



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 14, 2026 – 02:35 PM UTC

PDB ID : 5MP5 / pdb_00005mp5
Title : Crystal structure of DC8E8 Fab in the complex with a 14-mer tau peptide at pH 6.5
Authors : Skrabana, R.; Novak, M.
Deposited on : 2016-12-15
Resolution : 2.31 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

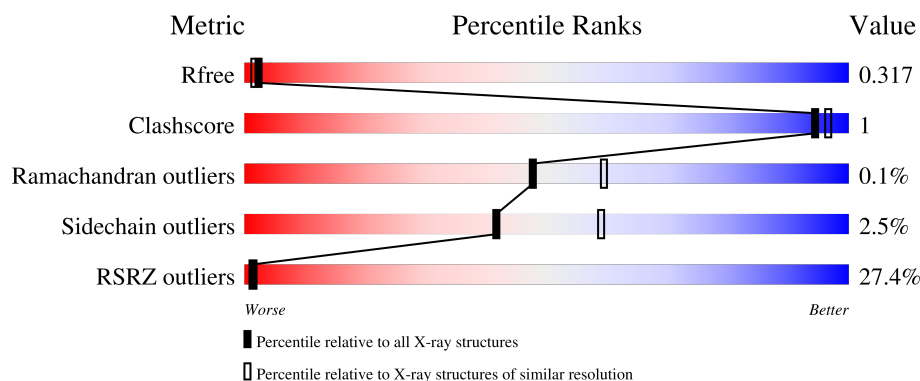
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.31 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	7754 (2.34-2.30)
Clashscore	190562	8383 (2.34-2.30)
Ramachandran outliers	187476	8303 (2.34-2.30)
Sidechain outliers	187428	8303 (2.34-2.30)
RSRZ outliers	180081	7760 (2.34-2.30)

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	A	220	27% 94% 5% ..
1	C	220	22% 93% 6%
1	E	220	30% 93% 6% .
1	H	220	20% 94% 5%
2	B	218	35% 97% .

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Mol	Chain	Length	Quality of chain
2	D	218	34% 96% .
2	F	218	35% 96% ..
2	L	218	11% 94% 6%
3	I	14	36% 14% 50%
3	J	14	36% 43% 57%
3	K	14	21% 36% 14% 50%

2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 13516 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 antibody Fab heavy chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	218	Total	C	N	O	S	0	0	0
			1646	1049	264	325	8			
1	C	220	Total	C	N	O	S	0	0	0
			1652	1051	265	328	8			
1	E	218	Total	C	N	O	S	0	0	0
			1636	1042	260	326	8			
1	H	219	Total	C	N	O	S	0	1	0
			1657	1057	265	327	8			

- Molecule 2 is a protein called antibody Fab light chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	217	Total	C	N	O	S	0	0	0
			1667	1040	280	340	7			
2	D	218	Total	C	N	O	S	0	0	0
			1671	1042	281	341	7			
2	F	216	Total	C	N	O	S	0	0	0
			1660	1036	279	338	7			
2	L	218	Total	C	N	O	S	0	0	0
			1684	1050	284	343	7			

- Molecule 3 is a protein called Microtubule-associated protein tau.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
3	I	7	Total	C	N	O	0	0	0
			42	25	9	8			
3	J	6	Total	C	N	O	0	0	0
			36	22	8	6			
3	K	7	Total	C	N	O	0	0	0
			42	25	9	8			

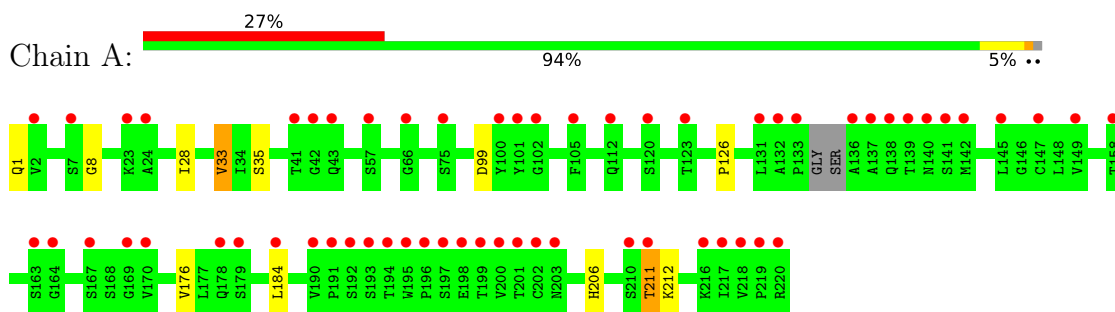
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	16	Total	O	0	0
			16	16		
4	B	15	Total	O	0	0
			15	15		
4	C	18	Total	O	0	0
			18	18		
4	D	14	Total	O	0	0
			14	14		
4	E	18	Total	O	0	0
			18	18		
4	F	10	Total	O	0	0
			10	10		
4	H	18	Total	O	0	0
			18	18		
4	L	14	Total	O	0	0
			14	14		

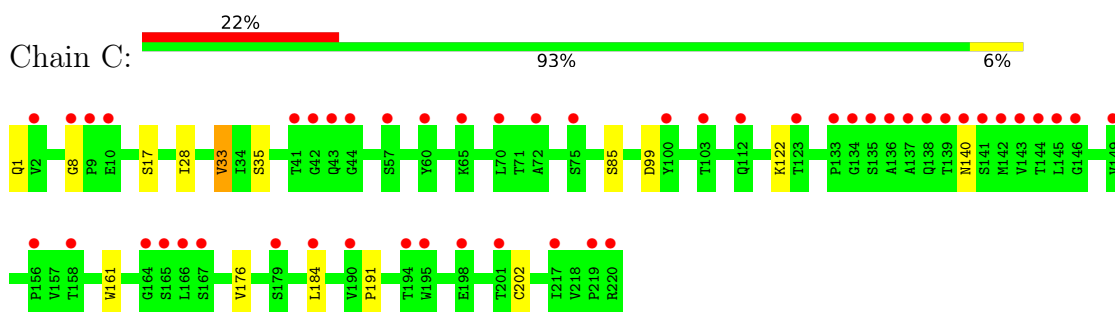
3 Residue-property plots [i](#)

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.

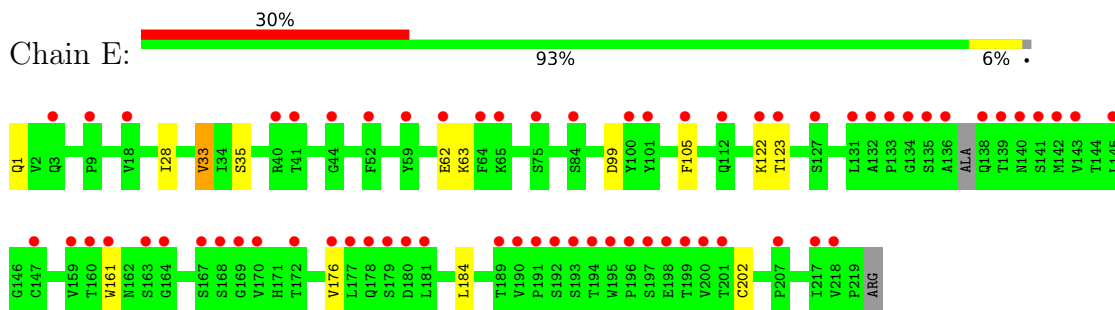
- Molecule 1: antibody Fab heavy chain



- Molecule 1: antibody Fab heavy chain

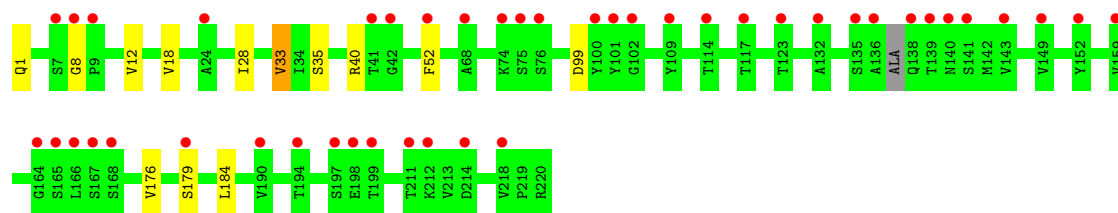


- Molecule 1: antibody Fab heavy chain

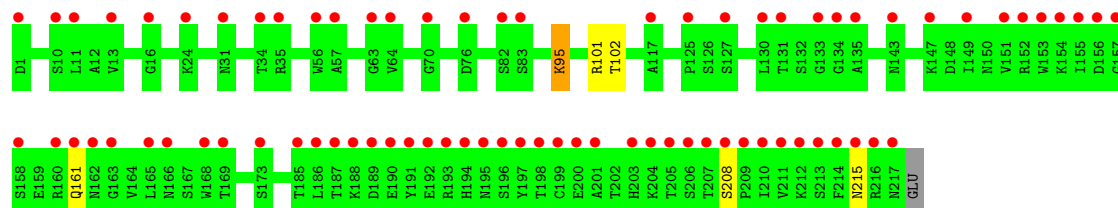


- Molecule 1: antibody Fab heavy chain

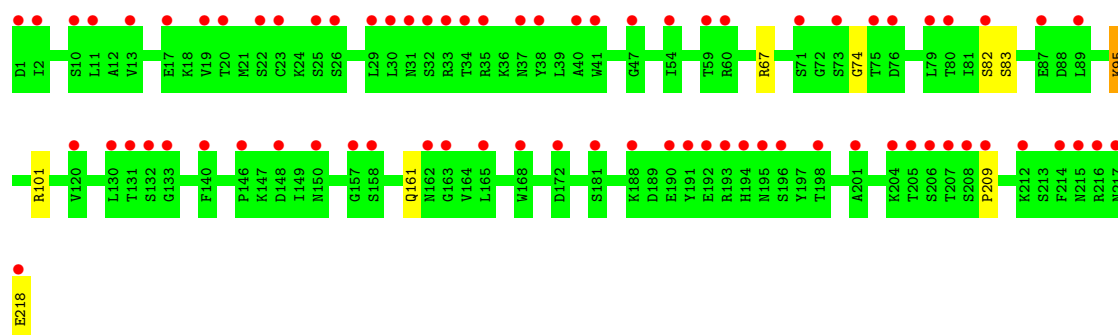




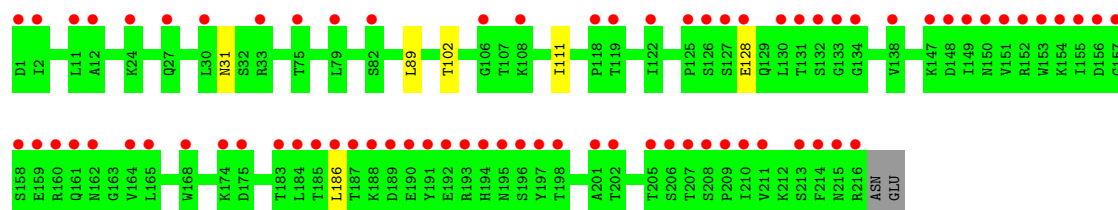
• Molecule 2: antibody Fab light chain



• Molecule 2: antibody Fab light chain



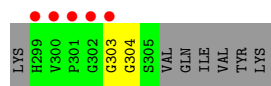
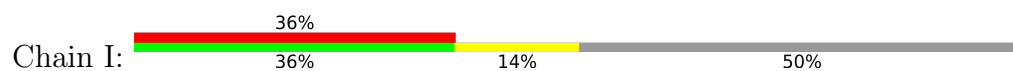
• Molecule 2: antibody Fab light chain



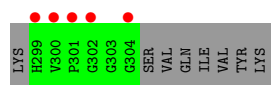
• Molecule 2: antibody Fab light chain



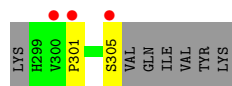
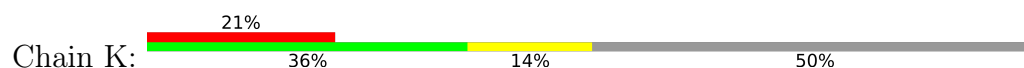
- Molecule 3: Microtubule-associated protein tau



- Molecule 3: Microtubule-associated protein tau



- Molecule 3: Microtubule-associated protein tau



4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	60.75Å 82.12Å 89.04Å 92.35° 95.36° 89.86°	Depositor
Resolution (Å)	34.50 – 2.31 34.50 – 2.31	Depositor EDS
% Data completeness (in resolution range)	85.7 (34.50-2.31) 90.5 (34.50-2.31)	Depositor EDS
R_{merge}	0.05	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.22 (at 2.31Å)	Xtriage
Refinement program	REFMAC 5.8.0135	Depositor
R, R_{free}	0.235 , 0.277 0.271 , 0.317	Depositor DCC
R_{free} test set	3343 reflections (4.43%)	wwPDB-VP
Wilson B-factor (Å ²)	37.1	Xtriage
Anisotropy	0.075	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 38.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.52$, $\langle L^2 \rangle = 0.37$	Xtriage
Estimated twinning fraction	0.000 for -h,k,-l	Xtriage
Reported twinning fraction	0.849 for H, K, L 0.151 for -H, K, -L	Depositor
Outliers	0 of 68044 reflections	Xtriage
F_o, F_c correlation	0.88	EDS
Total number of atoms	13516	wwPDB-VP
Average B, all atoms (Å ²)	38.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 17.46% 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: PCA

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	0.75	0/1683	0.93	2/2301 (0.1%)
1	C	0.77	0/1690	0.91	3/2312 (0.1%)
1	E	0.74	0/1673	0.90	1/2289 (0.0%)
1	H	0.73	0/1695	0.90	3/2318 (0.1%)
2	B	0.73	0/1703	0.90	0/2311
2	D	0.68	0/1707	0.86	0/2318
2	F	0.71	0/1696	0.90	0/2303
2	L	0.75	0/1720	0.91	0/2333
3	I	0.84	0/43	0.97	0/57
3	J	0.74	0/37	0.92	0/49
3	K	1.00	0/43	1.05	0/57
All	All	0.74	0/13690	0.90	9/18648 (0.0%)

There are no bond length outliers.

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	H	8	GLY	CA-C-N	7.38	127.39	119.78
1	H	8	GLY	C-N-CA	7.38	127.39	119.78
1	E	176	VAL	CB-CA-C	7.17	121.25	110.63
1	C	140	ASN	N-CA-C	-6.26	100.06	109.96
1	A	8	GLY	CA-C-N	5.93	125.94	119.89
1	A	8	GLY	C-N-CA	5.93	125.94	119.89
1	H	40	ARG	CG-CD-NE	5.63	124.39	112.00
1	C	8	GLY	CA-C-N	5.15	125.15	119.89
1	C	8	GLY	C-N-CA	5.15	125.15	119.89

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	1646	0	1598	4	0
1	C	1652	0	1594	4	0
1	E	1636	0	1577	6	0
1	H	1657	0	1597	6	0
2	B	1667	0	1594	1	0
2	D	1671	0	1587	3	0
2	F	1660	0	1586	3	0
2	L	1684	0	1618	7	0
3	I	42	0	36	3	0
3	J	36	0	30	0	0
3	K	42	0	36	1	0
4	A	16	0	0	0	0
4	B	15	0	0	0	0
4	C	18	0	0	0	0
4	D	14	0	0	0	0
4	E	18	0	0	1	0
4	F	10	0	0	0	0
4	H	18	0	0	1	0
4	L	14	0	0	1	0
All	All	13516	0	12853	34	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 1.

All (34) 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:A:206:HIS:HB3	1:A:211:THR:HG22	1.55	0.86
2:F:31:ASN:ND2	3:I:304:GLY:HA3	1.96	0.81
2:L:189:ASP:OD1	4:L:301:HOH:O	2.08	0.70
1:A:33:VAL:HG22	1:A:99:ASP:HB3	1.75	0.67
1:E:33:VAL:HG22	1:E:99:ASP:HB3	1.75	0.67
1:A:206:HIS:HB3	1:A:211:THR:CG2	2.25	0.67
1:C:33:VAL:HG22	1:C:99:ASP:HB3	1.76	0.65
1:H:12:VAL:HG21	1:H:18:VAL:HB	1.77	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:33:VAL:HG12	1:H:52[B]:PHE:CD1	2.33	0.62
1:H:33:VAL:HG22	1:H:99:ASP:HB3	1.80	0.62
1:H:33:VAL:HG11	1:H:52[B]:PHE:CE1	2.37	0.60
2:D:95:LYS:HE2	2:D:101:ARG:HD2	1.93	0.51
1:H:33:VAL:CG1	1:H:52[B]:PHE:CE1	2.93	0.50
2:B:95:LYS:HE2	2:B:101:ARG:HD2	1.94	0.50
2:L:95:LYS:HE2	2:L:101:ARG:HD2	1.95	0.48
1:E:62:GLU:H	1:E:62:GLU:CD	2.22	0.48
1:H:33:VAL:CG1	1:H:52[B]:PHE:CD1	2.97	0.47
1:A:126:PRO:HD2	1:A:211:THR:HG21	1.99	0.45
2:L:152:ARG:NH2	2:L:200:GLU:OE2	2.50	0.45
1:E:105:PHE:CE1	3:I:303:GLY:HA2	2.53	0.43
1:E:123:THR:HG21	4:E:311:HOH:O	2.18	0.43
3:K:301:PRO:HD2	3:K:305:SER:OG	2.19	0.42
2:D:209:PRO:HG2	4:H:315:HOH:O	2.19	0.42
1:C:161:TRP:CZ3	1:C:202:CYS:HB3	2.55	0.42
1:E:122:LYS:HA	1:E:122:LYS:HD3	1.84	0.41
1:C:191:PRO:HG3	2:L:161:GLN:HG2	2.01	0.41
2:L:89:LEU:HB2	2:L:111:ILE:HD12	2.02	0.41
2:D:67:ARG:HB2	2:D:82:SER:O	2.21	0.41
1:C:122:LYS:HA	1:C:122:LYS:HD3	1.85	0.41
2:L:67:ARG:HB2	2:L:82:SER:O	2.21	0.41
1:E:161:TRP:CZ3	1:E:202:CYS:HB3	2.56	0.40
2:L:43:GLN:HB2	2:L:53:LEU:HD11	2.04	0.40
2:F:89:LEU:HB2	2:F:111:ILE:HD12	2.02	0.40
2:F:31:ASN:HD21	3:I:304:GLY:HA3	1.84	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	214/220 (97%)	210 (98%)	4 (2%)	0	100	100
1	C	218/220 (99%)	211 (97%)	7 (3%)	0	100	100
1	E	214/220 (97%)	209 (98%)	5 (2%)	0	100	100
1	H	216/220 (98%)	212 (98%)	4 (2%)	0	100	100
2	B	215/218 (99%)	206 (96%)	9 (4%)	0	100	100
2	D	216/218 (99%)	207 (96%)	7 (3%)	2 (1%)	14	16
2	F	214/218 (98%)	204 (95%)	10 (5%)	0	100	100
2	L	216/218 (99%)	208 (96%)	8 (4%)	0	100	100
3	I	5/14 (36%)	4 (80%)	1 (20%)	0	100	100
3	J	4/14 (29%)	4 (100%)	0	0	100	100
3	K	5/14 (36%)	5 (100%)	0	0	100	100
All	All	1737/1794 (97%)	1680 (97%)	55 (3%)	2 (0%)	48	59

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	D	83	SER
2	D	74	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	185/189 (98%)	178 (96%)	7 (4%)	29	43
1	C	185/189 (98%)	178 (96%)	7 (4%)	29	43
1	E	184/189 (97%)	179 (97%)	5 (3%)	39	56
1	H	185/189 (98%)	179 (97%)	6 (3%)	34	50
2	B	188/194 (97%)	183 (97%)	5 (3%)	39	56
2	D	187/194 (96%)	184 (98%)	3 (2%)	55	72
2	F	187/194 (96%)	184 (98%)	3 (2%)	55	72

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	L	191/194 (98%)	189 (99%)	2 (1%)	68	81
3	I	4/11 (36%)	4 (100%)	0	100	100
3	J	3/11 (27%)	3 (100%)	0	100	100
3	K	4/11 (36%)	4 (100%)	0	100	100
All	All	1503/1565 (96%)	1465 (98%)	38 (2%)	42	59

All (38) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	28	ILE
1	A	33	VAL
1	A	35	SER
1	A	176	VAL
1	A	184	LEU
1	A	211	THR
1	A	212	LYS
2	B	95	LYS
2	B	102	THR
2	B	161	GLN
2	B	208	SER
2	B	215	ASN
1	C	17	SER
1	C	28	ILE
1	C	33	VAL
1	C	35	SER
1	C	85	SER
1	C	176	VAL
1	C	184	LEU
2	D	95	LYS
2	D	161	GLN
2	D	218	GLU
1	E	28	ILE
1	E	33	VAL
1	E	35	SER
1	E	63	LYS
1	E	184	LEU
2	F	102	THR
2	F	128	GLU
2	F	186	LEU
1	H	28	ILE
1	H	33	VAL

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Mol	Chain	Res	Type
1	H	35	SER
1	H	176	VAL
1	H	179	SER
1	H	184	LEU
2	L	95	LYS
2	L	148	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (11) such sidechains are listed below:

Mol	Chain	Res	Type
2	B	85	GLN
2	B	143	ASN
2	B	195	ASN
2	D	85	GLN
2	D	143	ASN
2	D	161	GLN
1	E	171	HIS
2	F	143	ASN
2	F	195	ASN
2	F	215	ASN
2	L	85	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

4 non-standard protein/DNA/RNA residues 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	$\# Z > 2$
1	PCA	H	1	1	7,8,9	0.32	0	9,10,12	1.68	2 (22%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
1	PCA	C	1	1	7,8,9	0.71	0	9,10,12	1.32	1 (11%)
1	PCA	A	1	1	7,8,9	0.59	0	9,10,12	1.19	1 (11%)
1	PCA	E	1	1	7,8,9	0.65	0	9,10,12	1.73	1 (11%)

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
1	PCA	H	1	1	-	0/0/11/13	0/1/1/1
1	PCA	C	1	1	-	0/0/11/13	0/1/1/1
1	PCA	A	1	1	-	0/0/11/13	0/1/1/1
1	PCA	E	1	1	-	0/0/11/13	0/1/1/1

There are no bond length outliers.

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	1	PCA	CB-CA-C	-4.25	106.83	112.66
1	H	1	PCA	CB-CA-C	-3.70	107.58	112.66
1	C	1	PCA	OE-CD-CG	-2.49	122.28	126.72
1	H	1	PCA	OE-CD-CG	-2.42	122.40	126.72
1	A	1	PCA	OE-CD-CG	-2.17	122.84	126.72

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

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	217/220 (98%)	1.52	60 (27%) 1 1	19, 34, 60, 76	0
1	C	219/220 (99%)	1.35	49 (22%) 2 2	18, 31, 59, 84	0
1	E	217/220 (98%)	1.64	66 (30%) 1 1	22, 36, 70, 87	0
1	H	218/220 (99%)	1.29	44 (20%) 3 3	18, 32, 52, 71	1 (0%)
2	B	217/218 (99%)	1.71	77 (35%) 1 1	19, 37, 75, 96	0
2	D	218/218 (100%)	1.72	75 (34%) 1 1	25, 41, 67, 88	0
2	F	216/218 (99%)	1.69	76 (35%) 1 1	21, 38, 77, 100	0
2	L	218/218 (100%)	1.01	23 (10%) 11 13	17, 31, 49, 78	0
3	I	7/14 (50%)	2.43	5 (71%) 0 0	42, 46, 49, 51	0
3	J	6/14 (42%)	4.08	5 (83%) 0 0	38, 39, 41, 45	6 (100%)
3	K	7/14 (50%)	2.12	3 (42%) 0 0	42, 47, 53, 54	0
All	All	1760/1794 (98%)	1.51	483 (27%) 1 1	17, 35, 67, 100	7 (0%)

All (483) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	J	300	VAL	6.9
1	C	138	GLN	6.5
2	D	30	LEU	6.3
1	H	138	GLN	6.3
1	A	139	THR	6.2
2	D	31	ASN	5.7
2	B	197	TYR	5.4
2	D	208	SER	5.3
1	E	138	GLN	5.3
1	C	135	SER	5.3
2	F	155	ILE	5.3
1	H	139	THR	5.2

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Mol	Chain	Res	Type	RSRZ
1	H	7	SER	5.2
1	E	199	THR	5.2
2	B	211	VAL	5.1
2	D	207	THR	5.1
1	E	140	ASN	5.0
1	C	139	THR	4.9
2	F	195	ASN	4.9
2	B	162	ASN	4.8
3	J	301	PRO	4.6
2	F	157	GLY	4.6
1	E	200	VAL	4.6
2	B	207	THR	4.6
3	J	302	GLY	4.6
1	A	197	SER	4.5
1	E	179	SER	4.5
2	D	33	ARG	4.5
1	E	142	MET	4.5
1	H	136	ALA	4.5
2	D	217	ASN	4.5
2	B	134	GLY	4.5
2	B	215	ASN	4.5
1	A	193	SER	4.4
1	A	199	THR	4.4
1	E	197	SER	4.4
1	H	9	PRO	4.4
2	F	189	ASP	4.4
2	L	217	ASN	4.4
1	E	195	TRP	4.3
2	F	197	TYR	4.3
1	H	141	SER	4.3
2	F	196	SER	4.3
2	F	214	PHE	4.2
2	F	215	ASN	4.2
1	E	136	ALA	4.2
1	E	196	PRO	4.2
2	B	161	GLN	4.1
2	D	204	LYS	4.1
2	B	206	SER	4.1
2	L	1	ASP	4.1
2	F	192	GLU	4.1
2	F	158	SER	4.1
1	A	2	VAL	4.1

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Mol	Chain	Res	Type	RSRZ
2	F	125	PRO	4.1
1	C	134	GLY	4.1
2	D	198	THR	4.0
2	F	149	ILE	4.0
1	C	137	ALA	4.0
2	F	207	THR	4.0
2	F	165	LEU	4.0
1	C	136	ALA	3.9
1	E	134	GLY	3.9
2	D	34	THR	3.9
2	F	132	SER	3.9
1	E	9	PRO	3.9
2	B	193	ARG	3.9
1	H	197	SER	3.9
1	A	133	PRO	3.9
1	H	101	TYR	3.9
2	B	195	ASN	3.9
2	F	156	ASP	3.8
1	C	123	THR	3.8
2	B	155	ILE	3.8
1	A	169	GLY	3.8
2	B	131	THR	3.7
1	A	192	SER	3.7
1	H	52[A]	PHE	3.7
1	C	141	SER	3.7
1	E	193	SER	3.7
1	C	103	THR	3.6
1	A	217	ILE	3.6
2	B	165	LEU	3.6
2	F	216	ARG	3.6
1	A	137	ALA	3.6
1	E	178	GLN	3.6
2	D	205	THR	3.6
2	F	122	ILE	3.6
2	D	215	ASN	3.6
1	A	132	ALA	3.6
1	E	141	SER	3.5
2	B	196	SER	3.5
2	B	163	GLY	3.5
3	J	304	GLY	3.5
1	H	166	LEU	3.5
1	E	194	THR	3.5

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Mol	Chain	Res	Type	RSRZ
2	L	161	GLN	3.5
2	F	174	LYS	3.5
2	B	16	GLY	3.5
2	B	130	LEU	3.5
2	B	186	LEU	3.5
1	A	194	THR	3.5
2	B	13	VAL	3.5
3	K	300	VAL	3.5
1	E	192	SER	3.5
2	B	1	ASP	3.5
1	A	219	PRO	3.5
1	C	142	MET	3.5
2	D	188	LYS	3.5
2	B	168	TRP	3.5
1	H	8	GLY	3.5
2	B	151	VAL	3.4
2	L	32	SER	3.4
1	A	140	ASN	3.4
2	B	205	THR	3.4
2	B	194	HIS	3.4
3	J	299	HIS	3.4
1	C	166	LEU	3.4
2	F	131	THR	3.4
1	A	190	VAL	3.4
1	E	143	VAL	3.4
1	E	190	VAL	3.4
2	D	218	GLU	3.4
2	F	153	TRP	3.3
2	F	193	ARG	3.3
2	B	213	SER	3.3
2	F	211	VAL	3.3
1	A	42	GLY	3.3
2	B	11	LEU	3.3
1	E	101	TYR	3.3
2	F	191	TYR	3.3
1	A	216	LYS	3.3
1	E	189	THR	3.3
3	I	299	HIS	3.3
1	A	198	GLU	3.3
2	B	157	GLY	3.2
2	B	156	ASP	3.2
1	E	198	GLU	3.2

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Mol	Chain	Res	Type	RSRZ
2	F	190	GLU	3.2
1	C	167	SER	3.2
2	D	32	SER	3.2
1	H	214	ASP	3.2
1	H	165	SER	3.2
1	H	190	VAL	3.2
2	D	19	VAL	3.2
1	H	140	ASN	3.2
2	F	130	LEU	3.2
3	K	301	PRO	3.2
2	F	213	SER	3.2
1	E	133	PRO	3.2
2	L	160	ARG	3.1
1	A	136	ALA	3.1
2	F	151	VAL	3.1
1	H	100	TYR	3.1
3	I	301	PRO	3.1
2	F	168	TRP	3.1
2	B	160	ARG	3.1
2	D	216	ARG	3.1
2	F	152	ARG	3.1
1	C	194	THR	3.1
1	A	120	SER	3.1
2	B	217	ASN	3.1
1	E	145	LEU	3.1
2	B	153	TRP	3.1
2	D	25	SER	3.1
2	B	214	PHE	3.1
2	D	23	CYS	3.1
2	D	1	ASP	3.1
2	L	19	VAL	3.1
1	C	220	ARG	3.1
1	A	105	PHE	3.1
1	C	8	GLY	3.1
2	D	195	ASN	3.1
2	B	57	ALA	3.1
1	A	220	ARG	3.1
1	E	180	ASP	3.0
2	F	1	ASP	3.0
2	D	60	ARG	3.0
1	H	194	THR	3.0
2	B	198	THR	3.0

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Mol	Chain	Res	Type	RSRZ
2	F	119	THR	3.0
1	A	195	TRP	3.0
2	F	160	ARG	3.0
2	F	134	GLY	3.0
1	C	9	PRO	3.0
2	F	159	GLU	3.0
2	D	75	THR	3.0
2	F	24	LYS	3.0
1	C	57	SER	3.0
1	E	135	SER	3.0
1	A	196	PRO	3.0
1	A	147	CYS	3.0
1	H	168	SER	3.0
2	D	82	SER	3.0
1	A	66	GLY	3.0
1	C	44	GLY	3.0
1	C	219	PRO	3.0
2	F	186	LEU	2.9
1	C	217	ILE	2.9
2	F	185	THR	2.9
2	B	34	THR	2.9
2	B	208	SER	2.9
1	A	164	GLY	2.9
2	D	163	GLY	2.9
3	I	302	GLY	2.9
2	B	135	ALA	2.9
1	C	158	THR	2.9
2	F	187	THR	2.9
2	B	133	GLY	2.9
2	D	194	HIS	2.9
1	C	70	LEU	2.9
2	F	201	ALA	2.9
1	A	163	SER	2.8
1	H	167	SER	2.8
2	F	194	HIS	2.8
1	E	105	PHE	2.8
2	D	2	ILE	2.8
1	E	164	GLY	2.8
2	F	206	SER	2.8
1	E	191	PRO	2.8
1	E	52	PHE	2.8
1	A	200	VAL	2.8

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Mol	Chain	Res	Type	RSRZ
2	F	154	LYS	2.8
2	F	188	LYS	2.8
2	B	189	ASP	2.8
3	I	303	GLY	2.8
2	F	138	VAL	2.8
1	E	41	THR	2.8
1	E	172	THR	2.8
1	E	201	THR	2.8
1	A	202	CYS	2.8
1	A	138	GLN	2.8
2	D	206	SER	2.8
2	F	209	PRO	2.8
2	D	130	LEU	2.8
2	B	212	LYS	2.8
1	A	201	THR	2.7
1	H	199	THR	2.7
2	L	27	GLN	2.7
2	D	158	SER	2.7
2	F	208	SER	2.7
1	A	191	PRO	2.7
2	D	29	LEU	2.7
1	A	75	SER	2.7
1	H	75	SER	2.7
2	B	125	PRO	2.7
1	C	195	TRP	2.7
2	B	200	GLU	2.7
2	L	168	TRP	2.7
2	D	165	LEU	2.7
2	F	161	GLN	2.7
2	F	150	ASN	2.7
2	F	198	THR	2.7
2	D	133	GLY	2.7
1	E	65	LYS	2.7
2	D	11	LEU	2.7
1	C	43	GLN	2.7
1	E	59	TYR	2.7
1	E	159	VAL	2.7
2	L	162	ASN	2.7
1	H	135	SER	2.7
1	E	177	LEU	2.7
2	B	56	TRP	2.7
1	C	145	LEU	2.6

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Mol	Chain	Res	Type	RSRZ
1	C	112	GLN	2.6
1	H	212	LYS	2.6
2	D	37	ASN	2.6
1	A	102	GLY	2.6
1	C	146	GLY	2.6
1	C	201	THR	2.6
1	C	179	SER	2.6
2	B	199	CYS	2.6
2	D	38	TYR	2.6
2	F	126	SER	2.6
2	B	188	LYS	2.6
1	A	170	VAL	2.6
1	C	133	PRO	2.6
2	B	185	THR	2.6
1	H	218	VAL	2.6
2	L	64	VAL	2.6
1	A	167	SER	2.6
1	E	75	SER	2.6
2	F	82	SER	2.6
2	B	147	LYS	2.6
2	B	117	ALA	2.5
2	D	157	GLY	2.5
2	B	154	LYS	2.5
2	D	212	LYS	2.5
1	E	131	LEU	2.5
2	F	162	ASN	2.5
2	F	175	ASP	2.5
1	E	123	THR	2.5
1	A	218	VAL	2.5
1	E	167	SER	2.5
2	F	27	GLN	2.5
2	B	149	ILE	2.5
2	D	191	TYR	2.5
1	C	140	ASN	2.5
2	B	201	ALA	2.5
2	D	172	ASP	2.5
1	A	43	GLN	2.5
2	D	13	VAL	2.5
2	D	26	SER	2.5
2	B	204	LYS	2.5
2	L	150	ASN	2.5
1	H	164	GLY	2.5

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Mol	Chain	Res	Type	RSRZ
1	C	198	GLU	2.4
2	F	205	THR	2.4
2	D	132	SER	2.4
2	D	196	SER	2.4
1	C	143	VAL	2.4
2	B	64	VAL	2.4
1	H	109	TYR	2.4
2	D	162	ASN	2.4
1	E	112	GLN	2.4
2	B	152	ARG	2.4
1	E	139	THR	2.4
1	E	168	SER	2.4
2	D	10	SER	2.4
2	F	127	SER	2.4
2	F	210	ILE	2.4
2	F	147	LYS	2.4
2	B	209	PRO	2.4
1	A	179	SER	2.4
2	B	158	SER	2.4
2	L	147	LYS	2.4
1	C	2	VAL	2.4
2	F	164	VAL	2.4
2	D	193	ARG	2.4
2	D	76	ASP	2.4
2	L	218	GLU	2.4
1	C	42	GLY	2.4
1	E	132	ALA	2.4
1	H	132	ALA	2.4
1	C	165	SER	2.4
2	B	10	SER	2.4
1	E	18	VAL	2.4
1	H	159	VAL	2.4
2	D	140	PHE	2.4
2	L	214	PHE	2.4
1	A	112	GLN	2.4
2	B	192	GLU	2.4
2	B	76	ASP	2.3
1	A	123	THR	2.3
1	H	211	THR	2.3
2	B	83	SER	2.3
2	D	73	SER	2.3
1	A	142	MET	2.3

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Mol	Chain	Res	Type	RSRZ
2	B	210	ILE	2.3
2	L	3	VAL	2.3
2	D	148	ASP	2.3
1	C	60	TYR	2.3
2	L	114	ALA	2.3
1	E	160	THR	2.3
1	A	141	SER	2.3
2	F	33	ARG	2.3
2	D	54	ILE	2.3
2	F	2	ILE	2.3
2	F	148	ASP	2.3
1	E	169	GLY	2.3
1	A	211	THR	2.3
2	D	131	THR	2.3
1	E	40	ARG	2.3
2	B	127	SER	2.3
3	I	300	VAL	2.3
2	L	189	ASP	2.3
1	H	42	GLY	2.3
2	D	168	TRP	2.3
2	D	59	THR	2.3
1	H	179	SER	2.3
1	E	62	GLU	2.3
2	F	184	LEU	2.2
2	L	164	VAL	2.3
2	L	193	ARG	2.2
1	A	24	ALA	2.2
1	A	158	THR	2.2
1	C	144	THR	2.2
1	E	100	TYR	2.2
1	H	68	ALA	2.2
2	D	80	THR	2.2
2	F	128	GLU	2.2
1	A	57	SER	2.2
1	E	217	ILE	2.2
1	A	131	LEU	2.2
1	E	181	LEU	2.2
1	H	149	VAL	2.2
1	E	207	PRO	2.2
2	B	203	HIS	2.2
2	D	192	GLU	2.2
1	H	117	THR	2.2

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Mol	Chain	Res	Type	RSRZ
1	E	127	SER	2.2
1	E	163	SER	2.2
2	B	82	SER	2.2
1	A	145	LEU	2.2
1	E	170	VAL	2.2
1	E	218	VAL	2.2
1	H	143	VAL	2.2
2	B	216	ARG	2.2
1	C	164	GLY	2.2
1	E	44	GLY	2.2
2	B	70	GLY	2.2
2	D	87	GLU	2.2
1	A	41	THR	2.2
1	C	41	THR	2.2
1	H	41	THR	2.2
2	D	22	SER	2.2
1	C	184	LEU	2.2
2	F	30	LEU	2.2
2	F	79	LEU	2.2
1	C	190	VAL	2.2
2	D	214	PHE	2.2
2	F	118	PRO	2.2
2	D	17	GLU	2.2
2	D	190	GLU	2.2
2	B	63	GLY	2.2
1	A	7	SER	2.2
1	C	72	ALA	2.2
2	B	191	TYR	2.1
2	D	35	ARG	2.1
2	D	41	TRP	2.1
2	B	31	ASN	2.1
2	D	120	VAL	2.1
2	B	190	GLU	2.1
2	F	133	GLY	2.1
1	C	75	SER	2.1
1	H	76	SER	2.1
1	H	114	THR	2.1
2	B	187	THR	2.1
1	E	122	LYS	2.1
2	B	143	ASN	2.1
2	D	150	ASN	2.1
1	C	149	VAL	2.1

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Mol	Chain	Res	Type	RSRZ
1	C	156	PRO	2.1
1	E	3	GLN	2.1
1	A	210	SER	2.1
2	D	20	THR	2.1
2	D	181	SER	2.1
2	F	75	THR	2.1
1	A	23	LYS	2.1
2	F	108	LYS	2.1
1	A	184	LEU	2.1
1	C	10	GLU	2.1
1	H	198	GLU	2.1
2	D	89	LEU	2.1
2	L	87	GLU	2.1
1	C	100	TYR	2.1
1	A	149	VAL	2.1
1	E	161	TRP	2.1
2	D	47	GLY	2.1
2	F	106	GLY	2.1
2	B	173	SER	2.1
2	B	166	ASN	2.1
2	L	148	ASP	2.1
1	H	152	TYR	2.1
2	B	24	LYS	2.0
2	F	202	THR	2.0
2	D	40	ALA	2.0
2	F	12	ALA	2.0
2	L	12	ALA	2.0
1	A	203	ASN	2.0
2	F	11	LEU	2.0
2	D	146	PRO	2.0
2	D	209	PRO	2.0
1	A	100	TYR	2.0
1	A	101	TYR	2.0
1	E	176	VAL	2.0
2	B	35	ARG	2.0
1	H	102	GLY	2.0
1	E	64	PHE	2.0
1	E	84	SER	2.0
1	H	123	THR	2.0
2	B	169	THR	2.0
2	D	71	SER	2.0
2	F	183	THR	2.0

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Mol	Chain	Res	Type	RSRZ
3	K	305	SER	2.0
1	H	24	ALA	2.0
2	D	201	ALA	2.0
1	A	178	GLN	2.0
1	E	147	CYS	2.0
2	D	79	LEU	2.0
2	L	54	ILE	2.0
1	C	65	LYS	2.0
1	H	74	LYS	2.0

6.2 Non-standard residues in protein, DNA, RNA chains [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
1	PCA	A	1	8/9	0.70	0.17	36,37,39,46	0
1	PCA	C	1	8/9	0.73	0.23	31,40,43,47	0
1	PCA	E	1	8/9	0.76	0.15	32,38,39,42	0
1	PCA	H	1	8/9	0.86	0.15	28,39,41,45	0

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.