



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 06:47 PM UTC

PDB ID : 6FG1 / pdb_00006fg1
Title : CRYSTAL STRUCTURE OF FAB OF NATALIZUMAB IN COMPLEX
WITH FAB OF NAA32.
Authors : Bertrand, T.; Pouzieux, S.
Deposited on : 2018-01-09
Resolution : 2.03 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

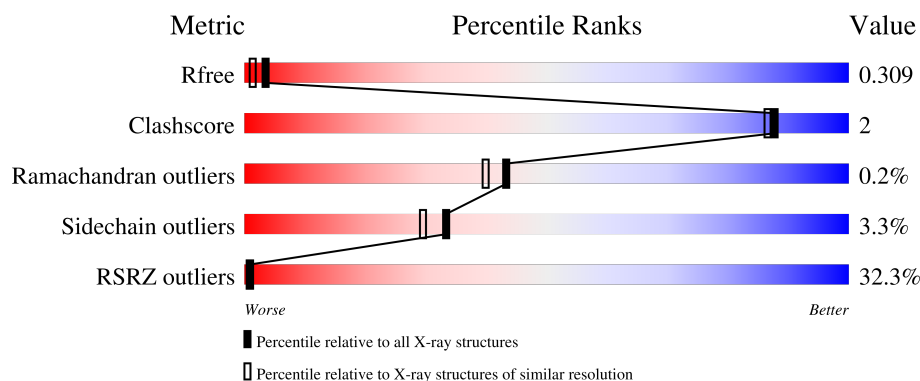
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.03 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	13299 (2.04-2.00)
Clashscore	190562	1022 (2.02-2.02)
Ramachandran outliers	187476	1014 (2.02-2.02)
Sidechain outliers	187428	1014 (2.02-2.02)
RSRZ outliers	180081	13314 (2.04-2.00)

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	241	27% 88%10%.
2	D	215	67% 88%11%.
3	H	234	21% 87%6%7%
4	L	213	12% 92%6%..

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 6993 atoms, of which 8 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 HEAVY CHAIN OF FAB NAA32.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	236	Total	C	N	O	S	0	0	0
			1790	1128	306	348	8			

- Molecule 2 is a protein called LIGHT CHAIN OF FAB NAA32.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	D	213	Total	C	N	O	S	0	0	0
			1627	1018	276	328	5			

- Molecule 3 is a protein called HEAVY CHAIN OF FAB NATALIZUMAB.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	H	218	Total	C	N	O	S	0	0	0
			1656	1045	276	327	8			

- Molecule 4 is a protein called LIGHT CHAIN OF FAB NATALIZUMAB.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	L	211	Total	C	N	O	S	0	0	0
			1641	1029	276	330	6			

- Molecule 5 is GLYCEROL (CCD ID: GOL) (formula: C₃H₈O₃).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	H	1	Total C O 6 3 3	0	0
5	H	1	Total C H O 14 3 8 3	0	0
5	L	1	Total C O 6 3 3	0	0

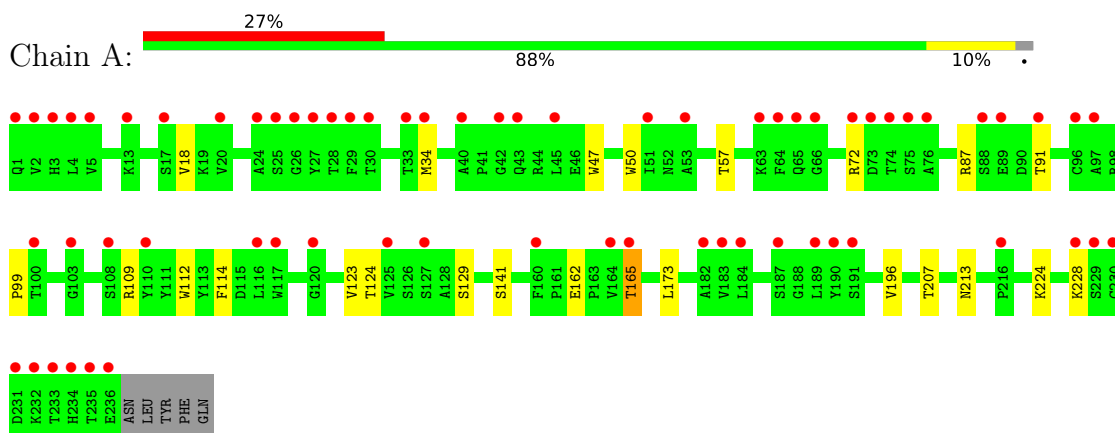
- Molecule 6 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	65	Total O 65 65	0	0
6	D	34	Total O 34 34	0	0
6	H	69	Total O 69 69	0	0
6	L	85	Total O 85 85	0	0

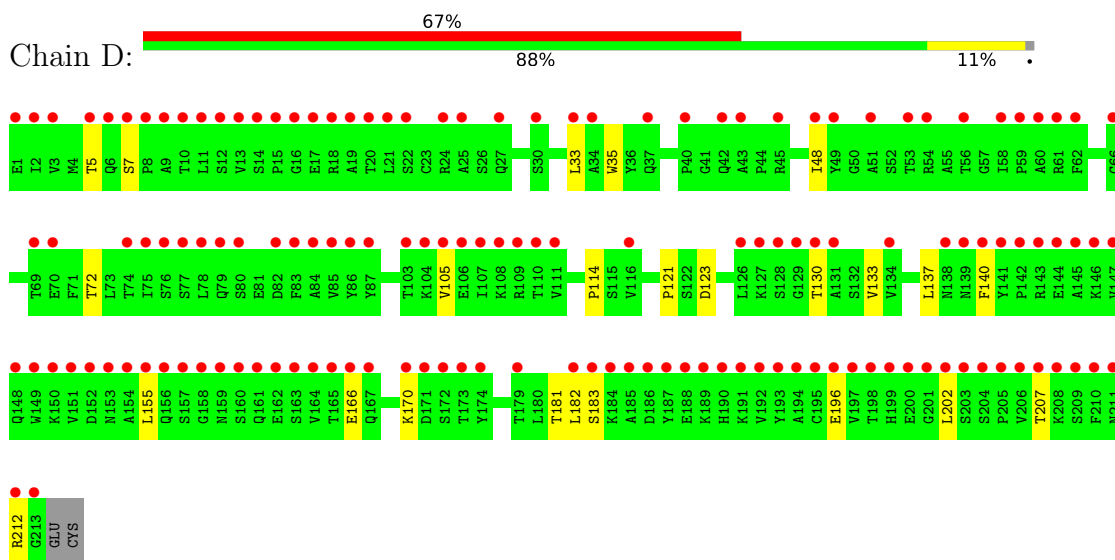
3 Residue-property plots

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.

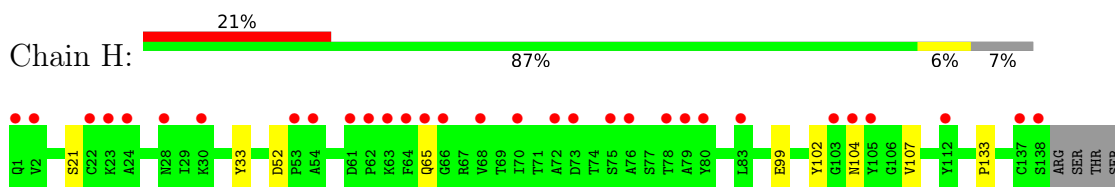
• Molecule 1: HEAVY CHAIN OF FAB NAA32

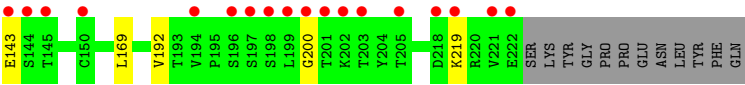


• Molecule 2: LIGHT CHAIN OF FAB NAA32

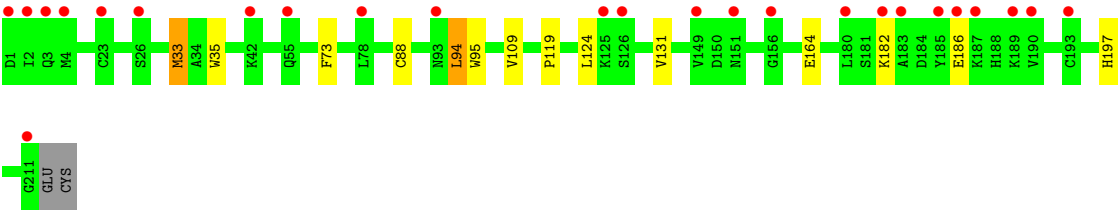


• Molecule 3: HEAVY CHAIN OF FAB NATALIZUMAB





● Molecule 4: LIGHT CHAIN OF FAB NATALIZUMAB



4 Data and refinement statistics

Property	Value	Source
Space group	P 4 21 2	Depositor
Cell constants a, b, c, α , β , γ	189.10Å 189.10Å 87.26Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	87.26 – 2.03 87.26 – 2.03	Depositor EDS
% Data completeness (in resolution range)	59.6 (87.26-2.03) 62.1 (87.26-2.03)	Depositor EDS
R_{merge}	0.13	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.41 (at 2.00Å)	Xtriage
Refinement program	BUSTER 2.11.7	Depositor
R, R_{free}	0.266 , 0.285 0.280 , 0.309	Depositor DCC
R_{free} test set	3195 reflections (5.03%)	wwPDB-VP
Wilson B-factor (Å ²)	35.2	Xtriage
Anisotropy	0.030	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 43.0	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	0.89	EDS
Total number of atoms	6993	wwPDB-VP
Average B, all atoms (Å ²)	39.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.09% 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

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	0.68	0/1838	1.17	0/2504
2	D	0.71	0/1663	1.17	4/2261 (0.2%)
3	H	0.68	0/1696	1.09	3/2309 (0.1%)
4	L	0.76	1/1678 (0.1%)	1.09	3/2280 (0.1%)
All	All	0.71	1/6875 (0.0%)	1.13	10/9354 (0.1%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	L	33	MET	SD-CE	-8.00	1.59	1.79

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	L	164	GLU	N-CA-C	-6.22	102.76	110.41
4	L	197	HIS	CA-C-N	6.09	128.72	120.38
4	L	197	HIS	C-N-CA	6.09	128.72	120.38
3	H	102	TYR	CA-C-N	5.61	126.31	120.03
3	H	102	TYR	C-N-CA	5.61	126.31	120.03
2	D	202	LEU	CA-C-N	5.34	129.68	121.19
2	D	202	LEU	C-N-CA	5.34	129.68	121.19
3	H	52	ASP	N-CA-C	-5.21	99.31	108.69
2	D	123	ASP	CA-C-N	5.18	127.22	120.28
2	D	123	ASP	C-N-CA	5.18	127.22	120.28

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	1790	0	1749	9	0
2	D	1627	0	1583	6	0
3	H	1656	0	1609	4	0
4	L	1641	0	1597	9	0
5	H	12	8	16	0	0
5	L	6	0	8	0	0
6	A	65	0	0	0	0
6	D	34	0	0	1	0
6	H	69	0	0	0	0
6	L	85	0	0	0	0
All	All	6985	8	6562	27	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 (27) 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)
4:L:33:MET:HE1	4:L:88:CYS:HB2	1.26	1.11
1:A:165:THR:HG23	1:A:213:ASN:HB3	1.74	0.68
4:L:33:MET:CE	4:L:88:CYS:HB2	2.16	0.60
3:H:169:LEU:HD21	3:H:192:VAL:HG21	1.87	0.56
1:A:47:TRP:HZ2	1:A:50:TRP:HE3	1.57	0.53
3:H:133:PRO:HD3	3:H:219:LYS:HE2	1.92	0.52
1:A:173:LEU:HD21	1:A:196:VAL:HG21	1.91	0.51
4:L:35:TRP:CZ3	4:L:88:CYS:HB3	2.48	0.49
1:A:91:THR:HG23	1:A:124:THR:HA	1.95	0.48
2:D:121:PRO:HD3	2:D:133:VAL:HG22	1.95	0.47
1:A:18:VAL:HG11	1:A:123:VAL:HG11	1.97	0.46
2:D:196:GLU:HG2	2:D:207:THR:HG22	1.96	0.46
1:A:57:THR:HG21	3:H:107:VAL:HG13	1.97	0.46
4:L:35:TRP:CE2	4:L:73:PHE:HB2	2.50	0.46
4:L:124:LEU:O	4:L:182:LYS:HD3	2.16	0.45
2:D:105:VAL:HB	6:D:301:HOH:O	2.16	0.45
2:D:182:LEU:HB3	2:D:183:SER:H	1.67	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:141:SER:HB3	1:A:228:LYS:HB2	1.98	0.44
1:A:99:PRO:HA	1:A:114:PHE:HA	2.00	0.43
2:D:114:PRO:HB3	2:D:140:PHE:HB3	2.01	0.43
4:L:35:TRP:CD2	4:L:73:PHE:HB2	2.54	0.43
2:D:35:TRP:HB2	2:D:48:ILE:HB	2.00	0.42
1:A:207:THR:HG23	1:A:224:LYS:HE2	2.01	0.42
4:L:94:LEU:C	4:L:95:TRP:CD1	2.98	0.42
4:L:94:LEU:HB3	4:L:95:TRP:H	1.74	0.41
3:H:33:TYR:HB2	3:H:99:GLU:HB3	2.02	0.41
4:L:119:PRO:HD3	4:L:131:VAL:HG22	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	234/241 (97%)	227 (97%)	7 (3%)	0	100	100
2	D	211/215 (98%)	196 (93%)	14 (7%)	1 (0%)	24	17
3	H	214/234 (92%)	207 (97%)	6 (3%)	1 (0%)	24	17
4	L	209/213 (98%)	204 (98%)	5 (2%)	0	100	100
All	All	868/903 (96%)	834 (96%)	32 (4%)	2 (0%)	43	40

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	D	212	ARG
3	H	200	GLY

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	200/205 (98%)	192 (96%)	8 (4%)	28	22
2	D	183/185 (99%)	173 (94%)	10 (6%)	19	12
3	H	183/198 (92%)	179 (98%)	4 (2%)	45	45
4	L	187/189 (99%)	184 (98%)	3 (2%)	55	56
All	All	753/777 (97%)	728 (97%)	25 (3%)	33	29

All (25) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	34	MET
1	A	72	ARG
1	A	87	ARG
1	A	109	ARG
1	A	112	TRP
1	A	129	SER
1	A	162	GLU
1	A	165	THR
2	D	5	THR
2	D	7	SER
2	D	33	LEU
2	D	72	THR
2	D	130	THR
2	D	137	LEU
2	D	155	LEU
2	D	166	GLU
2	D	170	LYS
2	D	181	THR
3	H	21	SER
3	H	65	GLN
3	H	104	ASN
3	H	143	GLU
4	L	94	LEU
4	L	109	VAL
4	L	186	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	55	HIS
2	D	32	ASN
2	D	190	HIS
4	L	3	GLN
4	L	159	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](#)

3 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	$\# Z > 2$
5	GOL	L	301	-	5,5,5	0.16	0	5,5,5	0.84	0
5	GOL	H	302	-	5,5,5	0.08	0	5,5,5	0.14	0
5	GOL	H	301	-	5,5,5	0.16	0	5,5,5	0.67	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
5	GOL	L	301	-	-	0/4/4/4	-
5	GOL	H	302	-	-	0/4/4/4	-
5	GOL	H	301	-	-	0/4/4/4	-

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.

No monomer is involved in short contacts.

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	236/241 (97%)	1.37	66 (27%) 1 1	15, 37, 62, 86	0
2	D	213/215 (99%)	2.70	144 (67%) 0 0	28, 51, 76, 82	0
3	H	218/234 (93%)	1.05	49 (22%) 2 2	16, 33, 63, 83	0
4	L	211/213 (99%)	0.70	25 (11%) 9 8	12, 28, 55, 67	0
All	All	878/903 (97%)	1.45	284 (32%) 1 1	12, 37, 67, 86	0

All (284) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	D	185	ALA	8.0
2	D	11	LEU	7.0
2	D	213	GLY	7.0
2	D	202	LEU	6.9
2	D	184	LYS	6.4
2	D	159	ASN	6.4
4	L	2	ILE	6.3
1	A	232	LYS	6.2
3	H	138	SER	5.6
4	L	211	GLY	5.5
2	D	205	PRO	5.5
2	D	206	VAL	5.4
2	D	207	THR	5.2
2	D	16	GLY	5.2
2	D	129	GLY	5.0
2	D	10	THR	4.9
1	A	235	THR	4.9
2	D	7	SER	4.9
2	D	141	TYR	4.9
2	D	156	GLN	4.9
2	D	201	GLY	4.9

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Mol	Chain	Res	Type	RSRZ
1	A	184	LEU	4.8
2	D	157	SER	4.7
2	D	150	LYS	4.6
2	D	13	VAL	4.6
2	D	170	LYS	4.6
2	D	83	PHE	4.5
1	A	42	GLY	4.4
1	A	183	VAL	4.3
2	D	158	GLY	4.3
1	A	65	GLN	4.3
2	D	8	PRO	4.3
1	A	3	HIS	4.3
2	D	75	ILE	4.3
2	D	9	ALA	4.2
2	D	24	ARG	4.2
2	D	108	LYS	4.2
2	D	196	GLU	4.2
2	D	204	SER	4.2
4	L	189	LYS	4.2
2	D	200	GLU	4.1
2	D	155	LEU	4.0
1	A	2	VAL	4.0
2	D	203	SER	4.0
2	D	105	VAL	4.0
2	D	148	GLN	4.0
2	D	78	LEU	4.0
3	H	199	LEU	3.9
2	D	58	ILE	3.9
2	D	145	ALA	3.9
2	D	18	ARG	3.9
1	A	228	LYS	3.9
3	H	68	VAL	3.8
2	D	188	GLU	3.8
2	D	189	LYS	3.8
2	D	182	LEU	3.8
2	D	15	PRO	3.8
2	D	192	VAL	3.8
2	D	198	THR	3.8
2	D	126	LEU	3.8
2	D	208	LYS	3.8
1	A	4	LEU	3.7
2	D	183	SER	3.7

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Mol	Chain	Res	Type	RSRZ
2	D	107	ILE	3.7
2	D	84	ALA	3.7
2	D	62	PHE	3.7
2	D	187	TYR	3.7
4	L	187	LYS	3.7
2	D	138	ASN	3.7
3	H	2	VAL	3.7
3	H	197	SER	3.7
2	D	146	LYS	3.7
2	D	186	ASP	3.7
1	A	33	THR	3.7
2	D	193	TYR	3.7
2	D	77	SER	3.6
2	D	80	SER	3.6
2	D	82	ASP	3.6
2	D	151	VAL	3.6
1	A	233	THR	3.6
2	D	19	ALA	3.6
4	L	125	LYS	3.6
3	H	66	GLY	3.6
3	H	1	GLN	3.6
2	D	140	PHE	3.5
3	H	143	GLU	3.5
2	D	79	GLN	3.5
2	D	143	ARG	3.5
4	L	186	GLU	3.5
1	A	28	THR	3.5
2	D	56	THR	3.5
3	H	112	TYR	3.5
3	H	64	PHE	3.5
1	A	230	CYS	3.5
2	D	197	VAL	3.4
1	A	229	SER	3.4
3	H	202	LYS	3.4
2	D	49	TYR	3.4
3	H	75	SER	3.4
3	H	222	GLU	3.4
2	D	164	VAL	3.4
3	H	65	GLN	3.4
1	A	231	ASP	3.3
1	A	236	GLU	3.3
3	H	203	THR	3.3

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Mol	Chain	Res	Type	RSRZ
2	D	111	VAL	3.3
2	D	174	TYR	3.3
2	D	48	ILE	3.3
2	D	17	GLU	3.3
2	D	27	GLN	3.2
2	D	21	LEU	3.2
1	A	29	PHE	3.2
2	D	149	TRP	3.1
2	D	43	ALA	3.1
2	D	194	ALA	3.1
1	A	165	THR	3.1
3	H	201	THR	3.1
1	A	20	VAL	3.1
3	H	30	LYS	3.1
2	D	139	ASN	3.0
1	A	116	LEU	3.0
1	A	125	VAL	3.0
2	D	147	VAL	3.0
4	L	190	VAL	3.0
4	L	3	GLN	3.0
2	D	211	ASN	3.0
2	D	70	GLU	3.0
3	H	23	LYS	3.0
1	A	97	ALA	3.0
3	H	54	ALA	3.0
2	D	12	SER	3.0
4	L	180	LEU	3.0
2	D	69	THR	3.0
3	H	218	ASP	3.0
4	L	1	ASP	3.0
1	A	234	HIS	3.0
2	D	199	HIS	3.0
3	H	150	CYS	2.9
1	A	75	SER	2.9
2	D	142	PRO	2.9
2	D	45	ARG	2.9
1	A	182	ALA	2.9
2	D	152	ASP	2.9
1	A	30	THR	2.9
2	D	53	THR	2.9
1	A	64	PHE	2.9
2	D	154	ALA	2.9

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Mol	Chain	Res	Type	RSRZ
2	D	20	THR	2.8
2	D	40	PRO	2.8
2	D	144	GLU	2.8
3	H	219	LYS	2.8
2	D	22	SER	2.8
1	A	1	GLN	2.8
2	D	60	ALA	2.8
2	D	3	VAL	2.8
2	D	163	SER	2.8
3	H	198	SER	2.8
1	A	103	GLY	2.8
1	A	40	ALA	2.8
2	D	127	LYS	2.8
2	D	190	HIS	2.8
3	H	200	GLY	2.8
3	H	83	LEU	2.8
1	A	63	LYS	2.8
3	H	62	PRO	2.8
2	D	76	SER	2.7
1	A	27	TYR	2.7
3	H	105	TYR	2.7
1	A	96	CYS	2.7
2	D	166	GLU	2.7
3	H	72	ALA	2.7
2	D	1	GLU	2.7
2	D	74	THR	2.7
2	D	160	SER	2.7
2	D	209	SER	2.7
4	L	23	CYS	2.7
2	D	212	ARG	2.7
3	H	103	GLY	2.6
1	A	53	ALA	2.6
3	H	61	ASP	2.6
2	D	61	ARG	2.6
1	A	13	LYS	2.6
2	D	191	LYS	2.6
2	D	162	GLU	2.6
2	D	130	THR	2.6
2	D	161	GLN	2.5
3	H	78	THR	2.5
3	H	144	SER	2.5
1	A	164	VAL	2.5

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Mol	Chain	Res	Type	RSRZ
4	L	126	SER	2.5
3	H	63	LYS	2.5
4	L	42	LYS	2.5
3	H	137	CYS	2.5
1	A	74	THR	2.5
1	A	88	SER	2.5
1	A	45	LEU	2.5
2	D	104	LYS	2.5
2	D	109	ARG	2.5
2	D	153	ASN	2.5
2	D	6	GLN	2.4
2	D	171	ASP	2.4
2	D	59	PRO	2.4
3	H	104	ASN	2.4
2	D	165	THR	2.4
3	H	53	PRO	2.4
2	D	86	TYR	2.4
2	D	25	ALA	2.4
3	H	24	ALA	2.4
1	A	66	GLY	2.4
2	D	116	VAL	2.4
1	A	108	SER	2.4
1	A	187	SER	2.4
2	D	14	SER	2.4
2	D	134	VAL	2.3
4	L	193	CYS	2.3
1	A	26	GLY	2.3
4	L	156	GLY	2.3
1	A	24	ALA	2.3
1	A	73	ASP	2.3
1	A	120	GLY	2.3
1	A	191	SER	2.3
2	D	210	PHE	2.3
1	A	51	ILE	2.3
2	D	2	ILE	2.3
3	H	205	THR	2.3
2	D	51	ALA	2.3
2	D	33	LEU	2.3
1	A	89	GLU	2.2
2	D	172	SER	2.2
3	H	196	SER	2.2
1	A	76	ALA	2.2

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Mol	Chain	Res	Type	RSRZ
2	D	34	ALA	2.2
2	D	66	GLY	2.2
2	D	131	ALA	2.2
3	H	79	ALA	2.2
4	L	55	GLN	2.2
2	D	54	ARG	2.2
3	H	76	ALA	2.2
3	H	22	CYS	2.2
2	D	42	GLN	2.2
1	A	110	TYR	2.2
1	A	190	TYR	2.2
2	D	128	SER	2.2
2	D	110	THR	2.2
3	H	145	THR	2.2
4	L	183	ALA	2.2
1	A	25	SER	2.2
4	L	26	SER	2.2
3	H	80	TYR	2.2
3	H	28	ASN	2.2
2	D	179	THR	2.2
1	A	72	ARG	2.1
1	A	17	SER	2.1
1	A	127	SER	2.1
2	D	87	TYR	2.1
2	D	5	THR	2.1
1	A	43	GLN	2.1
1	A	160	PHE	2.1
3	H	221	VAL	2.1
4	L	149	VAL	2.1
1	A	34	MET	2.1
4	L	4	MET	2.1
4	L	151	ASN	2.1
1	A	5	VAL	2.1
2	D	106	GLU	2.1
2	D	195	CYS	2.1
4	L	93	ASN	2.1
3	H	73	ASP	2.1
1	A	100	THR	2.1
2	D	173	THR	2.1
4	L	185	TYR	2.1
3	H	70	ILE	2.1
2	D	30	SER	2.1

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Mol	Chain	Res	Type	RSRZ
4	L	78	LEU	2.0
2	D	37	GLN	2.0
2	D	167	GLN	2.0
1	A	91	THR	2.0
2	D	85	VAL	2.0
3	H	194	VAL	2.0
1	A	117	TRP	2.0
1	A	189	LEU	2.0
4	L	182	LYS	2.0
1	A	216	PRO	2.0
2	D	103	THR	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
5	GOL	H	302	6/6	0.77	0.23	61,62,65,65	0
5	GOL	L	301	6/6	0.83	0.18	32,33,37,41	0
5	GOL	H	301	6/6	0.88	0.12	24,26,28,30	0

6.5 Other polymers [i](#)

There are no such residues in this entry.