



Full wwPDB X-ray Structure Validation Report ⓘ

Jun 11, 2026 – 06:08 PM EDT

PDB ID : 13FJ / pdb_000013fj
Title : TGFB1 IN COMPLEX WITH NIS793 FAB
Authors : Zhou, Z.; Zhu, X.; Clark, K.
Deposited on : 2026-05-04
Resolution : 2.75 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

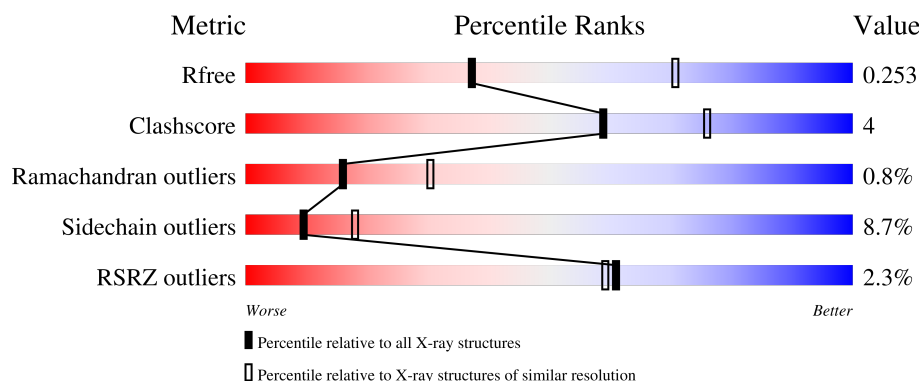
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION


The reported resolution of this entry is 2.75 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	1009 (2.76-2.76)
Clashscore	190562	1044 (2.76-2.76)
Ramachandran outliers	187476	1024 (2.76-2.76)
Sidechain outliers	187428	1024 (2.76-2.76)
RSRZ outliers	180081	1009 (2.76-2.76)

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	112	
1	B	112	
2	H	224	
2	I	224	
3	L	214	

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Mol	Chain	Length	Quality of chain
3	M	214	<div><div></div><div>4%</div><div>81%</div><div>15%</div><div>••</div></div>

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 8336 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 Transforming growth factor beta-1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	112	Total	C	N	O	S	0	0	0
			897	576	152	159	10			
1	B	112	Total	C	N	O	S	0	0	0
			897	576	152	159	10			

- Molecule 2 is a protein called NIS793 Fab heavy chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	H	218	Total	C	N	O	S	0	0	0
			1620	1025	271	317	7			
2	I	218	Total	C	N	O	S	0	0	0
			1617	1024	271	316	6			

- Molecule 3 is a protein called NIS793 Fab light chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	L	213	Total	C	N	O	S	0	0	0
			1600	996	270	329	5			
3	M	211	Total	C	N	O	S	0	0	0
			1585	988	268	325	4			

- Molecule 4 is SULFATE ION (CCD ID: SO4) (formula: O₄S).



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

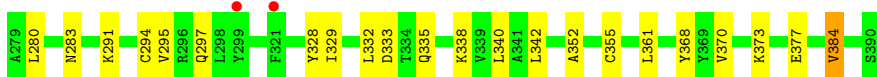
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	12	Total	O	0	0
			12	12		
5	B	7	Total	O	0	0
			7	7		
5	H	14	Total	O	0	0
			14	14		
5	I	29	Total	O	0	0
			29	29		
5	L	18	Total	O	0	0
			18	18		
5	M	15	Total	O	0	0
			15	15		

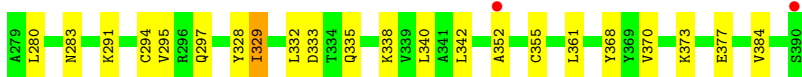
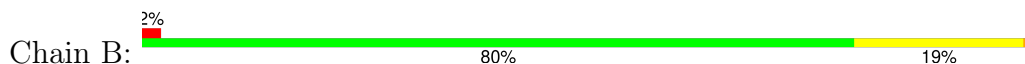
3 Residue-property plots [i](#)

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.

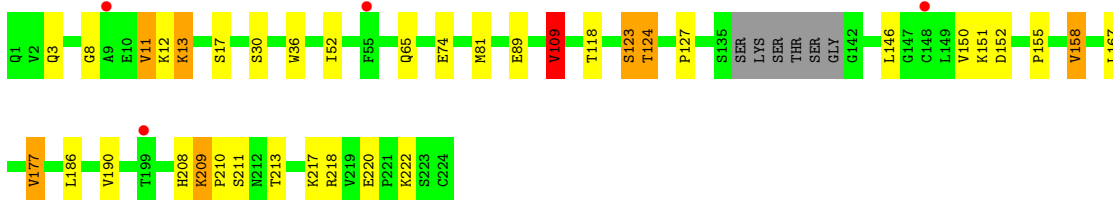
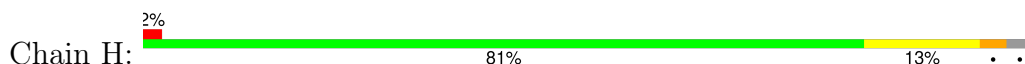
- Molecule 1: Transforming growth factor beta-1



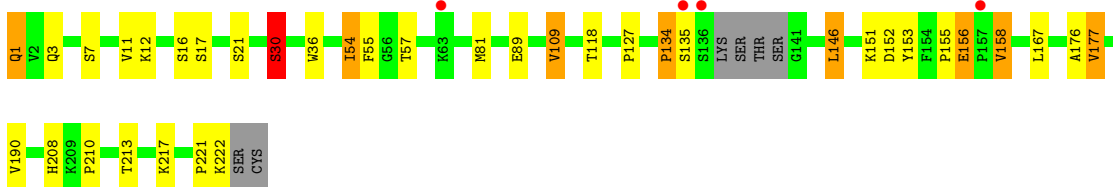
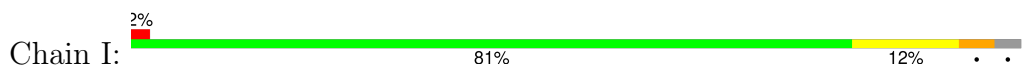
- Molecule 1: Transforming growth factor beta-1



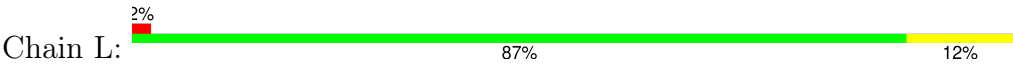
- Molecule 2: NIS793 Fab heavy chain



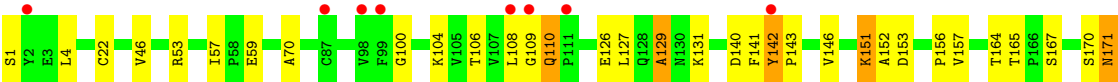
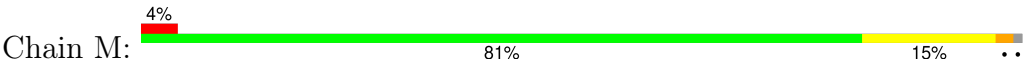
- Molecule 2: NIS793 Fab heavy chain



- Molecule 3: NIS793 Fab light chain



● Molecule 3: NIS793 Fab light chain



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	98.70Å 100.96Å 138.91Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	81.67 – 2.75 81.67 – 2.75	Depositor EDS
% Data completeness (in resolution range)	99.5 (81.67-2.75) 99.5 (81.67-2.75)	Depositor EDS
R_{merge}	0.15	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.34 (at 2.73Å)	Xtriage
Refinement program	BUSTER 2.11.8 (16-JUL-2021)	Depositor
R, R_{free}	0.217 , 0.254 0.211 , 0.253	Depositor DCC
R_{free} test set	1735 reflections (4.72%)	wwPDB-VP
Wilson B-factor (Å ²)	73.9	Xtriage
Anisotropy	0.568	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 69.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.095 for k,h,-l	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	8336	wwPDB-VP
Average B, all atoms (Å ²)	89.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.47% 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: 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	A	0.78	0/925	1.11	3/1258 (0.2%)
1	B	0.78	0/925	1.12	3/1258 (0.2%)
2	H	0.74	0/1658	1.07	6/2259 (0.3%)
2	I	0.78	0/1655	1.05	5/2256 (0.2%)
3	L	0.70	0/1637	1.04	4/2239 (0.2%)
3	M	0.75	0/1622	1.08	5/2219 (0.2%)
All	All	0.75	0/8422	1.07	26/11489 (0.2%)

There are no bond length outliers.

All (26) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	328	TYR	CA-C-N	9.13	138.40	121.97
1	B	328	TYR	C-N-CA	9.13	138.40	121.97
1	A	328	TYR	CA-C-N	8.75	137.72	121.97
1	A	328	TYR	C-N-CA	8.75	137.72	121.97
2	H	123	SER	CA-C-N	8.06	132.32	120.87
2	H	123	SER	C-N-CA	8.06	132.32	120.87
2	H	52	ILE	N-CA-C	-7.60	100.64	107.56
3	L	157	VAL	CA-C-N	7.39	130.05	120.44
3	L	157	VAL	C-N-CA	7.39	130.05	120.44
3	M	129	ALA	N-CA-C	-6.77	98.59	109.96
2	I	156	GLU	N-CA-C	6.26	122.05	113.16
2	H	158	VAL	N-CA-CB	6.16	119.91	111.41
1	B	333	ASP	CA-CB-CG	6.15	118.75	112.60
3	L	129	ALA	CA-C-N	6.03	130.69	122.07
3	L	129	ALA	C-N-CA	6.03	130.69	122.07
2	I	109	VAL	N-CA-CB	-6.02	105.16	112.33
1	A	333	ASP	CA-CB-CG	5.97	118.57	112.60
2	H	109	VAL	N-CA-CB	-5.76	105.88	112.21

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	I	176	ALA	N-CA-C	5.33	117.61	110.35
3	M	141	PHE	CA-CB-CG	5.26	119.06	113.80
2	I	109	VAL	CB-CA-C	5.25	116.29	110.62
3	M	109	GLY	CA-C-N	5.24	134.59	121.80
3	M	109	GLY	C-N-CA	5.24	134.59	121.80
2	H	30	SER	N-CA-C	5.18	121.84	110.80
3	M	140	ASP	N-CA-C	5.16	117.47	111.02
2	I	30	SER	N-CA-C	5.14	121.76	110.80

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	897	0	868	5	0
1	B	897	0	868	6	0
2	H	1620	0	1602	22	0
2	I	1617	0	1601	18	0
3	L	1600	0	1547	8	0
3	M	1585	0	1537	18	0
4	H	10	0	0	0	0
4	I	10	0	0	0	0
4	M	5	0	0	0	0
5	A	12	0	0	0	0
5	B	7	0	0	0	0
5	H	14	0	0	0	0
5	I	29	0	0	0	0
5	L	18	0	0	0	0
5	M	15	0	0	0	0
All	All	8336	0	8023	71	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 (71) 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:M:151:LYS:HZ1	3:M:156:PRO:HA	1.29	0.97
2:I:134:PRO:HD2	2:I:221:PRO:HA	1.61	0.81
3:M:151:LYS:HZ1	3:M:156:PRO:CA	1.95	0.78
3:M:151:LYS:NZ	3:M:156:PRO:HA	1.99	0.77
2:H:158:VAL:HG12	2:H:208:HIS:HD2	1.53	0.73
2:I:158:VAL:HG23	2:I:208:HIS:HD2	1.55	0.71
2:H:11:VAL:CG2	2:H:210:PRO:HB3	2.22	0.68
2:H:11:VAL:HG22	2:H:210:PRO:HB3	1.76	0.66
2:H:158:VAL:HG12	2:H:208:HIS:CD2	2.31	0.66
3:M:108:LEU:HD13	3:M:110:GLN:HB3	1.82	0.62
2:I:55:PHE:CE2	2:I:57:THR:HB	2.34	0.62
1:A:340:LEU:HD11	1:A:352:ALA:HB1	1.82	0.60
2:H:13:LYS:NZ	2:H:13:LYS:H	2.04	0.56
3:L:169:GLN:HB2	3:L:173:LYS:O	2.05	0.56
2:I:134:PRO:HG3	2:I:146:LEU:HB3	1.87	0.55
3:M:126:GLU:O	3:M:129:ALA:O	2.24	0.55
3:M:152:ALA:HB2	3:M:157:VAL:HG21	1.88	0.55
2:H:177:VAL:HG13	3:L:164:THR:CG2	2.40	0.52
2:H:11:VAL:HG13	2:H:155:PRO:HG3	1.92	0.52
2:H:150:VAL:HG11	2:H:158:VAL:HG21	1.92	0.51
2:H:36:TRP:CE2	2:H:81:MET:HB2	2.45	0.51
2:I:177:VAL:HG13	3:M:164:THR:CG2	2.40	0.51
3:M:152:ALA:HB2	3:M:157:VAL:CG2	2.41	0.51
2:I:36:TRP:CE2	2:I:81:MET:HB2	2.46	0.51
2:I:177:VAL:HG13	3:M:164:THR:HG23	1.93	0.50
2:I:158:VAL:CG2	2:I:208:HIS:HD2	2.25	0.50
3:M:4:LEU:HB2	3:M:100:GLY:HA2	1.95	0.49
2:H:177:VAL:HG13	3:L:164:THR:HG23	1.95	0.48
3:L:46:VAL:HG12	3:L:57:ILE:HD12	1.95	0.48
3:M:108:LEU:HD21	3:M:142:TYR:CE1	2.48	0.48
2:H:124:THR:HG22	2:H:211:SER:HB3	1.96	0.48
3:M:46:VAL:HG12	3:M:57:ILE:HD12	1.95	0.48
3:L:4:LEU:HB2	3:L:100:GLY:HA2	1.96	0.47
2:H:12:LYS:HD3	2:H:13:LYS:HZ1	1.78	0.47
2:H:158:VAL:HG22	2:H:186:LEU:HD21	1.95	0.47
2:I:167:LEU:HD21	2:I:190:VAL:HG21	1.97	0.47
2:H:158:VAL:CG1	2:H:208:HIS:HD2	2.24	0.47
3:L:13:ALA:O	3:L:16:GLN:HB2	2.14	0.47
1:B:332:LEU:HD13	1:B:338:LYS:HA	1.98	0.46
3:L:22:CYS:HB3	3:L:70:ALA:HB3	1.98	0.46
2:H:167:LEU:HD21	2:H:190:VAL:HG21	1.97	0.45
2:H:222:LYS:HD2	3:L:213:CYS:HB2	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:M:146:VAL:HG12	3:M:199:HIS:HB2	1.99	0.45
2:H:81:MET:HE3	2:H:81:MET:HB3	1.87	0.45
1:B:340:LEU:HD11	1:B:352:ALA:HB1	1.99	0.44
1:B:368:TYR:HE1	1:B:377:GLU:HG3	1.81	0.44
3:M:151:LYS:HZ1	3:M:156:PRO:CB	2.31	0.44
2:H:127:PRO:HD2	2:H:213:THR:HG21	1.99	0.43
3:M:22:CYS:HB3	3:M:70:ALA:HB3	1.99	0.43
2:I:127:PRO:HD2	2:I:213:THR:HG21	2.01	0.43
3:M:127:LEU:HD23	3:M:184:PRO:HB3	2.00	0.43
2:H:13:LYS:H	2:H:13:LYS:HZ3	1.66	0.43
1:A:283:ASN:H	1:A:283:ASN:HD22	1.66	0.43
2:I:12:LYS:HB3	2:I:16:SER:OG	2.19	0.43
1:A:332:LEU:HD13	1:A:338:LYS:HA	2.00	0.42
1:B:329:ILE:HD13	2:H:109:VAL:HG21	2.01	0.42
1:B:361:LEU:HD23	1:B:384:VAL:HA	2.01	0.42
1:A:368:TYR:HE1	1:A:377:GLU:HG3	1.83	0.42
2:I:1:GLN:HE21	2:I:1:GLN:HB3	1.70	0.42
2:I:30:SER:O	2:I:54:ILE:HG13	2.20	0.42
2:I:155:PRO:HD2	2:I:210:PRO:HB2	2.01	0.42
3:M:143:PRO:HD2	3:M:199:HIS:NE2	2.35	0.41
1:B:283:ASN:H	1:B:283:ASN:HD22	1.68	0.41
2:I:127:PRO:HB3	2:I:153:TYR:HB3	2.03	0.41
2:H:8:GLY:HA3	2:H:209:LYS:HD2	2.02	0.41
2:I:81:MET:HB3	2:I:81:MET:HE3	1.84	0.41
2:I:54:ILE:HG13	2:I:54:ILE:H	1.71	0.41
3:M:171:ASN:O	3:M:172:ASN:HB2	2.20	0.41
2:I:7:SER:HB3	2:I:21:SER:H	1.85	0.41
1:A:361:LEU:HD23	1:A:384:VAL:HA	2.02	0.41
2:H:11:VAL:HG21	2:H:124:THR:HG23	2.03	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	110/112 (98%)	104 (94%)	5 (4%)	1 (1%)	14	28
1	B	110/112 (98%)	105 (96%)	4 (4%)	1 (1%)	14	28
2	H	214/224 (96%)	201 (94%)	12 (6%)	1 (0%)	24	43
2	I	214/224 (96%)	199 (93%)	11 (5%)	4 (2%)	6	12
3	L	211/214 (99%)	201 (95%)	10 (5%)	0	100	100
3	M	209/214 (98%)	199 (95%)	8 (4%)	2 (1%)	12	24
All	All	1068/1100 (97%)	1009 (94%)	50 (5%)	9 (1%)	16	30

All (9) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	I	135	SER
2	H	152	ASP
2	I	152	ASP
3	M	153	ASP
1	A	329	ILE
2	I	30	SER
3	M	110	GLN
1	B	329	ILE
2	I	134	PRO

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	100/100 (100%)	89 (89%)	11 (11%)	6	11
1	B	100/100 (100%)	90 (90%)	10 (10%)	7	14
2	H	181/186 (97%)	163 (90%)	18 (10%)	7	15
2	I	180/186 (97%)	165 (92%)	15 (8%)	10	19
3	L	180/181 (99%)	168 (93%)	12 (7%)	15	28
3	M	178/181 (98%)	164 (92%)	14 (8%)	11	21
All	All	919/934 (98%)	839 (91%)	80 (9%)	9	18

All (80) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	280	LEU
1	A	291	LYS
1	A	294	CYS
1	A	295	VAL
1	A	297	GLN
1	A	335	GLN
1	A	342	LEU
1	A	355	CYS
1	A	370	VAL
1	A	373	LYS
1	A	384	VAL
1	B	280	LEU
1	B	291	LYS
1	B	294	CYS
1	B	295	VAL
1	B	297	GLN
1	B	335	GLN
1	B	342	LEU
1	B	355	CYS
1	B	370	VAL
1	B	373	LYS
2	H	3	GLN
2	H	11	VAL
2	H	13	LYS
2	H	17	SER
2	H	65	GLN
2	H	74	GLU
2	H	89	GLU
2	H	109	VAL
2	H	118	THR
2	H	123	SER
2	H	124	THR
2	H	146	LEU
2	H	151	LYS
2	H	177	VAL
2	H	209	LYS
2	H	217	LYS
2	H	218	ARG
2	H	220	GLU
2	I	1	GLN
2	I	3	GLN
2	I	11	VAL

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Mol	Chain	Res	Type
2	I	17	SER
2	I	54	ILE
2	I	89	GLU
2	I	109	VAL
2	I	118	THR
2	I	146	LEU
2	I	151	LYS
2	I	156	GLU
2	I	158	VAL
2	I	177	VAL
2	I	217	LYS
2	I	222	LYS
3	L	1	SER
3	L	53	ARG
3	L	104	LYS
3	L	106	THR
3	L	125	GLU
3	L	131	LYS
3	L	158	LYS
3	L	165	THR
3	L	167	SER
3	L	168	LYS
3	L	185	GLU
3	L	202	SER
3	M	1	SER
3	M	53	ARG
3	M	59	GLU
3	M	104	LYS
3	M	106	THR
3	M	131	LYS
3	M	142	TYR
3	M	151	LYS
3	M	165	THR
3	M	167	SER
3	M	170	SER
3	M	171	ASN
3	M	185	GLU
3	M	202	SER

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

Mol	Chain	Res	Type
1	A	283	ASN
1	A	359	GLN
1	B	283	ASN
1	B	381	ASN
2	H	212	ASN
2	I	1	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	SO4	H	302	-	4,4,4	0.30	0	6,6,6	0.16	0
4	SO4	I	301	-	4,4,4	0.29	0	6,6,6	0.21	0
4	SO4	I	302	-	4,4,4	0.29	0	6,6,6	0.06	0
4	SO4	M	301	-	4,4,4	0.33	0	6,6,6	0.24	0
4	SO4	H	301	-	4,4,4	0.36	0	6,6,6	0.25	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.

No monomer is involved in short contacts.

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

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	112/112 (100%)	-0.04	2 (1%) 67 65	63, 76, 94, 103	0
1	B	112/112 (100%)	-0.13	2 (1%) 67 65	59, 74, 91, 97	0
2	H	218/224 (97%)	0.14	4 (1%) 67 65	64, 90, 119, 133	0
2	I	218/224 (97%)	0.08	4 (1%) 67 65	58, 85, 116, 130	0
3	L	213/214 (99%)	0.29	5 (2%) 61 59	66, 100, 128, 141	0
3	M	211/214 (98%)	0.21	8 (3%) 44 41	60, 89, 134, 150	0
All	All	1084/1100 (98%)	0.13	25 (2%) 61 59	58, 87, 125, 150	0

All (25) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	M	108	LEU	4.2
3	M	142	TYR	3.1
3	M	111	PRO	2.9
2	H	148	CYS	2.7
3	M	99	PHE	2.6
1	B	352	ALA	2.5
1	B	390	SER	2.4
3	L	109	GLY	2.3
1	A	321	PHE	2.3
2	H	199	THR	2.3
3	M	87	CYS	2.3
2	H	55	PHE	2.3
3	L	145	ALA	2.2
2	I	157	PRO	2.2
2	I	135	SER	2.2
3	M	98	VAL	2.2
1	A	299	TYR	2.2
3	L	108	LEU	2.2
3	M	2	TYR	2.1

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Mol	Chain	Res	Type	RSRZ
2	H	9	ALA	2.1
2	I	63	LYS	2.1
3	L	112	LYS	2.1
3	L	128	GLN	2.0
2	I	136	SER	2.0
3	M	109	GLY	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(\AA^2)	Q<0.9
4	SO4	H	302	5/5	0.71	0.14	164,164,165,165	0
4	SO4	I	302	5/5	0.78	0.12	160,160,160,160	0
4	SO4	H	301	5/5	0.80	0.11	132,132,133,133	0
4	SO4	I	301	5/5	0.90	0.11	104,105,105,105	0
4	SO4	M	301	5/5	0.93	0.08	111,112,112,112	0

6.5 Other polymers [i](#)

There are no such residues in this entry.