



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 03:37 PM UTC

PDB ID : 8YX9 / pdb_00008yx9
Title : CD40 in complex with Dacetuzumab Fab
Authors : Caaveiro, J.M.M.; Fernandez-Perez, J.; Tsumoto, K.
Deposited on : 2024-04-02
Resolution : 2.80 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

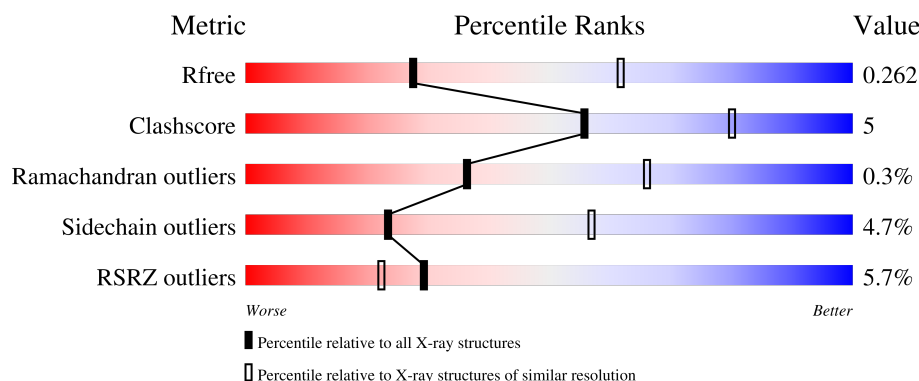
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.80 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	3866 (2.80-2.80)
Clashscore	190562	4276 (2.80-2.80)
Ramachandran outliers	187476	4196 (2.80-2.80)
Sidechain outliers	187428	4198 (2.80-2.80)
RSRZ outliers	180081	3869 (2.80-2.80)

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	223	5% 72% 20% • 5%
1	E	223	2% 78% 15% • 5%
1	G	223	8% 79% 15% • 5%
1	H	223	4% 83% 12% 5%
2	C	219	87% 11% ••

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
2	F	219	% 80% 17% ..
2	I	219	7% 85% 10% ...
2	L	219	2% 85% 14% .
3	A	179	13% 75% 12% .. 12%
3	D	179	9% 59% 7% . 34%
3	J	179	3% 37% . 62%
3	K	179	8% 73% 8% 20%

2 Entry composition [i](#)

There are 5 unique types of molecules in this entry. The entry contains 16889 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 Dacetuzumab, Heavy chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	H	212	Total	C	N	O	S	0	0	0
			1587	1007	269	306	5			
1	B	211	Total	C	N	O	S	0	0	0
			1578	1002	268	303	5			
1	E	211	Total	C	N	O	S	0	0	0
			1583	1005	268	305	5			
1	G	211	Total	C	N	O	S	0	0	0
			1583	1005	268	305	5			

- Molecule 2 is a protein called Dacetuzumab, light chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	L	217	Total	C	N	O	S	0	0	0
			1674	1048	286	335	5			
2	C	217	Total	C	N	O	S	0	0	0
			1674	1048	286	335	5			
2	F	217	Total	C	N	O	S	0	0	0
			1674	1048	286	335	5			
2	I	215	Total	C	N	O	S	0	0	0
			1659	1040	281	333	5			

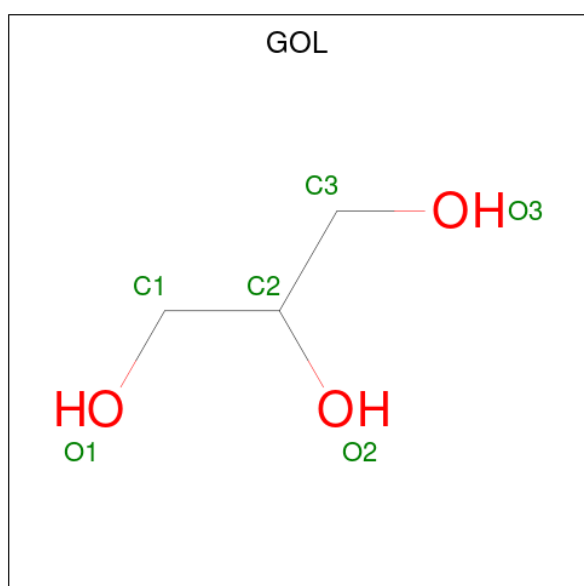
- Molecule 3 is a protein called Tumor necrosis factor receptor superfamily member 5.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	A	157	Total	C	N	O	S	0	1	0
			1206	735	206	245	20			
3	D	119	Total	C	N	O	S	0	1	0
			923	556	161	190	16			
3	J	68	Total	C	N	O	S	0	0	0
			533	322	91	112	8			
3	K	144	Total	C	N	O	S	0	1	0
			1115	683	191	223	18			

There are 24 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	194	HIS	-	expression tag	UNP P25942
A	195	HIS	-	expression tag	UNP P25942
A	196	HIS	-	expression tag	UNP P25942
A	197	HIS	-	expression tag	UNP P25942
A	198	HIS	-	expression tag	UNP P25942
A	199	HIS	-	expression tag	UNP P25942
D	194	HIS	-	expression tag	UNP P25942
D	195	HIS	-	expression tag	UNP P25942
D	196	HIS	-	expression tag	UNP P25942
D	197	HIS	-	expression tag	UNP P25942
D	198	HIS	-	expression tag	UNP P25942
D	199	HIS	-	expression tag	UNP P25942
J	194	HIS	-	expression tag	UNP P25942
J	195	HIS	-	expression tag	UNP P25942
J	196	HIS	-	expression tag	UNP P25942
J	197	HIS	-	expression tag	UNP P25942
J	198	HIS	-	expression tag	UNP P25942
J	199	HIS	-	expression tag	UNP P25942
K	194	HIS	-	expression tag	UNP P25942
K	195	HIS	-	expression tag	UNP P25942
K	196	HIS	-	expression tag	UNP P25942
K	197	HIS	-	expression tag	UNP P25942
K	198	HIS	-	expression tag	UNP P25942
K	199	HIS	-	expression tag	UNP P25942

- Molecule 4 is GLYCEROL (CCD ID: GOL) (formula: $C_3H_8O_3$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	H	1	Total C O 6 3 3	0	0
4	B	1	Total C O 6 3 3	0	0
4	E	1	Total C O 6 3 3	0	0
4	A	1	Total C O 6 3 3	0	0
4	D	1	Total C O 6 3 3	0	0
4	J	1	Total C O 6 3 3	0	0
4	K	1	Total C O 6 3 3	0	0

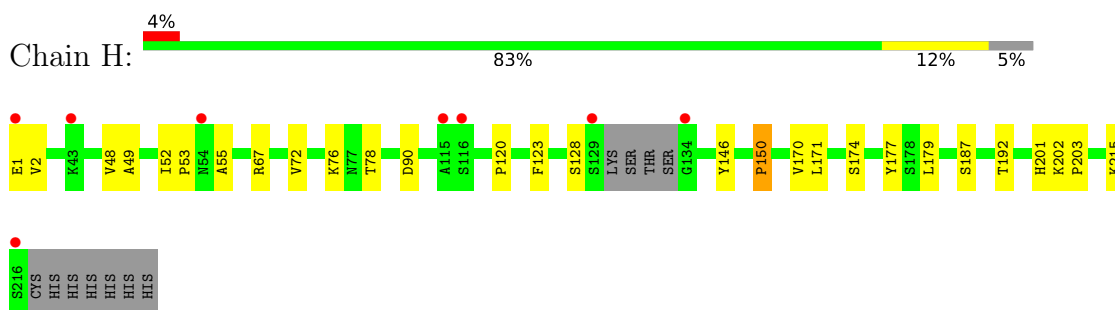
- Molecule 5 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	H	5	Total O 5 5	0	0
5	L	8	Total O 8 8	0	0
5	B	2	Total O 2 2	0	0
5	C	7	Total O 7 7	0	0
5	E	5	Total O 5 5	0	0
5	F	10	Total O 10 10	0	0
5	G	2	Total O 2 2	0	0
5	I	6	Total O 6 6	0	0
5	A	5	Total O 5 5	0	0
5	D	3	Total O 3 3	0	0
5	J	2	Total O 2 2	0	0
5	K	3	Total O 3 3	0	0

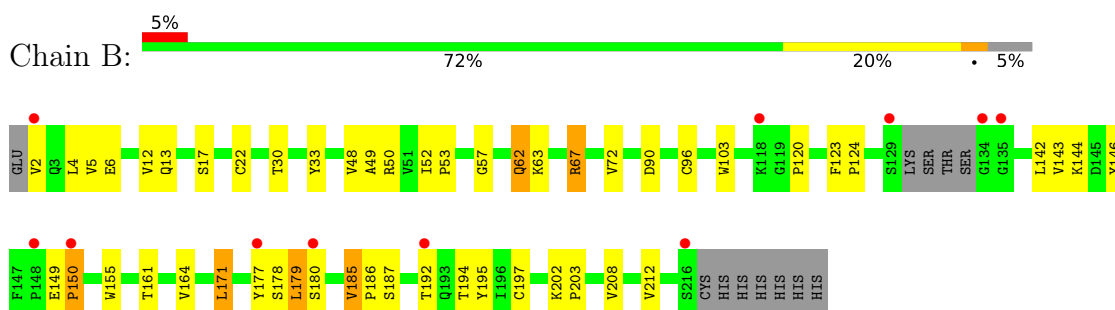
3 Residue-property plots [i](#)

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.

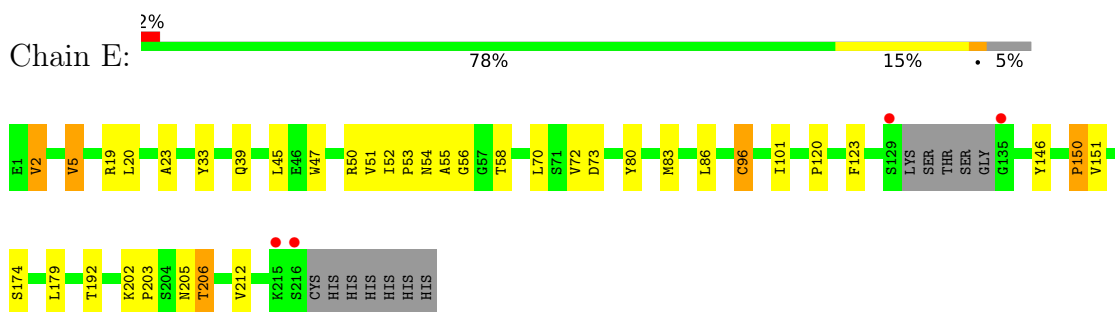
- Molecule 1: Dacetuzumab, Heavy chain



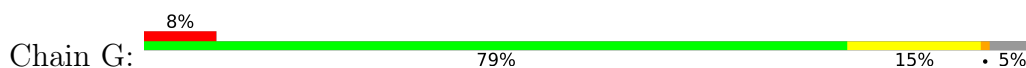
- Molecule 1: Dacetuzumab, Heavy chain

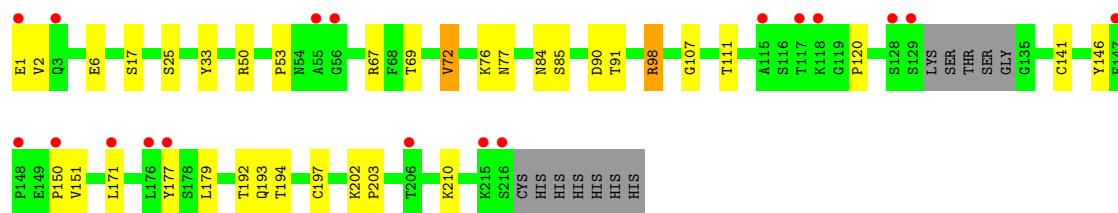


- Molecule 1: Dacetuzumab, Heavy chain

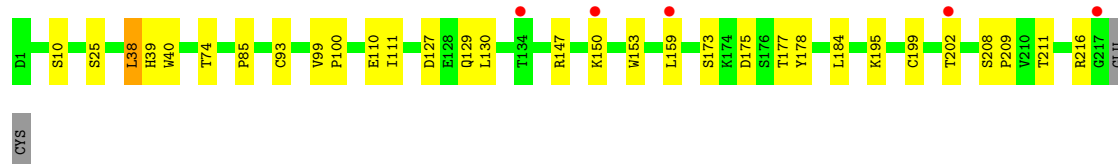
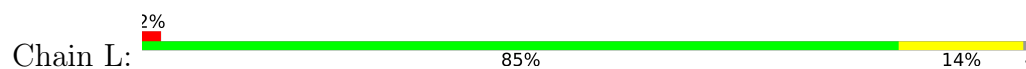


- Molecule 1: Dacetuzumab, Heavy chain





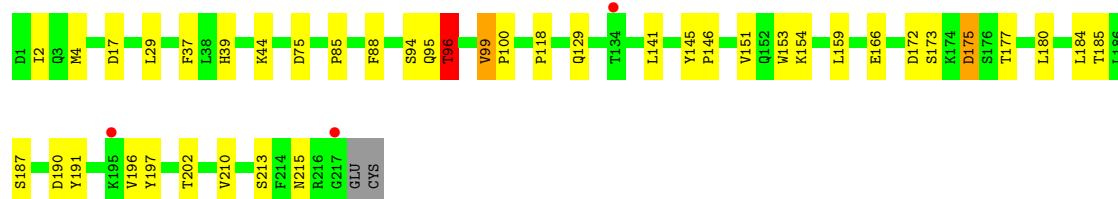
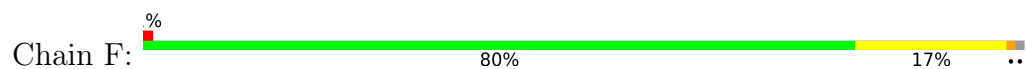
• Molecule 2: Dacetuzumab, light chain



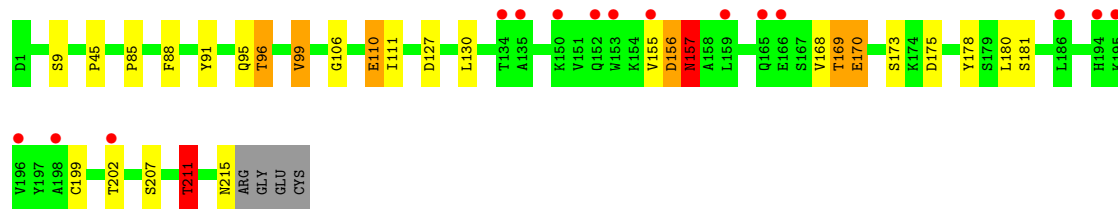
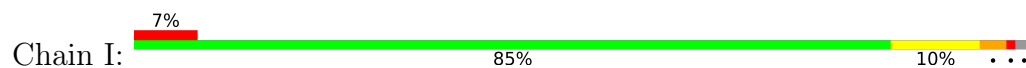
• Molecule 2: Dacetuzumab, light chain



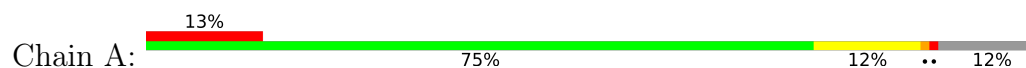
• Molecule 2: Dacetuzumab, light chain

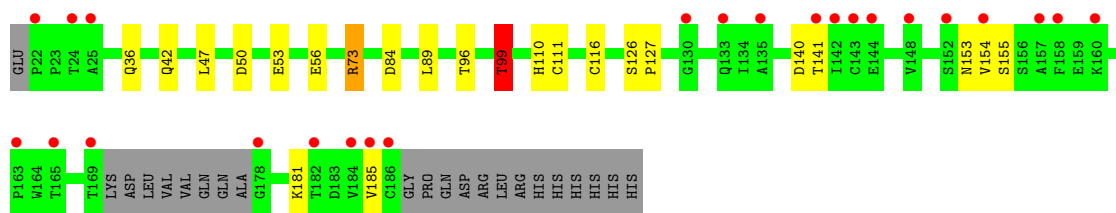


• Molecule 2: Dacetuzumab, light chain

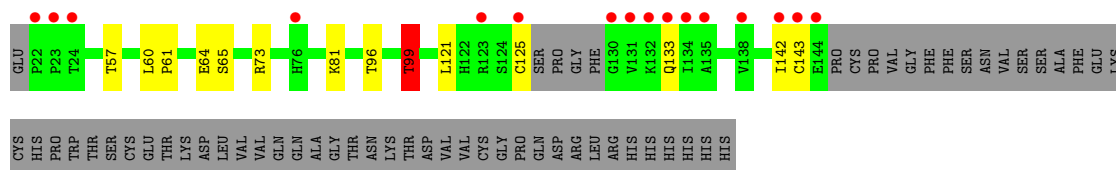


• Molecule 3: Tumor necrosis factor receptor superfamily member 5

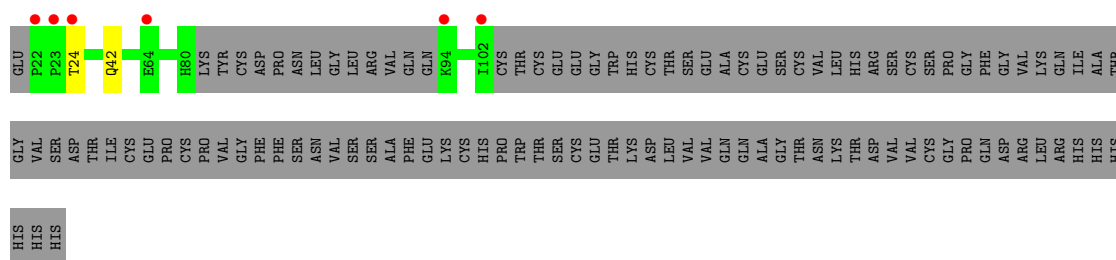




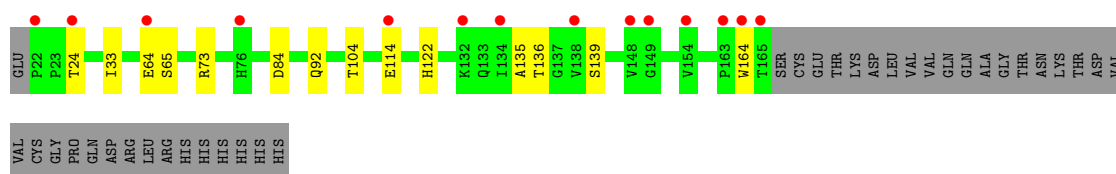
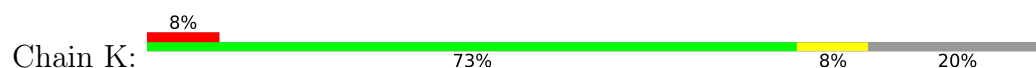
- Molecule 3: Tumor necrosis factor receptor superfamily member 5



- Molecule 3: Tumor necrosis factor receptor superfamily member 5



- Molecule 3: Tumor necrosis factor receptor superfamily member 5



4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α , β , γ	199.19Å 208.17Å 198.06Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.80 – 2.80 49.80 – 2.80	Depositor EDS
% Data completeness (in resolution range)	100.0 (49.80-2.80) 100.0 (49.80-2.80)	Depositor EDS
R_{merge}	0.15	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.39 (at 2.81Å)	Xtriage
Refinement program	REFMAC 5.8.0425	Depositor
R, R_{free}	0.209 , 0.262 0.213 , 0.262	Depositor DCC
R_{free} test set	4995 reflections (4.94%)	wwPDB-VP
Wilson B-factor (Å ²)	56.9	Xtriage
Anisotropy	0.477	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 33.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.004 for -k,-h,-l	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	16889	wwPDB-VP
Average B, all atoms (Å ²)	68.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.39% 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	B	0.54	0/1618	0.99	2/2205 (0.1%)
1	E	0.53	0/1623	1.00	4/2212 (0.2%)
1	G	0.52	0/1623	0.95	0/2212
1	H	0.53	0/1627	1.02	2/2217 (0.1%)
2	C	0.58	0/1713	1.01	5/2327 (0.2%)
2	F	0.56	0/1713	1.02	4/2327 (0.2%)
2	I	0.55	0/1698	1.01	3/2308 (0.1%)
2	L	0.56	0/1713	1.00	0/2327
3	A	0.54	0/1237	1.01	3/1679 (0.2%)
3	D	0.50	0/943	0.99	1/1276 (0.1%)
3	J	0.53	0/543	1.02	1/734 (0.1%)
3	K	0.50	0/1147	0.98	1/1558 (0.1%)
All	All	0.54	0/17198	1.00	26/23382 (0.1%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	B	0	1
1	G	0	1
2	F	0	1
All	All	0	3

There are no bond length outliers.

All (26) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	I	96	THR	CA-CB-OG1	-7.28	98.69	109.60

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	150	PRO	N-CA-CB	-7.26	94.61	102.60
1	B	150	PRO	N-CA-CB	-7.16	94.73	102.60
1	H	150	PRO	N-CA-CB	-6.71	95.21	102.60
3	J	42	GLN	CB-CA-C	-6.67	97.73	109.61
2	F	96	THR	CA-CB-OG1	-6.38	100.03	109.60
2	C	175	ASP	CB-CA-C	-6.36	100.04	110.85
2	C	96	THR	CA-CB-OG1	-6.33	100.11	109.60
3	A	56	GLU	CB-CA-C	6.23	120.74	109.83
2	F	175	ASP	CB-CA-C	-5.99	98.16	110.38
2	C	37	PHE	N-CA-CB	-5.97	102.92	110.45
1	B	13	GLN	CB-CA-C	5.91	117.98	109.11
2	F	99	VAL	N-CA-CB	-5.90	102.95	111.21
1	E	96	CYS	CB-CA-C	5.85	121.00	109.66
3	K	84	ASP	CA-CB-CG	5.56	118.16	112.60
1	E	206	THR	CA-CB-OG1	-5.42	101.47	109.60
2	C	175	ASP	CA-CB-CG	5.42	118.02	112.60
2	I	99	VAL	N-CA-CB	-5.33	104.50	109.99
2	I	211	THR	CA-CB-OG1	-5.25	101.72	109.60
3	A	99	THR	CA-CB-OG1	-5.25	101.72	109.60
2	C	114	THR	CA-CB-OG1	-5.24	101.74	109.60
1	H	192	THR	CA-CB-OG1	-5.24	101.74	109.60
3	A	50	ASP	CA-CB-CG	5.21	117.81	112.60
1	E	73	ASP	CA-CB-CG	5.20	117.80	112.60
3	D	99	THR	CA-CB-OG1	-5.16	101.87	109.60
2	F	185	THR	CA-CB-OG1	-5.05	102.03	109.60

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	57	GLY	Peptide
2	F	118	PRO	Peptide
1	G	98	ARG	Sidechain

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	1578	0	1547	30	0
1	E	1583	0	1553	18	0
1	G	1583	0	1553	16	0
1	H	1587	0	1556	14	0
2	C	1674	0	1625	13	0
2	F	1674	0	1625	24	0
2	I	1659	0	1609	12	0
2	L	1674	0	1625	17	0
3	A	1206	0	1098	8	0
3	D	923	0	842	5	0
3	J	533	0	482	0	0
3	K	1115	0	1013	5	0
4	A	6	0	8	0	0
4	B	6	0	8	1	0
4	D	6	0	8	0	0
4	E	6	0	8	0	0
4	H	6	0	8	0	0
4	J	6	0	8	0	0
4	K	6	0	8	0	0
5	A	5	0	0	1	0
5	B	2	0	0	0	0
5	C	7	0	0	0	0
5	D	3	0	0	0	0
5	E	5	0	0	0	0
5	F	10	0	0	0	0
5	G	2	0	0	0	0
5	H	5	0	0	0	0
5	I	6	0	0	0	0
5	J	2	0	0	0	0
5	K	3	0	0	0	0
5	L	8	0	0	0	0
All	All	16889	0	16184	155	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 (155) 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)
1:H:171:LEU:HD13	1:H:177:TYR:CE1	2.22	0.74
1:B:161:THR:O	1:B:164:VAL:HG12	1.88	0.74
2:C:37:PHE:HB3	2:C:96:THR:HG22	1.76	0.67

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:4:MET:HE3	2:F:95:GLN:HG2	1.77	0.66
1:G:197:CYS:SG	1:G:197:CYS:O	2.54	0.66
2:F:2:ILE:HG22	2:F:4:MET:HE2	1.78	0.65
1:B:146:TYR:CE2	1:B:177:TYR:HB2	2.32	0.65
2:F:2:ILE:HG22	2:F:4:MET:CE	2.26	0.64
2:F:37:PHE:HB3	2:F:96:THR:HG22	1.79	0.64
1:B:179:LEU:HD12	1:B:179:LEU:C	2.24	0.62
1:B:123:PHE:CE1	2:C:129:GLN:HG3	2.34	0.62
1:G:33:TYR:CD2	1:G:50:ARG:HD2	2.35	0.62
2:L:85:PRO:HB2	2:L:173:SER:O	2.01	0.61
2:I:155:VAL:C	2:I:157:ASN:H	2.09	0.61
2:I:156:ASP:O	2:I:157:ASN:HB2	2.02	0.60
1:H:67:ARG:NH2	1:H:90:ASP:OD2	2.37	0.57
2:F:175:ASP:HB3	2:F:177:THR:HG23	1.87	0.57
2:L:150:LYS:HB3	2:L:202:THR:OG1	2.06	0.56
1:B:185:VAL:HG21	1:B:195:TYR:OH	2.05	0.56
3:A:96:THR:OG1	3:A:99:THR:HB	2.06	0.56
2:F:187:SER:OG	2:F:190:ASP:OD1	2.24	0.55
3:D:96:THR:OG1	3:D:99:THR:HB	2.06	0.55
1:G:53:PRO:HB3	1:G:72:VAL:HG11	1.88	0.55
1:G:171:LEU:HD13	1:G:177:TYR:CE1	2.41	0.55
1:B:179:LEU:HD12	1:B:180:SER:N	2.21	0.55
1:H:123:PHE:CE2	2:L:129:GLN:HG3	2.42	0.55
1:B:6:GLU:HG3	1:B:96:CYS:HB3	1.88	0.55
1:B:171:LEU:CD1	1:B:177:TYR:CE1	2.91	0.54
2:I:180:LEU:HD23	2:I:181:SER:N	2.23	0.53
1:E:33:TYR:CD1	1:E:50:ARG:HD2	2.44	0.53
1:E:179:LEU:HD12	1:E:179:LEU:C	2.35	0.52
1:G:141:CYS:SG	1:G:197:CYS:CB	2.98	0.52
3:K:73:ARG:O	3:K:73:ARG:HG3	2.09	0.52
1:B:185:VAL:HG22	1:B:186:PRO:HD2	1.91	0.52
1:E:51:VAL:HG23	1:E:58:THR:HG22	1.92	0.51
2:I:45:PRO:HG2	2:I:170:GLU:HG2	1.91	0.51
2:C:18:ARG:HH22	2:F:75:ASP:CG	2.17	0.51
1:B:142:LEU:HD22	1:B:144:LYS:HB2	1.92	0.51
2:F:145:TYR:CG	2:F:146:PRO:HA	2.45	0.51
2:F:151:VAL:HG12	2:F:166:GLU:OE2	2.11	0.51
1:E:120:PRO:HB3	1:E:146:TYR:HB3	1.93	0.51
1:B:171:LEU:HD13	1:B:177:TYR:CE1	2.46	0.51
1:E:47:TRP:CE3	2:F:100:PRO:HB3	2.45	0.51
1:B:67:ARG:NH2	1:B:90:ASP:OD2	2.26	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:110:GLU:HG3	2:I:178:TYR:OH	2.11	0.50
2:L:175:ASP:HB3	2:L:177:THR:HG23	1.92	0.49
3:A:84:ASP:O	3:A:89:LEU:HB2	2.12	0.49
3:A:73:ARG:HG2	3:A:73:ARG:O	2.11	0.49
2:I:199:CYS:O	2:I:211:THR:HA	2.12	0.49
2:F:44:LYS:HE3	2:F:88:PHE:O	2.13	0.49
2:L:199:CYS:O	2:L:211:THR:HA	2.13	0.48
1:E:19:ARG:HD3	1:E:80:TYR:HB3	1.94	0.48
1:H:179:LEU:C	1:H:179:LEU:HD12	2.38	0.48
2:C:196:VAL:HG22	2:C:215:ASN:ND2	2.28	0.48
3:A:111:CYS:HB3	3:A:116:CYS:HA	1.95	0.48
2:C:42:GLN:HB2	2:C:52:LEU:HD11	1.96	0.48
2:F:154:LYS:HG2	2:F:159:LEU:HD23	1.95	0.48
1:G:67:ARG:NH2	1:G:90:ASP:OD1	2.47	0.48
1:E:5:VAL:HG22	1:E:23:ALA:HB3	1.95	0.47
2:F:196:VAL:HG22	2:F:215:ASN:OD1	2.14	0.47
2:F:191:TYR:HA	2:F:197:TYR:OH	2.14	0.47
1:G:202:LYS:N	1:G:203:PRO:CD	2.78	0.47
1:H:53:PRO:C	1:H:55:ALA:H	2.23	0.47
1:B:179:LEU:CD1	1:B:180:SER:N	2.78	0.47
1:E:151:VAL:CG1	1:E:179:LEU:HD21	2.44	0.47
3:D:133:GLN:HB3	3:D:142:ILE:HD13	1.97	0.47
1:E:39:GLN:HB2	1:E:45:LEU:HD23	1.96	0.46
3:K:73:ARG:O	3:K:73:ARG:CG	2.63	0.46
2:F:85:PRO:HB2	2:F:173:SER:O	2.15	0.46
2:L:110:GLU:HG3	2:L:178:TYR:OH	2.16	0.46
1:B:202:LYS:N	1:B:203:PRO:CD	2.78	0.46
1:E:2:VAL:HG21	1:E:101:ILE:HG13	1.97	0.46
1:H:215:LYS:NZ	2:L:127:ASP:OD2	2.42	0.46
2:C:191:TYR:HA	2:C:197:TYR:OH	2.15	0.46
1:H:171:LEU:HD13	1:H:177:TYR:CZ	2.49	0.46
1:G:6:GLU:OE1	1:G:107:GLY:N	2.44	0.46
1:E:83:MET:HB3	1:E:86:LEU:HD21	1.98	0.46
1:B:149:GLU:HG2	1:B:177:TYR:CZ	2.51	0.46
2:C:55:THR:OG1	2:C:58:ASN:ND2	2.48	0.46
1:H:202:LYS:N	1:H:203:PRO:CD	2.79	0.45
2:L:127:ASP:HA	2:L:130:LEU:HD12	1.97	0.45
2:I:168:VAL:HG12	2:I:169:THR:O	2.16	0.45
1:B:62:GLN:OE1	1:B:63:LYS:N	2.49	0.45
1:B:124:PRO:HB3	1:B:212:VAL:HG12	1.99	0.45
2:C:7:SER:HB3	2:F:17:ASP:HB3	1.99	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:1:GLU:HG2	1:G:2:VAL:HG13	1.97	0.45
1:B:185:VAL:HG21	1:B:195:TYR:CZ	2.52	0.45
2:C:52:LEU:HA	2:C:63:VAL:HG21	1.98	0.45
1:E:54:ASN:C	1:E:56:GLY:N	2.75	0.45
1:E:123:PHE:CE2	2:F:129:GLN:HG3	2.51	0.45
2:L:25:SER:OG	2:L:74:THR:HA	2.18	0.44
1:B:33:TYR:CD1	1:B:50:ARG:HD2	2.52	0.44
1:B:142:LEU:HD23	1:B:143:VAL:N	2.32	0.44
2:C:88:PHE:O	2:C:89:ALA:HB2	2.17	0.44
3:K:122:HIS:CD2	3:K:135:ALA:HB1	2.52	0.44
1:E:202:LYS:N	1:E:203:PRO:CD	2.81	0.44
3:A:110:HIS:CE1	3:A:140:ASP:OD1	2.71	0.44
2:L:99:VAL:HA	2:L:100:PRO:C	2.42	0.44
2:L:147:ARG:HG2	2:L:147:ARG:O	2.17	0.44
1:B:30:THR:HA	1:B:53:PRO:HB2	2.00	0.44
1:B:120:PRO:HB3	1:B:146:TYR:HB3	1.99	0.44
1:B:144:LYS:HA	1:B:178:SER:HB2	1.98	0.44
2:I:85:PRO:HA	2:I:111:ILE:HG13	1.99	0.44
3:A:126:SER:HB2	3:A:127:PRO:HD2	1.99	0.44
3:D:142:ILE:C	3:D:143:CYS:SG	3.01	0.44
2:F:172:ASP:HB3	2:F:175:ASP:HB2	2.00	0.43
1:G:192:THR:OG1	1:G:193:GLN:N	2.51	0.43
2:L:111:ILE:N	2:L:111:ILE:HD12	2.33	0.43
1:B:179:LEU:C	1:B:179:LEU:CD1	2.91	0.43
2:F:2:ILE:CG2	2:F:4:MET:CE	2.94	0.43
1:G:120:PRO:HB3	1:G:146:TYR:HB3	2.00	0.43
1:G:151:VAL:CG1	1:G:179:LEU:HD21	2.48	0.43
1:B:52:ILE:HA	1:B:53:PRO:HD3	1.89	0.43
2:F:39:HIS:HE2	2:F:96:THR:HB	1.84	0.43
1:H:201:HIS:C	1:H:203:PRO:HD2	2.43	0.43
2:I:88:PHE:CE1	2:I:170:GLU:HB3	2.53	0.43
1:G:91:THR:HG23	1:G:111:THR:HA	2.00	0.42
3:D:60:LEU:HD12	3:D:61:PRO:HD2	2.01	0.42
2:F:141:LEU:HD12	2:F:141:LEU:N	2.35	0.42
2:F:180:LEU:HD23	2:F:180:LEU:C	2.45	0.42
2:I:91:TYR:O	2:I:106:GLY:HA2	2.20	0.42
3:A:153:ASN:ND2	3:A:181:LYS:O	2.52	0.42
2:C:180:LEU:C	2:C:180:LEU:HD23	2.44	0.42
1:E:120:PRO:HD2	1:E:206:THR:HG21	2.01	0.42
3:A:42:GLN:HG2	5:A:304:HOH:O	2.18	0.42
1:H:52:ILE:HA	1:H:53:PRO:HD3	1.80	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:L:38:LEU:HG	2:L:39:HIS:N	2.34	0.42
1:B:4:LEU:HD12	1:B:22:CYS:SG	2.59	0.42
1:E:20:LEU:HG	1:E:83:MET:HE2	2.01	0.42
2:F:153:TRP:CE2	2:F:184:LEU:HB2	2.55	0.42
1:H:120:PRO:HB3	1:H:146:TYR:HB3	2.00	0.42
1:B:62:GLN:OE1	1:B:62:GLN:C	2.63	0.42
1:G:76:LYS:O	1:G:77:ASN:C	2.63	0.42
1:H:48:VAL:O	1:H:49:ALA:HB2	2.20	0.41
1:H:67:ARG:HH22	1:H:90:ASP:CG	2.29	0.41
3:D:64:GLU:O	3:D:65:SER:HB2	2.20	0.41
1:H:76:LYS:O	1:H:78:THR:OG1	2.28	0.41
1:E:19:ARG:HD2	1:E:19:ARG:C	2.45	0.41
2:I:95:GLN:CD	2:I:95:GLN:C	2.88	0.41
1:B:48:VAL:O	1:B:49:ALA:HB2	2.20	0.41
2:L:159:LEU:HD12	2:L:159:LEU:N	2.36	0.41
1:B:155:TRP:CH2	1:B:197:CYS:HB3	2.56	0.41
2:F:4:MET:HE1	2:F:29:LEU:HD21	2.02	0.41
1:G:179:LEU:HD12	1:G:179:LEU:C	2.45	0.41
1:E:52:ILE:HA	1:E:53:PRO:HD3	1.85	0.41
2:I:127:ASP:HA	2:I:130:LEU:HD23	2.03	0.41
3:K:64:GLU:O	3:K:65:SER:HB2	2.21	0.41
3:K:136:THR:OG1	3:K:139:SER:HB3	2.21	0.41
2:L:153:TRP:NE1	2:L:184:LEU:HB2	2.36	0.40
1:B:103:TRP:HZ3	4:B:301:GOL:H31	1.85	0.40
2:C:175:ASP:HB3	2:C:177:THR:HG23	2.03	0.40
1:G:84:ASN:O	1:G:85:SER:C	2.64	0.40
2:L:40:TRP:CZ3	2:L:93:CYS:HB3	2.57	0.40
2:L:208:SER:O	2:L:209:PRO:C	2.64	0.40
2:C:141:LEU:N	2:C:141:LEU:HD12	2.37	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	207/223 (93%)	195 (94%)	11 (5%)	1 (0%)	24	55
1	E	207/223 (93%)	194 (94%)	12 (6%)	1 (0%)	24	55
1	G	207/223 (93%)	188 (91%)	19 (9%)	0	100	100
1	H	208/223 (93%)	194 (93%)	13 (6%)	1 (0%)	24	55
2	C	215/219 (98%)	206 (96%)	9 (4%)	0	100	100
2	F	215/219 (98%)	203 (94%)	12 (6%)	0	100	100
2	I	213/219 (97%)	197 (92%)	14 (7%)	2 (1%)	14	41
2	L	215/219 (98%)	207 (96%)	7 (3%)	1 (0%)	24	55
3	A	154/179 (86%)	145 (94%)	9 (6%)	0	100	100
3	D	116/179 (65%)	110 (95%)	6 (5%)	0	100	100
3	J	64/179 (36%)	57 (89%)	7 (11%)	0	100	100
3	K	143/179 (80%)	131 (92%)	12 (8%)	0	100	100
All	All	2164/2484 (87%)	2027 (94%)	131 (6%)	6 (0%)	36	66

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	I	157	ASN
1	H	174	SER
1	B	192	THR
2	L	216	ARG
1	E	55	ALA
2	I	207	SER

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	173/185 (94%)	159 (92%)	14 (8%)	11	33
1	E	174/185 (94%)	164 (94%)	10 (6%)	18	49
1	G	174/185 (94%)	166 (95%)	8 (5%)	24	58

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	H	174/185 (94%)	167 (96%)	7 (4%)	28	63
2	C	194/196 (99%)	187 (96%)	7 (4%)	31	66
2	F	194/196 (99%)	188 (97%)	6 (3%)	35	70
2	I	193/196 (98%)	180 (93%)	13 (7%)	15	42
2	L	194/196 (99%)	191 (98%)	3 (2%)	57	84
3	A	144/163 (88%)	135 (94%)	9 (6%)	16	45
3	D	110/163 (68%)	104 (94%)	6 (6%)	19	51
3	J	64/163 (39%)	63 (98%)	1 (2%)	55	83
3	K	132/163 (81%)	126 (96%)	6 (4%)	24	58
All	All	1920/2176 (88%)	1830 (95%)	90 (5%)	23	57

All (90) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	H	1	GLU
1	H	2	VAL
1	H	72	VAL
1	H	128	SER
1	H	150	PRO
1	H	170	VAL
1	H	187	SER
2	L	10	SER
2	L	38	LEU
2	L	195	LYS
1	B	2	VAL
1	B	5	VAL
1	B	12	VAL
1	B	17	SER
1	B	62	GLN
1	B	67	ARG
1	B	72	VAL
1	B	150	PRO
1	B	171	LEU
1	B	179	LEU
1	B	185	VAL
1	B	187	SER
1	B	194	THR
1	B	208	VAL
2	C	1	ASP

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	C	10	SER
2	C	94	SER
2	C	96	THR
2	C	174	LYS
2	C	210	VAL
2	C	211	THR
1	E	2	VAL
1	E	5	VAL
1	E	70	LEU
1	E	72	VAL
1	E	96	CYS
1	E	150	PRO
1	E	174	SER
1	E	192	THR
1	E	205	ASN
1	E	212	VAL
2	F	94	SER
2	F	96	THR
2	F	99	VAL
2	F	202	THR
2	F	210	VAL
2	F	213	SER
1	G	17	SER
1	G	25	SER
1	G	69	THR
1	G	72	VAL
1	G	98	ARG
1	G	150	PRO
1	G	194	THR
1	G	210	LYS
2	I	9	SER
2	I	96	THR
2	I	99	VAL
2	I	110	GLU
2	I	156	ASP
2	I	157	ASN
2	I	169	THR
2	I	170	GLU
2	I	173	SER
2	I	175	ASP
2	I	202	THR
2	I	211	THR

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	I	215	ASN
3	A	36	GLN
3	A	47	LEU
3	A	53	GLU
3	A	73	ARG
3	A	99	THR
3	A	141	THR
3	A	154	VAL
3	A	155	SER
3	A	185	VAL
3	D	57	THR
3	D	73	ARG
3	D	81	LYS
3	D	99	THR
3	D	121	LEU
3	D	125	CYS
3	J	24	THR
3	K	24	THR
3	K	33	ILE
3	K	92	GLN
3	K	104	THR
3	K	114	GLU
3	K	164	TRP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (33) such sidechains are listed below:

Mol	Chain	Res	Type
1	H	106	GLN
1	H	205	ASN
2	L	35	ASN
2	L	152	GLN
2	L	215	ASN
1	B	193	GLN
2	C	58	ASN
2	C	84	GLN
2	C	152	GLN
2	C	157	ASN
2	C	204	GLN
2	C	215	ASN
1	E	39	GLN
1	E	62	GLN
1	E	82	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	F	35	ASN
2	F	43	GLN
2	F	142	ASN
1	G	172	GLN
2	I	58	ASN
2	I	84	GLN
2	I	98	HIS
2	I	204	GLN
3	A	34	ASN
3	A	93	GLN
3	A	122	HIS
3	A	153	ASN
3	A	162	HIS
3	D	110	HIS
3	D	122	HIS
3	J	30	GLN
3	J	79	GLN
3	K	34	ASN

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](#)

7 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	201	-	5,5,5	0.22	0	5,5,5	0.51	0
4	GOL	E	301	-	5,5,5	0.07	0	5,5,5	0.24	0
4	GOL	K	201	-	5,5,5	0.13	0	5,5,5	0.38	0
4	GOL	J	201	-	5,5,5	0.15	0	5,5,5	0.35	0
4	GOL	A	201	-	5,5,5	0.13	0	5,5,5	0.35	0
4	GOL	H	301	-	5,5,5	0.18	0	5,5,5	0.39	0
4	GOL	B	301	-	5,5,5	0.09	0	5,5,5	0.29	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	201	-	-	2/4/4/4	-
4	GOL	E	301	-	-	2/4/4/4	-
4	GOL	K	201	-	-	2/4/4/4	-
4	GOL	J	201	-	-	0/4/4/4	-
4	GOL	A	201	-	-	2/4/4/4	-
4	GOL	H	301	-	-	1/4/4/4	-
4	GOL	B	301	-	-	2/4/4/4	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (11) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	201	GOL	C1-C2-C3-O3
4	D	201	GOL	O1-C1-C2-O2
4	D	201	GOL	O1-C1-C2-C3
4	B	301	GOL	O1-C1-C2-O2
4	H	301	GOL	O1-C1-C2-C3
4	B	301	GOL	O1-C1-C2-C3
4	E	301	GOL	O1-C1-C2-C3
4	A	201	GOL	O2-C2-C3-O3
4	E	301	GOL	O1-C1-C2-O2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
4	K	201	GOL	O1-C1-C2-C3
4	K	201	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
4	B	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	211/223 (94%)	0.25	11 (5%) 33 25	42, 65, 103, 122	0
1	E	211/223 (94%)	0.06	4 (1%) 66 57	42, 64, 90, 126	0
1	G	211/223 (94%)	0.49	18 (8%) 16 12	46, 77, 112, 129	0
1	H	212/223 (95%)	0.12	8 (3%) 44 35	36, 64, 95, 112	0
2	C	217/219 (99%)	-0.21	1 (0%) 87 82	33, 50, 99, 115	0
2	F	217/219 (99%)	-0.19	3 (1%) 73 64	34, 47, 98, 111	0
2	I	215/219 (98%)	0.16	15 (6%) 22 16	37, 56, 110, 121	0
2	L	217/219 (99%)	-0.06	5 (2%) 61 51	31, 50, 110, 128	0
3	A	157/179 (87%)	0.52	24 (15%) 5 4	32, 70, 138, 154	1 (0%)
3	D	119/179 (66%)	0.39	16 (13%) 7 5	35, 66, 121, 136	1 (0%)
3	J	68/179 (37%)	0.15	6 (8%) 15 11	40, 62, 99, 114	0
3	K	144/179 (80%)	0.64	14 (9%) 13 10	40, 89, 126, 141	1 (0%)
All	All	2199/2484 (88%)	0.16	125 (5%) 29 22	31, 65, 112, 154	3 (0%)

All (125) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	D	22	PRO	6.0
3	J	102	ILE	5.2
3	J	22	PRO	5.1
3	A	22	PRO	4.9
3	K	22	PRO	4.6
2	L	217	GLY	4.5
3	A	148	VAL	4.3
1	G	216	SER	4.3
3	K	164	TRP	4.2
3	K	148	VAL	4.2
3	J	24	THR	4.1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	B	216	SER	4.0
1	E	216	SER	3.9
3	A	184	VAL	3.9
3	D	142	ILE	3.8
1	G	115	ALA	3.8
2	I	165	GLN	3.7
1	B	134	GLY	3.6
3	A	169	THR	3.6
3	D	23	PRO	3.6
3	K	64	GLU	3.6
1	G	129	SER	3.6
2	C	217	GLY	3.5
3	A	158	PHE	3.5
1	B	129	SER	3.5
3	D	131	VAL	3.4
1	H	1	GLU	3.4
2	L	150	LYS	3.4
1	B	150	PRO	3.3
1	H	134	GLY	3.3
3	A	25	ALA	3.2
2	I	198	ALA	3.2
3	A	142	ILE	3.2
3	D	76[A]	HIS	3.1
1	B	135	GLY	3.1
3	K	154	VAL	3.0
1	G	215	LYS	3.0
3	D	24	THR	3.0
3	K	132	LYS	3.0
3	A	163	PRO	3.0
2	L	202	THR	3.0
2	F	217	GLY	2.9
3	K	163	PRO	2.9
2	I	186	LEU	2.9
1	E	135	GLY	2.8
3	J	64	GLU	2.8
3	D	123	ARG	2.8
2	I	195	LYS	2.8
1	B	148	PRO	2.8
1	G	150	PRO	2.8
2	I	202	THR	2.8
2	I	159	LEU	2.7
3	A	186	CYS	2.7

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
3	K	76[A]	HIS	2.7
3	A	185	VAL	2.7
2	L	159	LEU	2.7
1	G	56	GLY	2.7
2	I	135	ALA	2.6
1	H	54	ASN	2.6
1	H	216	SER	2.6
3	A	152	SER	2.6
1	H	129	SER	2.6
1	E	215	LYS	2.6
2	I	134	THR	2.6
1	E	129	SER	2.5
1	G	1	GLU	2.5
1	G	118	LYS	2.5
3	D	138	VAL	2.5
3	A	135	ALA	2.5
3	J	94	LYS	2.5
3	D	125	CYS	2.5
3	K	138	VAL	2.4
1	B	177	TYR	2.4
3	A	154	VAL	2.4
3	D	130	GLY	2.4
1	G	206	THR	2.4
3	J	23	PRO	2.4
1	B	180	SER	2.4
1	G	55	ALA	2.4
3	A	24	THR	2.4
2	I	194	HIS	2.4
1	G	148	PRO	2.4
3	K	114	GLU	2.4
3	A	133	GLN	2.4
1	B	118	LYS	2.3
3	D	133	GLN	2.3
3	A	143	CYS	2.3
3	D	143	CYS	2.3
3	D	132	LYS	2.3
1	B	192	THR	2.3
3	A	178	GLY	2.3
1	G	147	PHE	2.3
3	D	144	GLU	2.3
2	L	134	THR	2.3
2	F	134	THR	2.3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
3	D	135	ALA	2.2
1	G	3	GLN	2.2
1	G	117	THR	2.2
3	A	182	THR	2.2
3	K	165	THR	2.2
1	H	116	SER	2.2
2	I	150	LYS	2.2
2	I	152	GLN	2.2
3	K	134	ILE	2.2
3	A	130	GLY	2.2
1	G	176	LEU	2.2
2	I	196	VAL	2.2
3	A	141	THR	2.2
2	F	195	LYS	2.2
2	I	166	GLU	2.2
1	B	2	VAL	2.1
3	A	160	LYS	2.1
3	K	149	GLY	2.1
2	I	153	TRP	2.1
1	G	128	SER	2.1
1	H	43	LYS	2.1
2	I	155	VAL	2.1
3	K	24	THR	2.1
3	A	144	GLU	2.1
3	D	134	ILE	2.1
3	A	157	ALA	2.1
1	G	177	TYR	2.1
1	G	171	LEU	2.0
3	A	165	THR	2.0
1	H	115	ALA	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	GOL	A	201	6/6	0.71	0.21	68,75,82,84	0
4	GOL	J	201	6/6	0.71	0.27	71,80,84,86	0
4	GOL	K	201	6/6	0.73	0.27	73,80,83,83	0
4	GOL	D	201	6/6	0.74	0.21	63,72,76,78	0
4	GOL	H	301	6/6	0.93	0.14	50,59,60,62	0
4	GOL	B	301	6/6	0.94	0.13	62,65,67,67	0
4	GOL	E	301	6/6	0.96	0.11	59,65,66,68	0

6.5 Other polymers [i](#)

There are no such residues in this entry.