



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 4, 2026 – 06:54 PM UTC

PDB ID : 9YIO / pdb_00009yio
Title : Crystal structure of 5B3 Fab in complex with PvRipr EGF7-8
Authors : Xiao, X.; Cowman, A.F.; Scally, S.W.
Deposited on : 2025-10-02
Resolution : 2.08 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

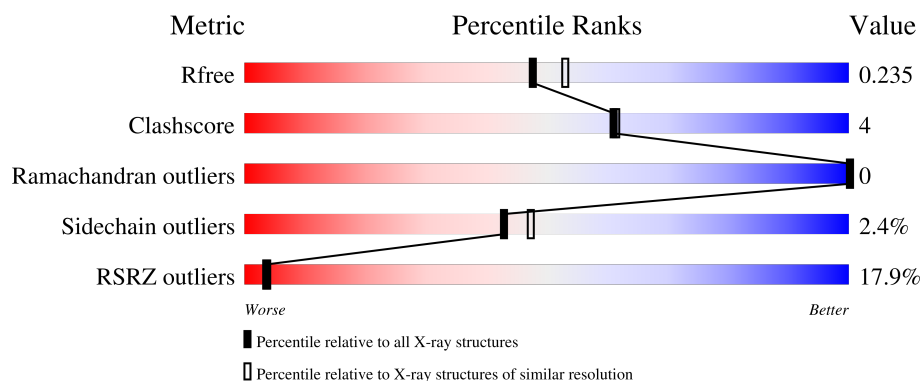
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.08 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	8172 (2.10-2.06)
Clashscore	190562	8714 (2.10-2.06)
Ramachandran outliers	187476	8641 (2.10-2.06)
Sidechain outliers	187428	8642 (2.10-2.06)
RSRZ outliers	180081	8177 (2.10-2.06)

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	B	83	24% 88% 11% .
2	C	213	21% 87% 11% .
3	D	224	12% 84% 15% .

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 4214 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 PvRipr EGF7-8.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	B	83	Total	C	N	O	S	0	0	0
			651	395	121	121	14			

There are 5 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	761	GLY	-	expression tag	UNP A0A564ZTL5
B	762	HIS	-	expression tag	UNP A0A564ZTL5
B	763	MET	-	expression tag	UNP A0A564ZTL5
B	767	GLN	ASN	engineered mutation	UNP A0A564ZTL5
B	780	GLN	ASN	engineered mutation	UNP A0A564ZTL5

- Molecule 2 is a protein called 5B3 kappa chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	C	209	Total	C	N	O	S	0	0	0
			1602	1006	268	322	6			

- Molecule 3 is a protein called 5B3 heavy chain.

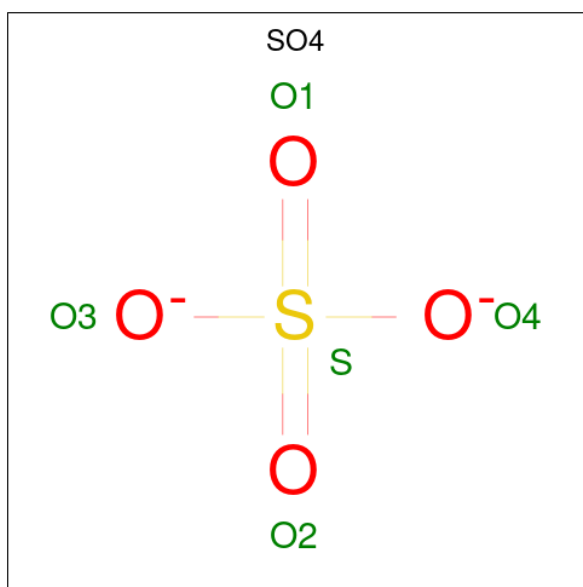
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	D	222	Total	C	N	O	S	0	1	0
			1695	1075	281	334	5			

- Molecule 4 is GLYCEROL (CCD ID: GOL) (formula: C₃H₈O₃).



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

- Molecule 5 is SULFATE ION (CCD ID: SO4) (formula: O₄S).



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

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

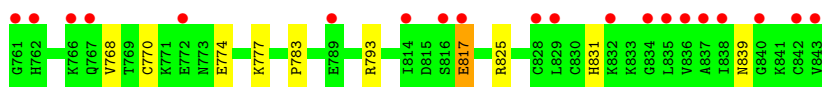
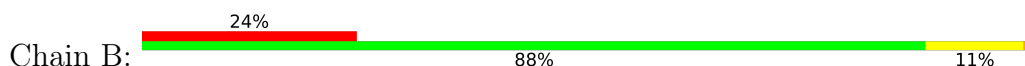
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	B	50	Total	O	0	0
			50	50		
6	C	71	Total	O	0	0
			71	71		
6	D	117	Total	O	0	0
			117	117		

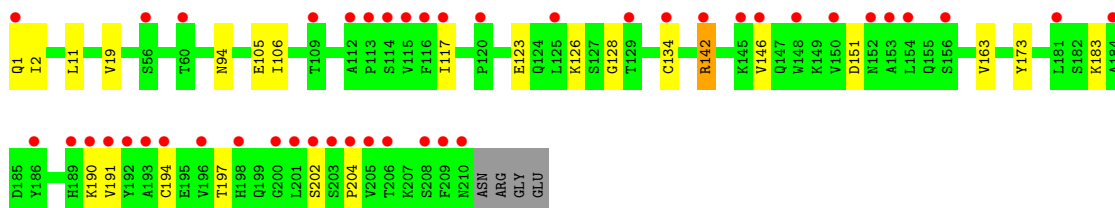
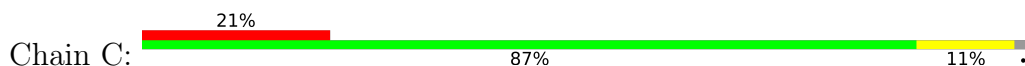
3 Residue-property plots [i](#)

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.

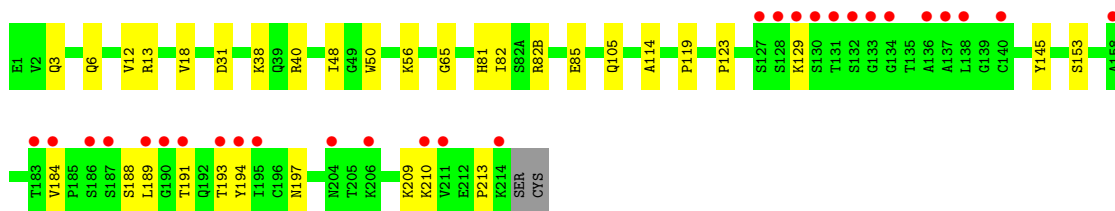
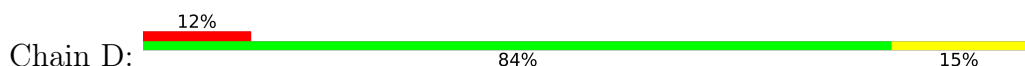
- Molecule 1: PvRipr EGF7-8



- Molecule 2: 5B3 kappa chain



- Molecule 3: 5B3 heavy chain



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, α , β , γ	80.27Å 81.75Å 92.15Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	48.64 – 2.08 48.64 – 2.08	Depositor EDS
% Data completeness (in resolution range)	99.2 (48.64-2.08) 91.0 (48.64-2.08)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	0.81 (at 2.08Å)	Xtriage
Refinement program	PHENIX 1.21_5207	Depositor
R, R_{free}	0.204 , 0.235 0.204 , 0.235	Depositor DCC
R_{free} test set	2001 reflections (5.41%)	wwPDB-VP
Wilson B-factor (Å ²)	27.6	Xtriage
Anisotropy	0.640	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 52.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.018 for k,h,-l	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	4214	wwPDB-VP
Average B, all atoms (Å ²)	55.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.12% 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: GOL, SO4

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	B	0.16	0/659	0.37	0/881
2	C	0.14	0/1643	0.34	0/2238
3	D	0.16	0/1743	0.34	0/2377
All	All	0.15	0/4045	0.35	0/5496

There are no bond length outliers.

There are no bond angle outliers.

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	B	651	0	636	5	0
2	C	1602	0	1548	11	0
3	D	1695	0	1657	19	0
4	B	6	0	8	0	0
4	D	12	0	16	2	0
5	D	10	0	0	0	0
6	B	50	0	0	0	0
6	C	71	0	0	0	0
6	D	117	0	0	0	0
All	All	4214	0	3865	33	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 4.

All (33) 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)
3:D:65:GLY:O	3:D:82(B):ARG:NH2	2.21	0.73
3:D:123:PRO:HD3	3:D:209:LYS:HE2	1.76	0.66
3:D:153:SER:HB2	3:D:197:ASN:HB2	1.79	0.64
3:D:188:SER:HA	3:D:191:THR:HB	1.83	0.61
3:D:6:GLN:H	3:D:105[A]:GLN:HE22	1.51	0.58
1:B:793:ARG:HG2	3:D:31:ASP:HB3	1.85	0.58
1:B:817:GLU:OE1	1:B:831:HIS:NE2	2.40	0.55
3:D:119:PRO:HB3	3:D:145:TYR:HB3	1.89	0.55
2:C:142:ARG:HD2	2:C:163:VAL:HG11	1.90	0.54
2:C:128:GLY:C	2:C:183:LYS:HB2	2.35	0.52
3:D:6:GLN:H	3:D:105[A]:GLN:NE2	2.08	0.52
2:C:123:GLU:HA	2:C:126:LYS:HE2	1.92	0.51
3:D:38:LYS:HB2	3:D:48:ILE:HD11	1.93	0.50
2:C:11:LEU:HD21	2:C:19:VAL:HB	1.98	0.46
2:C:190:LYS:HE3	2:C:191:VAL:HG23	1.97	0.46
3:D:193:THR:HG23	3:D:210:LYS:HE2	1.97	0.46
3:D:81:HIS:CE1	4:D:301:GOL:H31	2.51	0.46
2:C:151:ASP:HA	2:C:191:VAL:HB	1.99	0.45
3:D:184:VAL:HG11	3:D:194:TYR:CE1	2.52	0.45
2:C:117:ILE:HG22	3:D:129:LYS:HB3	2.00	0.44
3:D:40:ARG:NH1	3:D:85:GLU:OE1	2.51	0.44
3:D:189:LEU:HB3	3:D:213:PRO:HG2	2.00	0.44
2:C:2:ILE:HD12	2:C:94:ASN:HB2	2.00	0.43
2:C:197:THR:HG22	2:C:204:PRO:HB3	2.00	0.43
2:C:105:GLU:HG3	2:C:173:TYR:OH	2.19	0.43
2:C:105:GLU:HG2	2:C:106:ILE:N	2.34	0.43
3:D:13:ARG:NH1	3:D:114:ALA:O	2.49	0.42
1:B:770:CYS:HB3	1:B:774:GLU:HB2	2.02	0.42
3:D:56:LYS:O	4:D:302:GOL:H11	2.19	0.42
3:D:18:VAL:HB	3:D:82:ILE:HB	2.01	0.41
1:B:777:LYS:HE2	1:B:777:LYS:HB3	1.91	0.41
1:B:768:VAL:HG21	1:B:783:PRO:HB2	2.03	0.40
3:D:12:VAL:HG21	3:D:18:VAL:HG22	2.04	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	B	81/83 (98%)	74 (91%)	7 (9%)	0	100	100
2	C	207/213 (97%)	199 (96%)	8 (4%)	0	100	100
3	D	221/224 (99%)	214 (97%)	7 (3%)	0	100	100
All	All	509/520 (98%)	487 (96%)	22 (4%)	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	B	78/78 (100%)	75 (96%)	3 (4%)	29	30
2	C	182/185 (98%)	176 (97%)	6 (3%)	33	35
3	D	192/193 (100%)	190 (99%)	2 (1%)	68	75
All	All	452/456 (99%)	441 (98%)	11 (2%)	43	47

All (11) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	817	GLU
1	B	825	ARG
1	B	839	ASN
2	C	1	GLN
2	C	134	CYS

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Mol	Chain	Res	Type
2	C	142	ARG
2	C	146	VAL
2	C	194	CYS
2	C	202	SER
3	D	3	GLN
3	D	50	TRP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
2	C	38	GLN
3	D	39	GLN
3	D	192	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 oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

5 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
4	GOL	D	302	-	5,5,5	0.39	0	5,5,5	0.38	0
4	GOL	B	901	-	5,5,5	0.35	0	5,5,5	0.41	0
4	GOL	D	301	-	5,5,5	0.34	0	5,5,5	0.34	0
5	SO4	D	303	-	4,4,4	0.71	0	6,6,6	0.11	0
5	SO4	D	304	-	4,4,4	0.67	0	6,6,6	0.09	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	D	301	-	-	4/4/4/4	-
4	GOL	D	302	-	-	3/4/4/4	-
4	GOL	B	901	-	-	0/4/4/4	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (7) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	D	301	GOL	O1-C1-C2-O2
4	D	301	GOL	O1-C1-C2-C3
4	D	301	GOL	C1-C2-C3-O3
4	D	302	GOL	O1-C1-C2-C3
4	D	301	GOL	O2-C2-C3-O3
4	D	302	GOL	O2-C2-C3-O3
4	D	302	GOL	O1-C1-C2-O2

There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	D	302	GOL	1	0
4	D	301	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	B	83/83 (100%)	1.19	20 (24%) 2 2	27, 51, 94, 102	0
2	C	209/213 (98%)	0.87	44 (21%) 2 2	24, 57, 117, 134	0
3	D	222/224 (99%)	0.51	28 (12%) 8 8	19, 40, 103, 126	1 (0%)
All	All	514/520 (98%)	0.77	92 (17%) 3 4	19, 48, 109, 134	1 (0%)

All (92) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	836	VAL	4.6
1	B	838	ILE	4.2
2	C	154	LEU	4.2
1	B	761	GLY	4.1
3	D	130	SER	4.0
1	B	762	HIS	3.9
1	B	843	VAL	3.9
3	D	136	ALA	3.9
2	C	192	TYR	3.7
1	B	837	ALA	3.7
3	D	128	SER	3.7
2	C	209	PHE	3.7
2	C	194	CYS	3.7
2	C	153	ALA	3.6
2	C	125	LEU	3.6
2	C	115	VAL	3.5
2	C	191	VAL	3.3
3	D	195	ILE	3.2
3	D	133	GLY	3.2
1	B	842	CYS	3.2
2	C	210	ASN	3.1
3	D	158	ALA	3.0
1	B	829	LEU	3.0

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Mol	Chain	Res	Type	RSRZ
1	B	835	LEU	3.0
3	D	138	LEU	3.0
3	D	189	LEU	3.0
2	C	134	CYS	2.9
1	B	840	GLY	2.9
3	D	191	THR	2.9
2	C	156	SER	2.8
3	D	194	TYR	2.8
2	C	181	LEU	2.8
2	C	117	ILE	2.8
2	C	202	SER	2.7
3	D	131	THR	2.7
2	C	205	VAL	2.7
3	D	211	VAL	2.7
2	C	196	VAL	2.6
3	D	140	CYS	2.6
2	C	152	ASN	2.6
3	D	190	GLY	2.6
2	C	193	ALA	2.6
2	C	204	PRO	2.6
3	D	127	SER	2.6
2	C	116	PHE	2.5
2	C	129	THR	2.5
2	C	114	SER	2.4
2	C	208	SER	2.4
2	C	142	ARG	2.4
1	B	767	GLN	2.4
2	C	203	SER	2.4
2	C	206	THR	2.4
3	D	129	LYS	2.4
1	B	834	GLY	2.4
3	D	193	THR	2.4
2	C	113	PRO	2.4
2	C	112	ALA	2.4
2	C	60	THR	2.4
3	D	183	THR	2.4
2	C	120	PRO	2.4
2	C	198	HIS	2.3
1	B	772	GLU	2.3
1	B	817	GLU	2.3
2	C	148	TRP	2.3
2	C	184	ALA	2.3

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Mol	Chain	Res	Type	RSRZ
2	C	190	LYS	2.3
2	C	189	HIS	2.3
2	C	201	LEU	2.3
2	C	1	GLN	2.3
2	C	146	VAL	2.3
1	B	766	LYS	2.3
2	C	186	TYR	2.3
2	C	150	VAL	2.2
2	C	145	LYS	2.2
1	B	832	LYS	2.2
3	D	214	LYS	2.2
3	D	137	ALA	2.2
1	B	828	CYS	2.2
2	C	56	SER	2.2
3	D	132	SER	2.2
3	D	187	SER	2.2
3	D	204	ASN	2.2
3	D	184	VAL	2.1
1	B	816	SER	2.1
3	D	134	GLY	2.1
1	B	814	ILE	2.1
3	D	206	LYS	2.1
3	D	186	SER	2.1
1	B	789	GLU	2.1
2	C	200	GLY	2.1
2	C	109	THR	2.0
3	D	210	LYS	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
4	GOL	B	901	6/6	0.75	0.14	73,83,92,100	0
4	GOL	D	301	6/6	0.78	0.18	56,66,71,88	0
5	SO4	D	304	5/5	0.88	0.11	55,59,67,68	0
4	GOL	D	302	6/6	0.89	0.14	45,50,56,61	0
5	SO4	D	303	5/5	0.93	0.12	41,44,54,60	0

6.5 Other polymers [i](#)

There are no such residues in this entry.