



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 05:32 PM UTC

PDB ID : 8TFT / pdb_00008tft
Title : Fab of O13-1 human IgG1 antibody bound to IgV domain of human TIM-3
Authors : Oganessian, V.Y.; van Dyk, N.; Mazor, Y.; Yang, C.
Deposited on : 2023-07-11
Resolution : 2.30 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

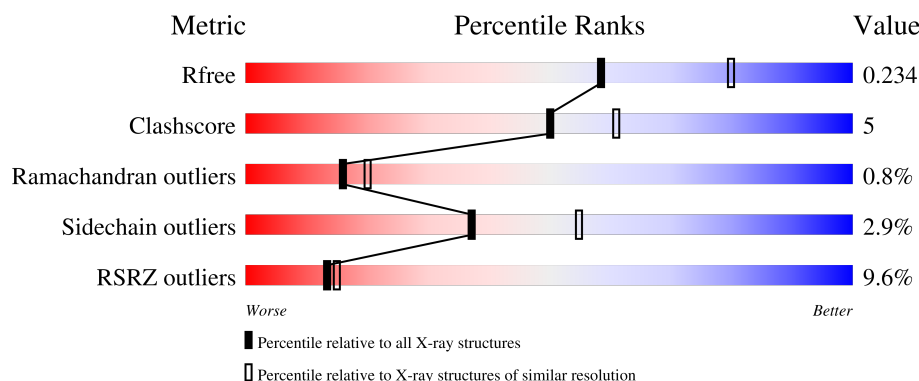
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.30 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	6319 (2.30-2.30)
Clashscore	190562	6919 (2.30-2.30)
Ramachandran outliers	187476	6854 (2.30-2.30)
Sidechain outliers	187428	6854 (2.30-2.30)
RSRZ outliers	180081	6325 (2.30-2.30)

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	H	227	11% 86% 12% ..
1	I	227	5% 90% 8% ..
2	L	213	15% 88% 11% .
2	M	213	3% 93% 6% .
3	F	109	17% 73% 21% 5% .

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Mol	Chain	Length	Quality of chain
3	G	109	12% 81% 17%

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 8313 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 O-13-1 IgG1 Fab heavy chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	I	224	Total	C	N	O	S	0	0	0
			1666	1050	278	332	6			
1	H	224	Total	C	N	O	S	0	0	0
			1666	1050	278	332	6			

- Molecule 2 is a protein called O-13-1 IgG1 Fab light chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	M	211	Total	C	N	O	S	0	0	0
			1592	998	272	318	4			
2	L	213	Total	C	N	O	S	0	0	0
			1608	1006	274	323	5			

- Molecule 3 is a protein called T-cell immunoglobulin mucin receptor 3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	F	109	Total	C	N	O	S	0	0	0
			863	550	145	161	7			
3	G	109	Total	C	N	O	S	0	0	0
			863	550	145	161	7			

- Molecule 4 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula: C₈H₁₅NO₆).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	F	1	Total	C	N	O	0	0
			14	8	1	5		
4	G	1	Total	C	N	O	0	0
			14	8	1	5		

- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	I	7	Total	O	0	0
			7	7		
5	F	3	Total	O	0	0
			3	3		
5	H	9	Total	O	0	0
			9	9		
5	L	1	Total	O	0	0
			1	1		
5	G	7	Total	O	0	0
			7	7		

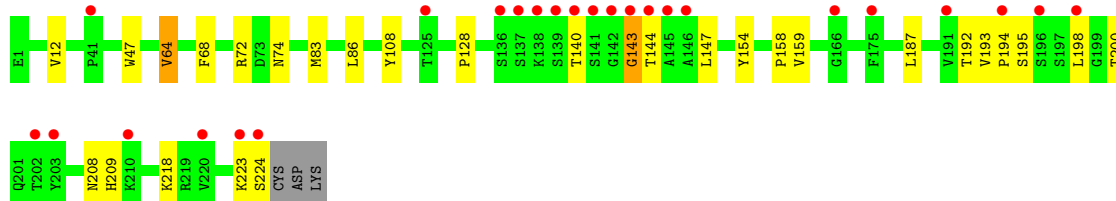
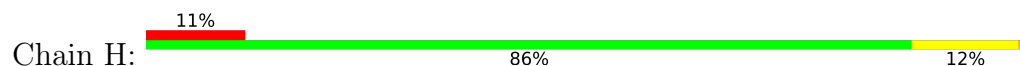
3 Residue-property plots [i](#)

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.

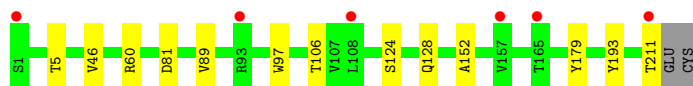
- Molecule 1: O-13-1 IgG1 Fab heavy chain



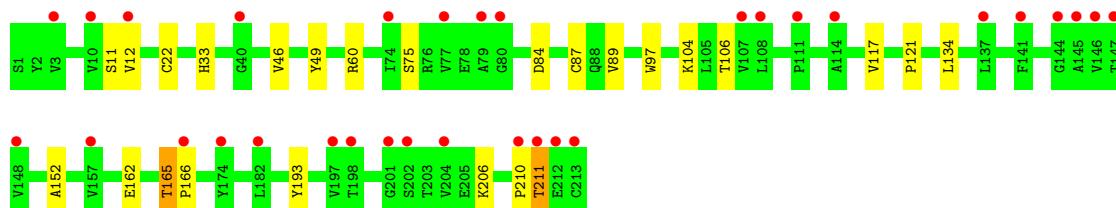
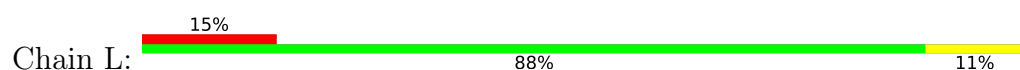
- Molecule 1: O-13-1 IgG1 Fab heavy chain



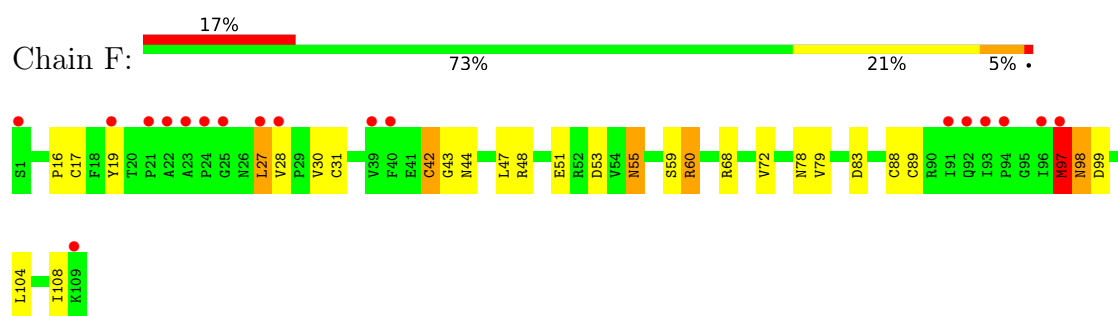
- Molecule 2: O-13-1 IgG1 Fab light chain



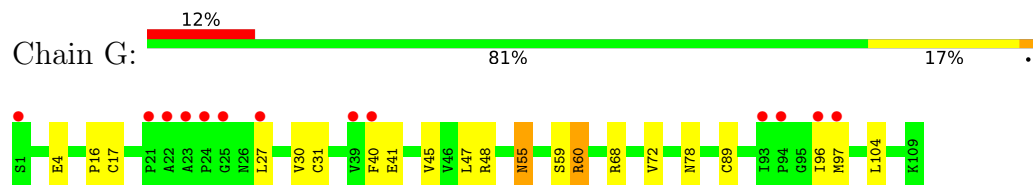
- Molecule 2: O-13-1 IgG1 Fab light chain



- Molecule 3: T-cell immunoglobulin mucin receptor 3



- Molecule 3: T-cell immunoglobulin mucin receptor 3



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	218.34Å 69.78Å 93.63Å 90.00° 99.90° 90.00°	Depositor
Resolution (Å)	37.00 – 2.30 37.00 – 2.30	Depositor EDS
% Data completeness (in resolution range)	98.2 (37.00-2.30) 98.2 (37.00-2.30)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.28 (at 2.20Å)	Xtriage
Refinement program	REFMAC 5.8.0415	Depositor
R, R_{free}	0.244 , 0.271 (Not available) , 0.234	Depositor DCC
R_{free} test set	1361 reflections (1.92%)	wwPDB-VP
Wilson B-factor (Å ²)	52.3	Xtriage
Anisotropy	0.058	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 28.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	8313	wwPDB-VP
Average B, all atoms (Å ²)	61.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 27.96 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 2.0037e-03. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

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: NAG

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	H	0.51	0/1707	0.79	0/2323
1	I	0.50	0/1707	0.79	0/2323
2	L	0.50	0/1649	0.78	0/2251
2	M	0.50	0/1633	0.79	0/2231
3	F	0.47	0/884	0.76	0/1202
3	G	0.46	0/884	0.81	0/1202
All	All	0.49	0/8464	0.78	0/11532

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	H	1666	0	1615	21	0
1	I	1666	0	1615	12	0
2	L	1608	0	1560	13	0
2	M	1592	0	1549	10	0
3	F	863	0	835	21	0
3	G	863	0	837	15	0
4	F	14	0	13	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	G	14	0	13	1	0
5	F	3	0	0	0	0
5	G	7	0	0	0	0
5	H	9	0	0	0	0
5	I	7	0	0	0	0
5	L	1	0	0	0	0
All	All	8313	0	8037	82	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 5.

All (82) 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:G:30:VAL:HG11	3:G:72:VAL:HG11	1.31	1.11
3:F:30:VAL:HG11	3:F:72:VAL:HG11	1.33	1.04
2:M:5:THR:HG21	3:G:40:PHE:O	1.67	0.94
2:L:210:PRO:O	2:L:211:THR:HG23	1.83	0.79
3:F:27:LEU:HD22	3:F:68:ARG:HD2	1.70	0.72
3:F:27:LEU:HD23	3:F:51:GLU:O	1.94	0.68
1:H:144:THR:HG23	1:H:192:THR:CG2	2.25	0.67
3:G:55:ASN:HD22	3:G:55:ASN:C	2.05	0.64
3:F:55:ASN:C	3:F:55:ASN:HD22	2.05	0.63
2:M:5:THR:CG2	3:G:41:GLU:HB3	2.31	0.60
2:M:124:SER:O	2:M:128:GLN:HG2	2.01	0.59
3:F:27:LEU:HG	3:F:28:VAL:N	2.16	0.59
1:I:187:LEU:C	1:I:187:LEU:HD12	2.27	0.58
3:F:30:VAL:HG11	3:F:72:VAL:CG1	2.22	0.58
1:H:187:LEU:C	1:H:187:LEU:HD12	2.29	0.57
2:M:5:THR:HG23	3:G:41:GLU:HB3	1.86	0.56
2:L:60:ARG:HD2	2:L:75:SER:O	2.05	0.56
3:F:27:LEU:HD22	3:F:68:ARG:CD	2.37	0.54
1:H:193:VAL:HG22	1:H:194:PRO:HD2	1.89	0.54
1:I:83:MET:HB3	1:I:86:LEU:HD21	1.89	0.53
1:I:193:VAL:HG22	1:I:194:PRO:HD2	1.91	0.53
3:G:27:LEU:HD22	3:G:68:ARG:HD2	1.91	0.52
1:H:72:ARG:CD	1:H:74:ASN:HD21	2.22	0.51
1:H:154:TYR:CE2	1:H:159:VAL:HG23	2.46	0.51
3:F:97:MET:O	3:F:99:ASP:N	2.42	0.51
3:F:47:LEU:HD23	3:F:48:ARG:N	2.26	0.50
1:H:223:LYS:O	1:H:224:SER:C	2.55	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:G:31:CYS:HB3	3:G:48:ARG:HG3	1.93	0.50
3:F:19:TYR:C	3:F:19:TYR:CD1	2.89	0.50
1:H:83:MET:HB3	1:H:86:LEU:HD21	1.93	0.50
2:M:60:ARG:NH2	2:M:81:ASP:OD2	2.36	0.50
2:L:165:THR:HG22	2:L:166:PRO:HD2	1.93	0.49
1:I:223:LYS:O	1:I:224:SER:C	2.55	0.49
3:G:47:LEU:HD23	3:G:48:ARG:N	2.27	0.49
3:F:42:CYS:HB3	3:F:88:CYS:SG	2.53	0.49
2:L:121:PRO:HA	2:L:134:LEU:HD23	1.95	0.49
1:H:72:ARG:HD3	1:H:74:ASN:ND2	2.28	0.48
2:L:84:ASP:OD1	2:L:104:LYS:HG2	2.14	0.48
1:H:47:TRP:CG	2:L:97:TRP:HB2	2.49	0.47
3:F:79:VAL:HG21	3:F:108:ILE:CD1	2.44	0.47
3:F:17:CYS:CB	3:F:89:CYS:SG	3.03	0.47
1:H:72:ARG:HD3	1:H:74:ASN:HD21	1.80	0.47
3:F:19:TYR:OH	3:F:27:LEU:HD12	2.15	0.46
1:H:147:LEU:C	1:H:147:LEU:HD12	2.41	0.46
1:H:198:LEU:C	1:H:200:THR:H	2.23	0.46
1:H:144:THR:HG23	1:H:192:THR:HG22	1.97	0.45
3:G:17:CYS:CB	3:G:89:CYS:SG	3.04	0.45
1:I:195:SER:HA	1:I:198:LEU:HD13	1.98	0.45
2:M:5:THR:CG2	3:G:41:GLU:CB	2.95	0.45
3:F:79:VAL:CG2	3:F:83:ASP:HB2	2.47	0.45
2:L:165:THR:HG22	2:L:166:PRO:CD	2.47	0.45
2:L:11:SER:O	2:L:12:VAL:HG23	2.16	0.45
1:I:147:LEU:C	1:I:147:LEU:HD12	2.42	0.44
1:I:178:VAL:HG21	2:M:179:TYR:CD1	2.52	0.44
3:G:59:SER:O	3:G:60:ARG:HB2	2.18	0.44
3:F:31:CYS:HB3	3:F:48:ARG:HG3	1.99	0.44
1:H:72:ARG:CD	1:H:74:ASN:ND2	2.80	0.44
1:H:64:VAL:HG13	1:H:68:PHE:HB2	2.00	0.44
3:F:27:LEU:HD23	3:F:51:GLU:C	2.42	0.44
1:I:47:TRP:CG	2:M:97:TRP:HB2	2.53	0.44
1:H:64:VAL:HG13	1:H:68:PHE:CG	2.53	0.44
3:F:78:ASN:HD21	4:F:201:NAG:C1	2.31	0.43
3:F:16:PRO:HD2	3:F:104:LEU:HD22	2.00	0.43
1:I:143:GLY:O	1:I:195:SER:N	2.51	0.43
2:M:5:THR:HG21	3:G:40:PHE:C	2.42	0.42
1:H:143:GLY:O	1:H:195:SER:N	2.52	0.42
2:L:22:CYS:SG	2:L:87:CYS:CB	3.08	0.42
2:L:117:VAL:O	2:L:206:LYS:HE3	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:108:TYR:HB3	2:L:33:HIS:CE1	2.54	0.42
1:H:208:ASN:HD22	1:H:209:HIS:N	2.18	0.42
1:H:12:VAL:HG11	1:H:86:LEU:HD13	2.02	0.41
1:I:12:VAL:HG11	1:I:86:LEU:HD13	2.02	0.41
3:F:98:ASN:O	3:F:99:ASP:C	2.62	0.41
1:I:52:SER:O	1:I:72:ARG:NH1	2.53	0.41
1:H:128:PRO:HB3	1:H:154:TYR:HB3	2.01	0.41
2:L:49:TYR:CG	3:G:68:ARG:HG3	2.55	0.41
2:M:152:ALA:HB2	2:M:193:TYR:CE2	2.55	0.41
3:G:16:PRO:HD2	3:G:104:LEU:HD22	2.02	0.41
1:I:210:LYS:N	1:I:211:PRO:CD	2.84	0.40
3:G:78:ASN:HD21	4:G:201:NAG:C1	2.35	0.40
3:F:59:SER:O	3:F:60:ARG:HB2	2.21	0.40
2:L:152:ALA:HB2	2:L:193:TYR:CE2	2.57	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	H	222/227 (98%)	213 (96%)	8 (4%)	1 (0%)	24	31
1	I	222/227 (98%)	216 (97%)	6 (3%)	0	100	100
2	L	211/213 (99%)	200 (95%)	10 (5%)	1 (0%)	24	31
2	M	209/213 (98%)	199 (95%)	10 (5%)	0	100	100
3	F	107/109 (98%)	94 (88%)	8 (8%)	5 (5%)	2	1
3	G	107/109 (98%)	97 (91%)	8 (8%)	2 (2%)	6	5
All	All	1078/1098 (98%)	1019 (94%)	50 (5%)	9 (1%)	16	20

All (9) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	G	97	MET
3	F	43	GLY
3	F	44	ASN
1	H	143	GLY
3	F	97	MET
2	L	211	THR
3	F	98	ASN
3	F	60	ARG
3	G	60	ARG

5.3.2 Protein sidechains [i](#)

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	H	184/187 (98%)	180 (98%)	4 (2%)	45	65
1	I	184/187 (98%)	180 (98%)	4 (2%)	45	65
2	L	179/179 (100%)	174 (97%)	5 (3%)	38	56
2	M	177/179 (99%)	173 (98%)	4 (2%)	44	63
3	F	94/94 (100%)	89 (95%)	5 (5%)	20	30
3	G	94/94 (100%)	90 (96%)	4 (4%)	26	39
All	All	912/920 (99%)	886 (97%)	26 (3%)	37	55

All (26) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	I	158	PRO
1	I	178	VAL
1	I	210	LYS
1	I	218	LYS
2	M	46	VAL
2	M	89	VAL
2	M	106	THR
2	M	211	THR
3	F	27	LEU
3	F	42	CYS

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Mol	Chain	Res	Type
3	F	53	ASP
3	F	55	ASN
3	F	97	MET
1	H	64	VAL
1	H	140	THR
1	H	158	PRO
1	H	218	LYS
2	L	46	VAL
2	L	89	VAL
2	L	106	THR
2	L	162	GLU
2	L	165	THR
3	G	4	GLU
3	G	45	VAL
3	G	55	ASN
3	G	96	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (12) such sidechains are listed below:

Mol	Chain	Res	Type
1	I	77	ASN
1	I	180	GLN
1	I	208	ASN
2	M	26	ASN
2	M	172	ASN
2	M	199	HIS
3	F	55	ASN
1	H	74	ASN
1	H	208	ASN
2	L	196	GLN
3	G	55	ASN
3	G	78	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 [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

2 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	NAG	G	201	-	14,14,15	0.43	0	17,19,21	1.78	1 (5%)
4	NAG	F	201	-	14,14,15	0.39	0	17,19,21	0.52	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	NAG	G	201	-	-	3/6/23/26	0/1/1/1
4	NAG	F	201	-	-	2/6/23/26	0/1/1/1

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	G	201	NAG	O5-C1-C2	6.67	121.61	111.29

There are no chirality outliers.

All (5) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	F	201	NAG	C8-C7-N2-C2
4	F	201	NAG	O7-C7-N2-C2

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Mol	Chain	Res	Type	Atoms
4	G	201	NAG	O5-C5-C6-O6
4	G	201	NAG	C4-C5-C6-O6
4	G	201	NAG	O7-C7-N2-C2

There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	G	201	NAG	1	0
4	F	201	NAG	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	H	224/227 (98%)	0.93	25 (11%) 10 11	32, 59, 106, 177	0
1	I	224/227 (98%)	0.55	11 (4%) 35 36	36, 52, 92, 135	0
2	L	213/213 (100%)	1.14	32 (15%) 5 6	40, 69, 95, 129	0
2	M	211/213 (99%)	0.49	6 (2%) 55 57	34, 54, 77, 89	0
3	F	109/109 (100%)	1.00	18 (16%) 4 5	36, 62, 137, 154	0
3	G	109/109 (100%)	0.60	13 (11%) 9 10	29, 45, 112, 143	0
All	All	1090/1098 (99%)	0.78	105 (9%) 13 15	29, 57, 102, 177	0

All (105) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	H	140	THR	6.5
3	F	22	ALA	6.4
1	H	137	SER	5.5
3	G	96	ILE	5.5
1	H	138	LYS	5.3
3	F	28	VAL	5.3
2	M	211	THR	5.1
3	G	23	ALA	5.0
3	G	22	ALA	5.0
3	F	96	ILE	4.9
1	H	139	SER	4.8
3	G	1	SER	4.6
1	H	136	SER	4.5
1	H	145	ALA	4.4
3	F	21	PRO	4.1
1	H	141	SER	4.1
1	I	138	LYS	4.1
1	I	140	THR	4.0
3	G	97	MET	4.0

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Mol	Chain	Res	Type	RSRZ
2	L	145	ALA	4.0
3	F	94	PRO	3.8
3	F	39	VAL	3.8
1	I	137	SER	3.7
3	F	24	PRO	3.7
3	F	93	ILE	3.7
3	F	19	TYR	3.7
3	F	27	LEU	3.6
3	F	25	GLY	3.6
2	L	213	CYS	3.5
1	I	141	SER	3.5
1	H	142	GLY	3.5
1	H	223	LYS	3.4
3	F	97	MET	3.4
1	H	143	GLY	3.4
1	I	200	THR	3.4
1	I	136	SER	3.4
1	I	139	SER	3.3
2	L	174	TYR	3.2
2	L	157	VAL	3.2
3	G	27	LEU	3.0
3	F	23	ALA	3.0
2	L	107	VAL	3.0
1	H	144	THR	3.0
1	H	224	SER	3.0
3	G	40	PHE	2.9
3	G	24	PRO	2.9
2	L	146	VAL	2.9
1	I	224	SER	2.8
1	H	198	LEU	2.7
1	I	223	LYS	2.7
2	L	12	VAL	2.7
3	G	39	VAL	2.7
2	L	10	VAL	2.7
2	L	108	LEU	2.7
1	H	146	ALA	2.6
2	L	79	ALA	2.6
2	L	77	VAL	2.6
2	L	198	THR	2.6
2	L	111	PRO	2.6
2	L	74	ILE	2.6
2	L	211	THR	2.6

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Mol	Chain	Res	Type	RSRZ
3	G	21	PRO	2.6
3	F	1	SER	2.6
2	M	108	LEU	2.5
1	H	194	PRO	2.5
2	L	144	GLY	2.5
2	L	204	VAL	2.4
3	F	92	GLN	2.4
1	H	191	VAL	2.4
3	F	40	PHE	2.4
3	F	109	LYS	2.4
2	L	210	PRO	2.4
2	L	201	GLY	2.4
2	L	137	LEU	2.4
2	L	197	VAL	2.4
2	L	212	GLU	2.4
3	G	94	PRO	2.3
1	H	166	GLY	2.3
2	L	40	GLY	2.3
1	H	202	THR	2.3
1	H	203	TYR	2.3
1	H	125	THR	2.3
2	M	165	THR	2.3
2	L	202	SER	2.3
2	M	93	ARG	2.3
3	G	93	ILE	2.3
1	H	210	LYS	2.3
1	I	181	SER	2.3
2	M	157	VAL	2.2
2	L	166	PRO	2.2
2	M	1	SER	2.2
2	L	3	VAL	2.2
2	L	148	VAL	2.2
2	L	141	PHE	2.2
2	L	80	GLY	2.2
2	L	114	ALA	2.2
1	H	175	PHE	2.1
1	I	142	GLY	2.1
3	G	25	GLY	2.1
3	F	91	ILE	2.1
1	H	41	PRO	2.1
1	H	196	SER	2.0
2	L	147	THR	2.0

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Mol	Chain	Res	Type	RSRZ
2	L	182	LEU	2.0
1	H	220	VAL	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
4	NAG	F	201	14/15	0.51	0.17	94,105,115,117	0
4	NAG	G	201	14/15	0.56	0.16	89,103,107,107	0

6.5 Other polymers [i](#)

There are no such residues in this entry.