å 86.50Å 66.47Å 90.00° 103.97° 90.00°	Depositor
Resolution (Å)	29.79 – 2.09 29.78 – 2.09	Depositor EDS
% Data completeness (in resolution range)	99.1 (29.79-2.09) 99.1 (29.78-2.09)	Depositor EDS
R_{merge}	0.05	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.90 (at 2.10Å)	Xtriage
Refinement program	REFMAC 5.5.0102	Depositor
R, R_{free}	0.206 , 0.266 0.205 , 0.265	Depositor DCC
R_{free} test set	2977 reflections (5.30%)	DCC
Wilson B-factor (Å ²)	32.4	Xtriage
Anisotropy	0.056	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.37 , 64.1	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.29$	Xtriage
Outliers	0 of 59136 reflections	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	7373	wwPDB-VP
Average B, all atoms (Å ²)	42.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.75% 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, 0.375 respectively for untwinned datasets, and 0.333, 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: GOL, LI

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	0.74	1/1552 (0.1%)	0.78	2/2099 (0.1%)
1	D	0.73	0/1613	0.90	6/2182 (0.3%)
2	B	0.57	0/1917	0.71	0/2614
2	E	0.74	0/1954	0.83	1/2661 (0.0%)
All	All	0.69	1/7036 (0.0%)	0.80	9/9556 (0.1%)

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	3
2	B	0	1
All	All	0	4

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	130	SER	CB-OG	16.77	1.64	1.42

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	159	LEU	CA-CB-CG	9.62	137.42	115.30
1	A	159	LEU	CA-CB-CG	7.84	133.34	115.30
1	D	159	LEU	CB-CG-CD2	7.09	123.06	111.00
1	A	87	LEU	CA-CB-CG	5.61	128.20	115.30
1	D	155	ASP	CB-CG-OD1	5.57	123.32	118.30
1	D	121	LEU	CB-CG-CD2	5.49	120.33	111.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	E	65	ASP	CB-CG-OD1	5.39	123.15	118.30
1	D	138	ASP	CB-CG-OD1	5.33	123.10	118.30
1	D	121	LEU	CA-CB-CG	5.17	127.20	115.30

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	126	SER	Peptide
1	A	127	SER	Peptide
1	A	173	ALA	Peptide
2	B	204	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	1516	0	1433	8	0
1	D	1573	0	1488	2	0
2	B	1868	0	1783	8	0
2	E	1905	0	1817	7	0
3	D	1	0	0	0	0
4	B	6	0	8	1	0
4	E	6	0	8	0	0
5	A	72	0	0	0	0
5	B	74	0	0	0	0
5	D	144	0	0	0	0
5	E	208	0	0	0	0
All	All	7373	0	6537	24	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 2.

All (24) 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:130:SER:CB	1:A:130:SER:OG	1.64	1.43
2:E:210:ARG:NH2	2:E:212:GLN:OE1	2.22	0.73
2:B:28:GLN:O	2:B:75:ASP:HB3	1.92	0.68
1:A:130:SER:CB	1:A:130:SER:HG	2.07	0.58
1:A:122:ARG:HD2	1:A:129:LYS:HD3	1.87	0.57
2:E:222:ASP:OD1	2:E:222:ASP:N	2.38	0.57
2:E:16:LEU:HD12	2:E:112:LEU:HD11	1.87	0.56
2:E:98:LEU:HD22	4:B:246:GOL:H11	1.89	0.54
1:A:130:SER:CA	1:A:130:SER:OG	2.52	0.54
2:E:186:ASP:N	2:E:186:ASP:OD1	2.43	0.51
1:A:127:SER:HA	1:A:129:LYS:HG3	1.93	0.50
1:A:122:ARG:HA	1:A:129:LYS:HB3	1.94	0.50
1:D:121:LEU:HB3	2:E:130:GLU:O	2.16	0.45
2:B:131:PRO:HD3	2:B:144:LEU:HG	1.99	0.44
2:E:113:THR:OG1	2:E:155:HIS:NE2	2.41	0.44
1:D:112:GLN:HG3	1:D:112:GLN:H	1.18	0.44
2:B:4:ILE:HD13	2:B:30:MET:HG2	1.99	0.44
2:B:14:GLN:HB3	2:B:112:LEU:HD13	2.00	0.43
2:B:16:LEU:HD12	2:B:112:LEU:HD11	2.00	0.43
2:B:154:ASP:HB2	2:B:177:PRO:HG2	2.01	0.43
1:A:112:GLN:HG2	1:A:112:GLN:H	1.53	0.42
2:B:16:LEU:HD21	2:B:22:MET:HB2	2.03	0.41
1:A:131:VAL:HG12	1:A:174:TRP:HB3	2.02	0.41
2:B:123:PRO:HD3	2:B:231:PRO:HB3	2.02	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	192/202 (95%)	171 (89%)	16 (8%)	5 (3%)	7 2
1	D	202/202 (100%)	200 (99%)	1 (0%)	1 (0%)	34 30

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	B	236/243 (97%)	227 (96%)	8 (3%)	1 (0%)	39	37
2	E	241/243 (99%)	239 (99%)	2 (1%)	0	100	100
All	All	871/890 (98%)	837 (96%)	27 (3%)	7 (1%)	24	17

All (7) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	127	SER
1	A	145	GLN
2	B	205	PRO
1	A	27	ARG
1	A	200	PRO
1	A	184	ASN
1	D	1	LYS

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	173/178 (97%)	162 (94%)	11 (6%)	22	18
1	D	180/178 (101%)	171 (95%)	9 (5%)	30	27
2	B	202/205 (98%)	190 (94%)	12 (6%)	24	20
2	E	205/205 (100%)	198 (97%)	7 (3%)	44	45
All	All	760/766 (99%)	721 (95%)	39 (5%)	29	26

All (39) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	D	1	LYS
1	D	26	ASP
1	D	27	ARG
1	D	30	GLN
1	D	56	GLU

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Mol	Chain	Res	Type
1	D	121	LEU
1	D	144	SER
1	D	159	LEU
1	D	197	PHE
2	E	12	THR
2	E	44	LEU
2	E	75	ASP
2	E	176	GLN
2	E	194	ARG
2	E	219	SER
2	E	222	ASP
1	A	25	SER
1	A	26	ASP
1	A	30	GLN
1	A	44	GLU
1	A	77	ASP
1	A	79	GLN
1	A	81	SER
1	A	112	GLN
1	A	138	ASP
1	A	164	MET
1	A	170	SER
2	B	42	LEU
2	B	44	LEU
2	B	75	ASP
2	B	133	GLU
2	B	149	THR
2	B	176	GLN
2	B	178	LEU
2	B	194	ARG
2	B	197	VAL
2	B	223	GLU
2	B	225	THR
2	B	239	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (6) such sidechains are listed below:

Mol	Chain	Res	Type
1	D	91	ASN
1	D	112	GLN
2	E	108	GLN
1	A	21	ASN

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Mol	Chain	Res	Type
2	B	140	GLN
2	B	226	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 carbohydrates in this entry.

5.6 Ligand geometry ⓘ

Of 3 ligands modelled in this entry, 1 is monoatomic - leaving 2 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the chemical component dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
4	GOL	B	246	-	5,5,5	0.13	0	5,5,5	1.13	0
4	GOL	E	2	-	5,5,5	0.35	0	5,5,5	0.29	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
4	GOL	B	246	-	-	0/4/4/4	0/0/0/0
4	GOL	E	2	-	-	0/4/4/4	0/0/0/0

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	B	246	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 ⓘ

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	195/202 (96%)	1.72	62 (31%) 1 1	23, 45, 118, 119	0
1	D	202/202 (100%)	0.50	11 (5%) 29 38	14, 29, 45, 53	0
2	B	238/243 (97%)	1.33	61 (25%) 1 1	22, 54, 78, 90	0
2	E	243/243 (100%)	0.30	12 (4%) 33 42	17, 27, 47, 60	0
All	All	878/890 (98%)	0.94	146 (16%) 2 3	14, 35, 83, 119	0

All (146) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	174	TRP	14.4
1	A	188	ASN	9.3
2	B	183	ALA	8.5
1	A	189	SER	8.4
1	A	200	PRO	8.3
2	B	225	THR	7.8
1	A	146	SER	7.5
1	A	186	PHE	7.4
1	A	187	ASN	7.4
1	A	128	ASP	6.9
1	A	201	GLU	6.6
1	A	130	SER	6.5
1	A	181	ALA	6.5
1	A	127	SER	6.4
1	A	199	SER	6.3
1	A	148	ASP	6.0
1	A	126	SER	6.0
1	A	147	LYS	5.9
1	A	196	PHE	5.5
2	B	224	TRP	5.4
1	A	184	ASN	5.4

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Mol	Chain	Res	Type	RSRZ
2	B	209	PHE	5.3
2	B	140	GLN	5.2
2	B	206	ARG	5.2
1	A	132	CYS	5.2
1	A	149	SER	5.0
1	D	128	ASP	5.0
1	A	122	ARG	4.9
1	A	124	SER	4.8
1	A	197	PHE	4.7
2	B	184	LEU	4.7
2	E	245	ASP	4.6
1	A	131	VAL	4.5
2	B	205	PRO	4.5
1	A	94	GLY	4.3
1	D	127	SER	4.3
2	B	137	SER	4.3
1	D	126	SER	4.3
2	B	219	SER	4.2
2	B	227	ASP	4.2
2	B	229	ALA	4.1
2	B	228	ARG	4.0
1	A	185	ALA	4.0
2	B	162	VAL	3.9
1	A	133	LEU	3.9
1	A	162	ARG	3.9
2	B	220	GLU	3.8
2	E	225	THR	3.7
2	B	119	ASN	3.6
1	A	182	CYS	3.6
2	B	222	ASP	3.6
1	A	163	SER	3.6
2	B	221	ASN	3.5
2	B	223	GLU	3.5
1	A	144	SER	3.5
1	A	125	LYS	3.5
1	A	145	GLN	3.5
2	B	210	ARG	3.5
2	B	164	GLY	3.4
1	D	50	TYR	3.4
2	B	185	ASN	3.4
2	B	147	LEU	3.4
1	A	113	ASN	3.4

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Mol	Chain	Res	Type	RSRZ
1	A	198	PRO	3.3
2	E	223	GLU	3.3
2	B	117	ASP	3.3
2	E	42	LEU	3.2
2	B	230	LYS	3.2
1	A	193	GLU	3.2
2	E	227	ASP	3.2
2	B	138	HIS	3.2
2	B	134	ALA	3.2
1	A	129	LYS	3.1
2	B	5	ALA	3.1
2	B	226	GLN	3.1
1	A	165	ASP	3.1
2	E	3	MET	3.1
2	B	100	PHE	3.1
1	A	190	ILE	3.1
1	A	192	PRO	3.1
2	B	203	GLN	3.1
2	B	125	GLU	3.0
1	A	151	VAL	3.0
1	A	164	MET	3.0
2	B	143	THR	3.0
2	B	122	PHE	3.0
2	B	204	ASP	3.0
2	B	44	LEU	3.0
2	B	200	THR	2.9
1	A	155	ASP	2.9
2	B	182	PRO	2.9
1	D	94	GLY	2.9
2	B	195	LEU	2.9
2	B	126	VAL	2.9
2	E	185	ASN	2.9
2	B	116	GLU	2.9
2	B	133	GLU	2.9
2	E	220	GLU	2.8
1	A	28	GLY	2.8
2	B	42	LEU	2.8
1	A	26	ASP	2.8
2	B	130	GLU	2.8
1	A	118	VAL	2.8
2	B	168	HIS	2.7
2	B	201	PHE	2.7

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Mol	Chain	Res	Type	RSRZ
2	B	136	ILE	2.7
1	A	150	ASP	2.7
2	B	16	LEU	2.7
2	E	100	PHE	2.7
2	B	86	PRO	2.7
1	D	27	ARG	2.6
1	A	1	LYS	2.6
2	E	145	VAL	2.6
2	B	124	PRO	2.6
1	A	191	ILE	2.6
2	B	115	VAL	2.6
2	E	221	ASN	2.6
1	A	152	TYR	2.6
2	B	118	LEU	2.5
1	D	201	GLU	2.5
1	A	120	GLN	2.5
2	B	241	TRP	2.5
1	A	183	ALA	2.5
1	D	0	ALA	2.5
2	B	145	VAL	2.5
2	B	161	TRP	2.5
1	A	195	THR	2.4
2	B	163	ASN	2.4
1	A	119	TYR	2.4
2	B	198	SER	2.4
1	D	93	GLY	2.4
1	A	158	VAL	2.4
1	D	179	ASP	2.3
1	A	116	PRO	2.3
1	A	134	PHE	2.3
2	B	4	ILE	2.2
1	D	171	ALA	2.2
2	B	112	LEU	2.2
1	A	135	THR	2.2
2	B	197	VAL	2.1
1	A	153	ILE	2.1
1	A	157	CYS	2.1
2	B	172	CYS	2.1
1	A	96	LYS	2.0
1	A	7	SER	2.0
2	E	219	SER	2.0

6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

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

6.3 Carbohydrates [i](#)

There are no carbohydrates 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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. 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	LLDF	B-factors(\AA^2)	Q<0.9
4	GOL	B	246	6/6	0.83	0.20	1.62	34,40,41,41	0
4	GOL	E	2	6/6	0.88	0.23	-	53,54,54,55	6
3	LI	D	202	1/1	0.93	0.09	-	2,2,2,2	0

6.5 Other polymers [i](#)

There are no such residues in this entry.