



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 13, 2026 – 11:24 PM UTC

PDB ID : 2ADF / pdb_00002adf
Title : Crystal Structure and Paratope Determination of 82D6A3, an Antithrombotic Antibody Directed Against the von Willebrand factor A3-Domain
Authors : Staelens, S.; Hadders, M.A.; Vauterin, S.; Platteau, C.; Vanhoorelbeke, K.; Huizinga, E.G.; Deckmyn, H.
Deposited on : 2005-07-20
Resolution : 1.90 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

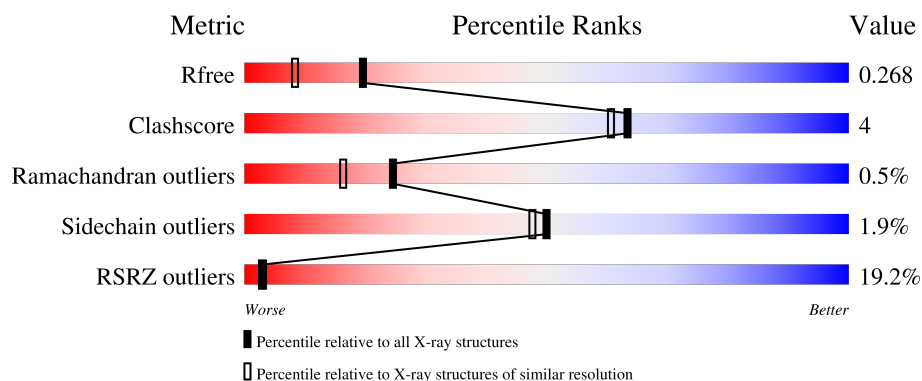
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.90 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	7789 (1.90-1.90)
Clashscore	190562	8410 (1.90-1.90)
Ramachandran outliers	187476	8333 (1.90-1.90)
Sidechain outliers	187428	8333 (1.90-1.90)
RSRZ outliers	180081	7790 (1.90-1.90)

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	196	
2	H	218	
3	L	209	

2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 5165 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 Von Willebrand factor.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	189	Total	C	N	O	S	0	0	0
			1414	894	242	272	6			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	916	GLY	-	expression tag	UNP P04275
A	917	SER	-	expression tag	UNP P04275
A	918	HIS	-	expression tag	UNP P04275
A	919	MET	-	expression tag	UNP P04275

- Molecule 2 is a protein called 82D6A3 IgG.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	H	218	Total	C	N	O	S	0	0	0
			1665	1056	272	330	7			

- Molecule 3 is a protein called 82D6A3 IgG.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	L	209	Total	C	N	O	S	0	0	0
			1624	1015	274	329	6			

- Molecule 4 is ACETIC ACID (CCD ID: ACY) (formula: C₂H₄O₂).



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

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



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

- Molecule 6 is GLYCEROL (CCD ID: GOL) (formula: C₃H₈O₃).



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

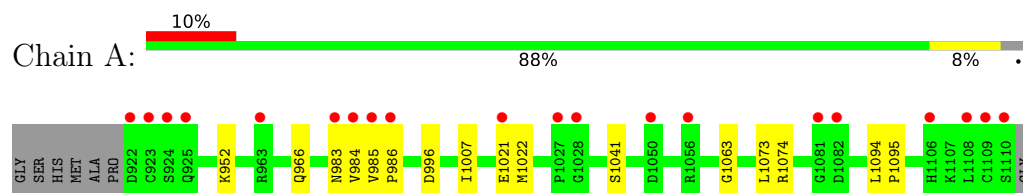
- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	136	Total	O	0	0
			136	136		
7	H	155	Total	O	0	0
			155	155		
7	L	151	Total	O	0	0
			151	151		

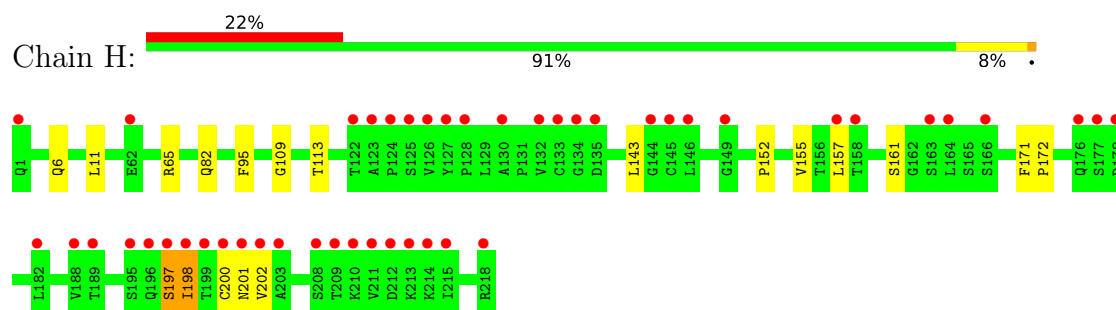
3 Residue-property plots [i](#)

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.

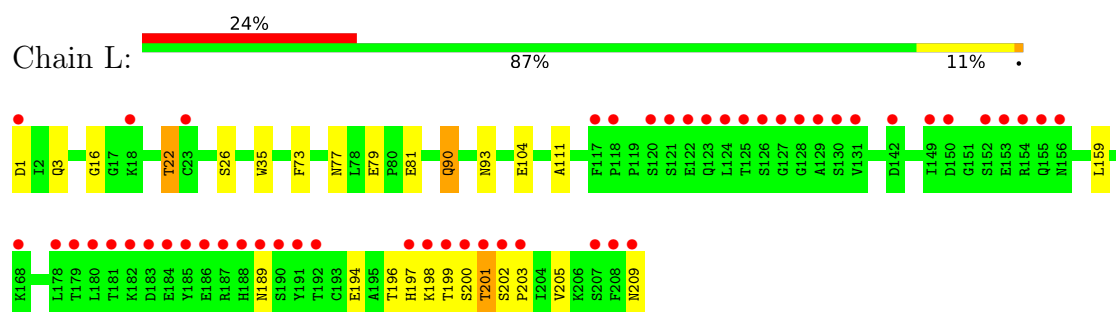
- Molecule 1: Von Willebrand factor



- Molecule 2: 82D6A3 IgG



- Molecule 3: 82D6A3 IgG



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	72.18Å 89.08Å 123.51Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	27.35 – 1.90 27.35 – 1.90	Depositor EDS
% Data completeness (in resolution range)	100.0 (27.35-1.90) 99.8 (27.35-1.90)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	4.25 (at 1.91Å)	Xtriage
Refinement program	REFMAC 5.2.0003	Depositor
R, R_{free}	0.191 , 0.220 0.246 , 0.268	Depositor DCC
R_{free} test set	3243 reflections (5.12%)	wwPDB-VP
Wilson B-factor (Å ²)	22.9	Xtriage
Anisotropy	0.246	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 36.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	5165	wwPDB-VP
Average B, all atoms (Å ²)	20.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.23% 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 [i](#)

5.1 Standard geometry [i](#)

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

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	0.59	0/1439	0.95	0/1957
2	H	0.53	0/1709	0.85	1/2333 (0.0%)
3	L	0.65	2/1662 (0.1%)	0.92	2/2253 (0.1%)
All	All	0.59	2/4810 (0.0%)	0.91	3/6543 (0.0%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	L	209	ASN	C-OXT	12.53	1.48	1.23
3	L	189	ASN	CG-OD1	5.46	1.33	1.23

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	L	198	LYS	N-CA-C	-6.64	103.13	113.02
3	L	201	THR	N-CA-C	-6.06	105.38	112.89
2	H	65	ARG	N-CA-C	5.70	120.35	113.17

There are no chirality outliers.

There are no planarity outliers.

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	1414	0	1425	9	0
2	H	1665	0	1621	13	0
3	L	1624	0	1567	14	0
4	A	4	0	3	0	0
5	H	5	0	0	0	0
5	L	5	0	0	0	0
6	H	6	0	8	1	0
7	A	136	0	0	2	0
7	H	155	0	0	4	0
7	L	151	0	0	2	0
All	All	5165	0	4624	37	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 (37) 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:L:200:SER:HB3	3:L:202:SER:O	1.63	0.99
2:H:161:SER:H	2:H:201:ASN:HD21	1.24	0.84
1:A:1021:GLU:HG2	7:A:1227:HOH:O	1.78	0.83
1:A:984:VAL:O	1:A:986:PRO:HD3	1.87	0.74
2:H:6:GLN:HE21	2:H:109:GLY:HA3	1.53	0.73
3:L:200:SER:CB	3:L:202:SER:O	2.37	0.72
3:L:22:THR:HG22	7:L:1049:HOH:O	1.93	0.66
2:H:161:SER:H	2:H:201:ASN:ND2	1.95	0.63
6:H:1004:GOL:H32	7:H:1066:HOH:O	1.99	0.62
2:H:157:LEU:HD11	2:H:200:CYS:HB2	1.82	0.61
3:L:16:GLY:HA2	3:L:77:ASN:HD22	1.65	0.61
1:A:952:LYS:NZ	1:A:996:ASP:OD1	2.34	0.58
2:H:157:LEU:HD13	2:H:202:VAL:HG22	1.84	0.58
3:L:200:SER:HB2	7:L:1024:HOH:O	2.04	0.57
2:H:113:THR:HG22	7:H:1014:HOH:O	2.02	0.57
3:L:199:THR:O	3:L:200:SER:HB2	2.06	0.55
3:L:79:GLU:OE1	3:L:81:GLU:OE2	2.27	0.53
1:A:966:GLN:HE21	1:A:983:ASN:H	1.57	0.52
3:L:202:SER:HB3	3:L:203:PRO:HD2	1.92	0.52
3:L:90:GLN:HE22	3:L:93:ASN:H	1.58	0.51
2:H:143:LEU:HD12	2:H:198:ILE:HG21	1.97	0.47
1:A:1007:ILE:HD12	1:A:1041:SER:HB2	1.97	0.46
3:L:35:TRP:CE2	3:L:73:PHE:HB2	2.51	0.45
2:H:6:GLN:HE22	2:H:95:PHE:HA	1.81	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1094:LEU:HB3	1:A:1095:PRO:HD3	1.99	0.45
1:A:952:LYS:CE	1:A:996:ASP:OD1	2.64	0.45
3:L:194:GLU:HG2	3:L:205:VAL:HG22	2.00	0.44
3:L:111:ALA:HA	3:L:199:THR:HB	1.99	0.44
2:H:6:GLN:HE21	2:H:109:GLY:CA	2.28	0.42
3:L:196:THR:CG2	3:L:203:PRO:HB3	2.49	0.42
1:A:1063:GLY:HA3	1:A:1073:LEU:HD11	2.00	0.42
2:H:11:LEU:HD22	2:H:152:PRO:HG3	2.01	0.41
2:H:171:PHE:HA	2:H:172:PRO:HD3	1.96	0.41
3:L:3:GLN:HG2	3:L:26:SER:HB3	2.02	0.41
1:A:1074:ARG:NH2	7:A:1242:HOH:O	2.50	0.40
2:H:82:GLN:NE2	7:H:1158:HOH:O	2.55	0.40
2:H:113:THR:HG21	7:H:1105:HOH:O	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	187/196 (95%)	180 (96%)	7 (4%)	0	100	100
2	H	216/218 (99%)	210 (97%)	4 (2%)	2 (1%)	14	6
3	L	207/209 (99%)	200 (97%)	6 (3%)	1 (0%)	24	16
All	All	610/623 (98%)	590 (97%)	17 (3%)	3 (0%)	24	16

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	H	197	SER
3	L	197	HIS
2	H	198	ILE

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	156/160 (98%)	154 (99%)	2 (1%)	61	61
2	H	187/187 (100%)	185 (99%)	2 (1%)	65	67
3	L	185/185 (100%)	179 (97%)	6 (3%)	34	27
All	All	528/532 (99%)	518 (98%)	10 (2%)	50	47

All (10) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	985	VAL
1	A	1022	MET
2	H	155	VAL
2	H	197	SER
3	L	1	ASP
3	L	22	THR
3	L	90	GLN
3	L	104	GLU
3	L	159	LEU
3	L	201	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (10) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	959	ASN
1	A	966	GLN
1	A	990	HIS
2	H	6	GLN
2	H	169	HIS
2	H	201	ASN
3	L	77	ASN
3	L	90	GLN
3	L	137	ASN
3	L	160	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

4 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	ACY	A	1112	-	3,3,3	0.80	0	3,3,3	0.76	0
5	SO4	L	1003	-	4,4,4	0.28	0	6,6,6	0.26	0
5	SO4	H	1002	-	4,4,4	0.21	0	6,6,6	0.18	0
6	GOL	H	1004	-	5,5,5	0.39	0	5,5,5	0.31	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	GOL	H	1004	-	-	2/4/4/4	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	H	1004	GOL	O1-C1-C2-C3
6	H	1004	GOL	O1-C1-C2-O2

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	H	1004	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	189/196 (96%)	0.58	20 (10%)	11 12	10, 16, 30, 38	0
2	H	218/218 (100%)	1.12	47 (21%)	2 2	10, 22, 34, 35	0
3	L	209/209 (100%)	1.50	51 (24%)	2 1	13, 17, 25, 43	0
All	All	616/623 (98%)	1.08	118 (19%)	3 3	10, 17, 33, 43	0

All (118) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	L	199	THR	8.9
1	A	985	VAL	8.9
3	L	201	THR	7.6
3	L	198	LYS	6.2
3	L	185	TYR	6.2
3	L	191	TYR	6.0
3	L	128	GLY	6.0
2	H	128	PRO	5.9
3	L	181	THR	5.8
3	L	190	SER	5.7
3	L	118	PRO	5.4
2	H	197	SER	5.2
3	L	125	THR	5.0
3	L	149	ILE	5.0
3	L	183	ASP	5.0
2	H	127	TYR	4.9
1	A	984	VAL	4.8
3	L	124	LEU	4.7
1	A	986	PRO	4.5
1	A	1021	GLU	4.4
2	H	133	CYS	4.4
3	L	200	SER	4.4
3	L	1	ASP	4.4

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Mol	Chain	Res	Type	RSRZ
3	L	187	ARG	4.3
3	L	121	SER	4.2
3	L	180	LEU	4.2
2	H	123	ALA	4.1
2	H	195	SER	4.1
3	L	129	ALA	4.1
3	L	122	GLU	4.1
3	L	184	GLU	4.0
3	L	189	ASN	4.0
1	A	923	CYS	3.9
3	L	123	GLN	3.8
2	H	198	ILE	3.8
3	L	202	SER	3.8
1	A	983	ASN	3.7
1	A	1110	SER	3.7
3	L	156	ASN	3.7
3	L	208	PHE	3.7
3	L	186	GLU	3.6
2	H	146	LEU	3.6
2	H	215	ILE	3.6
2	H	126	VAL	3.5
3	L	168	LYS	3.5
2	H	200	CYS	3.5
3	L	209	ASN	3.5
2	H	211	VAL	3.4
2	H	125	SER	3.4
3	L	131	VAL	3.4
3	L	182	LYS	3.4
3	L	188	HIS	3.4
3	L	207	SER	3.3
3	L	152	SER	3.3
2	H	134	GLY	3.2
1	A	925	GLN	3.2
2	H	213	LYS	3.2
2	H	214	LYS	3.2
2	H	149	GLY	3.2
3	L	203	PRO	3.1
3	L	179	THR	3.1
3	L	126	SER	3.1
3	L	192	THR	3.1
1	A	922	ASP	3.1
3	L	154	ARG	3.1

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Mol	Chain	Res	Type	RSRZ
2	H	164	LEU	3.0
2	H	132	VAL	3.0
3	L	155	GLN	3.0
2	H	203	ALA	3.0
3	L	18	LYS	2.9
2	H	210	LYS	2.9
1	A	1082	ASP	2.9
2	H	163	SER	2.9
1	A	1106	HIS	2.9
2	H	196	GLN	2.9
2	H	144	GLY	2.8
2	H	135	ASP	2.8
3	L	178	LEU	2.8
2	H	212	ASP	2.8
2	H	199	THR	2.8
3	L	120	SER	2.7
1	A	1081	GLY	2.7
3	L	127	GLY	2.6
2	H	189	THR	2.6
1	A	963	ARG	2.6
2	H	130	ALA	2.6
2	H	1	GLN	2.5
3	L	117	PHE	2.5
3	L	150	ASP	2.5
3	L	23	CYS	2.4
2	H	218	ARG	2.4
2	H	208	SER	2.4
2	H	188	VAL	2.4
2	H	176	GLN	2.4
2	H	166	SER	2.4
2	H	209	THR	2.4
1	A	1050	ASP	2.3
2	H	124	PRO	2.3
1	A	924	SER	2.3
1	A	1109	CYS	2.3
2	H	122	THR	2.3
3	L	153	GLU	2.3
3	L	197	HIS	2.3
1	A	1028	GLY	2.2
3	L	142	ASP	2.2
2	H	177	SER	2.2
1	A	1027	PRO	2.2

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Mol	Chain	Res	Type	RSRZ
2	H	158	THR	2.1
3	L	130	SER	2.1
1	A	1056	ARG	2.1
2	H	182	LEU	2.1
2	H	202	VAL	2.1
1	A	1108	LEU	2.1
2	H	201	ASN	2.1
2	H	62	GLU	2.0
2	H	145	CYS	2.0
2	H	157	LEU	2.0
2	H	178	ASP	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($\text{\AA}^2$)	Q<0.9
6	GOL	H	1004	6/6	0.83	0.13	41,42,43,43	0
5	SO4	L	1003	5/5	0.89	0.20	38,39,40,40	0
4	ACY	A	1112	4/4	0.93	0.13	35,35,35,35	0
5	SO4	H	1002	5/5	0.95	0.16	29,30,33,33	0

6.5 Other polymers [i](#)

There are no such residues in this entry.