



Full wwPDB X-ray Structure Validation Report ⓘ

Jun 23, 2024 – 07:53 AM EDT

PDB ID : 5BVJ
Title : The molecular mode of action and species specificity of canakinumab, a human monoclonal antibody neutralizing IL-1beta
Authors : Rondeau, J.M.
Deposited on : 2015-06-05
Resolution : 2.00 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 : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.37.1
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0158
CCP4 : 7.0.044 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.37.1

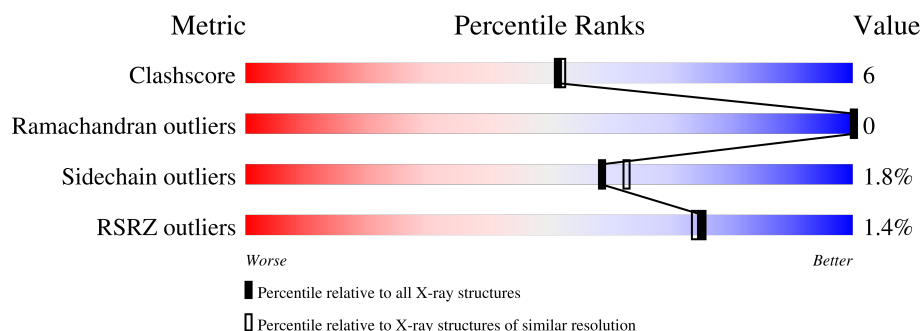
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.00 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))
Clashscore	141614	9178 (2.00-2.00)
Ramachandran outliers	138981	9054 (2.00-2.00)
Sidechain outliers	138945	9053 (2.00-2.00)
RSRZ outliers	127900	7900 (2.00-2.00)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	214	<div> <div>83%</div> <div>16%</div> <div>.</div> </div>
1	C	214	<div> <div>%</div> <div>82%</div> <div>17%</div> <div>.</div> </div>
1	E	214	<div> <div>%</div> <div>86%</div> <div>14%</div> <div>.</div> </div>
1	G	214	<div> <div>86%</div> <div>13%</div> <div>.</div> </div>
2	B	225	<div> <div>%</div> <div>88%</div> <div>11%</div> </div>
2	D	225	<div> <div>4%</div> <div>87%</div> <div>12%</div> <div>.</div> </div>

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Mol	Chain	Length	Quality of chain
2	F	225	<div><div>%</div><div><div></div><div>84%</div><div>10%</div><div>6%</div></div></div>
2	H	225	<div><div></div><div>87%</div><div>9%</div><div></div></div>

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 14437 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 canakinumab Fab light-chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	214	Total	C	N	O	S	0	0	0
			1645	1030	274	336	5			
1	C	214	Total	C	N	O	S	0	0	0
			1645	1030	274	336	5			
1	E	214	Total	C	N	O	S	0	0	0
			1645	1030	274	336	5			
1	G	214	Total	C	N	O	S	0	0	0
			1645	1030	274	336	5			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	224	Total	C	N	O	S	0	0	0
			1691	1066	288	330	7			
2	D	222	Total	C	N	O	S	0	0	0
			1675	1056	285	327	7			
2	F	212	Total	C	N	O	S	0	0	0
			1611	1022	274	309	6			
2	H	218	Total	C	N	O	S	0	0	0
			1646	1040	280	320	6			

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	149	Total	O	0	0
			149	149		
3	B	186	Total	O	0	0
			186	186		
3	C	101	Total	O	0	0
			101	101		
3	D	162	Total	O	0	0
			162	162		

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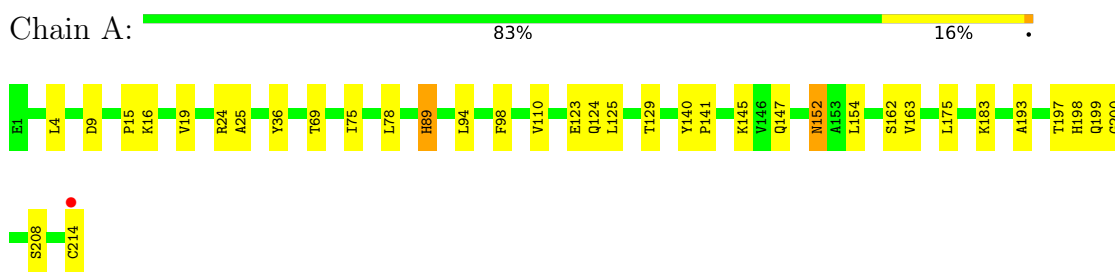
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	E	146	Total 146	O 146	0	0
3	F	123	Total 123	O 123	0	0
3	G	172	Total 172	O 172	0	0
3	H	195	Total 195	O 195	0	0

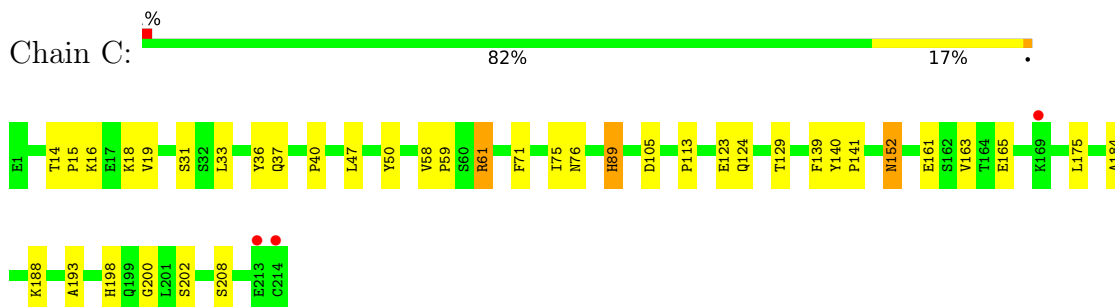
3 Residue-property plots

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

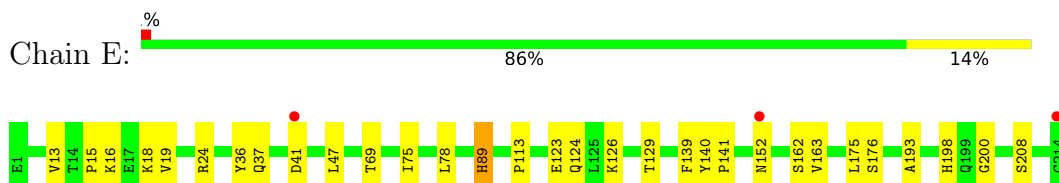
- Molecule 1: canakinumab Fab light-chain



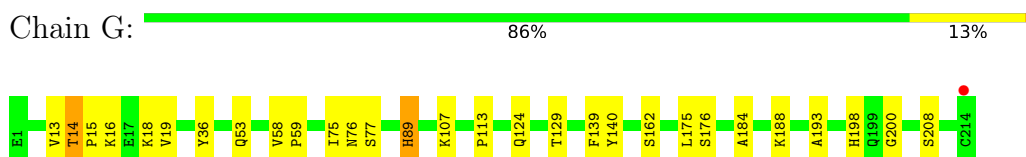
- Molecule 1: canakinumab Fab light-chain



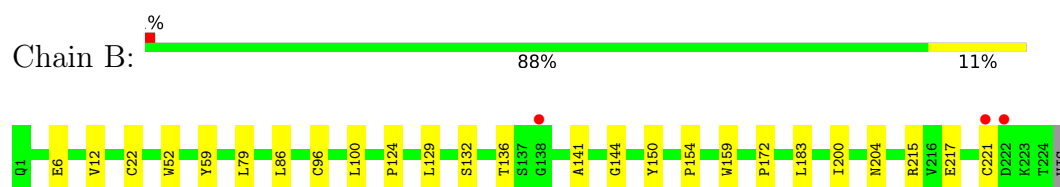
- Molecule 1: canakinumab Fab light-chain



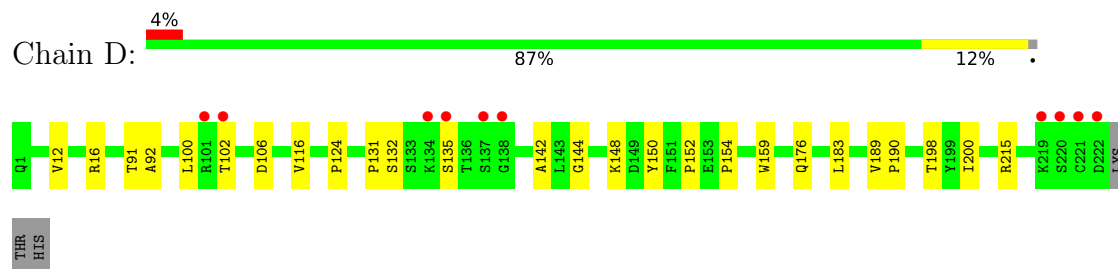
- Molecule 1: canakinumab Fab light-chain



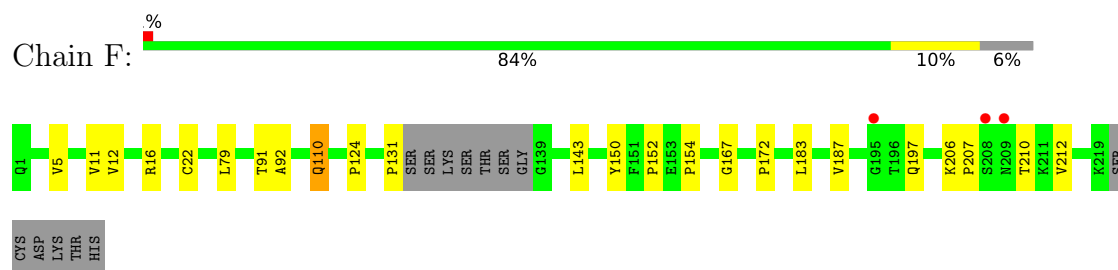
- Molecule 2: canakinumab Fab heavy-chain



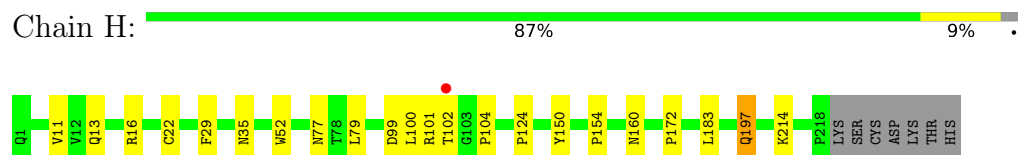
- Molecule 2: canakinumab Fab heavy-chain



- Molecule 2: canakinumab Fab heavy-chain



- Molecule 2: canakinumab Fab heavy-chain



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	80.62Å 142.26Å 83.80Å 90.00° 115.76° 90.00°	Depositor
Resolution (Å)	50.81 – 2.00 50.81 – 2.00	Depositor EDS
% Data completeness (in resolution range)	99.7 (50.81-2.00) 98.9 (50.81-2.00)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	5.26 (at 2.00Å)	Xtriage
Refinement program	CNS CNX2002	Depositor
R, R_{free}	0.186 , 0.228 0.180 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å ²)	22.0	Xtriage
Anisotropy	0.437	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 50.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.015 for l,-k,h	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	14437	wwPDB-VP
Average B, all atoms (Å ²)	24.0	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 23.09 % 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 4.9973e-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: 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	0.34	0/1682	0.67	0/2282
1	C	0.32	0/1682	0.65	0/2282
1	E	0.33	0/1682	0.64	0/2282
1	G	0.35	0/1682	0.67	0/2282
2	B	0.36	0/1725	0.68	1/2352 (0.0%)
2	D	0.33	0/1709	0.65	0/2331
2	F	0.34	0/1644	0.66	0/2243
2	H	0.35	0/1680	0.69	0/2293
All	All	0.34	0/13486	0.66	1/18347 (0.0%)

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	C	0	1
1	E	0	1
1	G	0	1
All	All	0	3

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	129	LEU	N-CA-C	-5.09	97.26	111.00

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	C	140	TYR	Sidechain
1	E	140	TYR	Sidechain
1	G	140	TYR	Sidechain

5.2 Too-close contacts [i](#)

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	1645	0	1594	24	0
1	C	1645	0	1595	24	0
1	E	1645	0	1595	21	0
1	G	1645	0	1595	22	0
2	B	1691	0	1647	15	0
2	D	1675	0	1628	16	0
2	F	1611	0	1570	17	0
2	H	1646	0	1601	13	0
3	A	149	0	0	1	0
3	B	186	0	0	1	0
3	C	101	0	0	2	0
3	D	162	0	0	4	0
3	E	146	0	0	3	0
3	F	123	0	0	2	0
3	G	172	0	0	2	0
3	H	195	0	0	3	0
All	All	14437	0	12825	145	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 6.

All (145) 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)
2:F:131:PRO:HG3	2:F:143:LEU:HB3	1.46	0.96
1:E:176:SER:HB3	3:E:335:HOH:O	1.70	0.91
1:G:13:VAL:HG21	1:G:19:VAL:HB	1.65	0.79
1:A:19:VAL:HG13	1:A:75:ILE:HB	1.63	0.79
1:E:13:VAL:HG21	1:E:19:VAL:HB	1.64	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:110:GLN:NE2	2:F:110:GLN:H	1.87	0.71
1:E:198:HIS:CD2	1:E:200:GLY:H	2.11	0.69
1:G:198:HIS:CD2	1:G:200:GLY:H	2.11	0.69
1:G:176:SER:HB3	3:G:395:HOH:O	1.93	0.68
2:H:35:ASN:ND2	2:H:99:ASP:HB2	2.09	0.67
1:C:19:VAL:HG22	1:C:75:ILE:HB	1.76	0.66
2:B:200:ILE:HD13	2:B:215:ARG:HA	1.77	0.66
1:E:124:GLN:HG2	1:E:129:THR:O	1.96	0.66
1:A:198:HIS:CD2	1:A:200:GLY:H	2.16	0.63
2:F:110:GLN:H	2:F:110:GLN:HE21	1.46	0.63
1:C:198:HIS:CD2	1:C:200:GLY:H	2.17	0.63
1:E:37:GLN:HB2	1:E:47:LEU:HD11	1.80	0.62
1:C:37:GLN:HB2	1:C:47:LEU:HD11	1.82	0.61
2:H:160:ASN:ND2	2:H:197:GLN:HE22	1.98	0.61
2:F:5:VAL:HA	2:F:110:GLN:HE22	1.65	0.61
1:G:15:PRO:O	1:G:16:LYS:HB2	2.01	0.60
1:C:36:TYR:HE1	1:C:89:HIS:HB3	1.66	0.60
1:A:147:GLN:HG3	1:A:154:LEU:HD11	1.84	0.59
1:C:113:PRO:HB3	1:C:139:PHE:HB3	1.85	0.59
1:E:19:VAL:HG12	1:E:75:ILE:HB	1.84	0.58
1:G:193:ALA:HB2	1:G:208:SER:HB3	1.85	0.58
2:D:200:ILE:HG12	2:D:215:ARG:HA	1.84	0.58
1:G:124:GLN:HG2	1:G:129:THR:O	2.03	0.58
1:E:123:GLU:O	1:E:126:LYS:HG2	2.04	0.58
1:A:124:GLN:HG2	1:A:129:THR:O	2.04	0.57
2:B:132:SER:O	2:B:136:THR:HG23	2.05	0.57
1:G:162:SER:OG	2:H:172:PRO:HD2	2.05	0.57
1:A:15:PRO:O	1:A:16:LYS:HB2	2.05	0.56
1:E:198:HIS:HD2	1:E:200:GLY:H	1.52	0.56
2:F:16:ARG:HH21	1:G:53:GLN:HG3	1.70	0.56
1:G:19:VAL:HG12	1:G:75:ILE:HB	1.85	0.56
2:B:124:PRO:HB3	2:B:150:TYR:HB3	1.87	0.56
1:C:124:GLN:HG2	1:C:129:THR:O	2.05	0.55
1:G:162:SER:HB3	3:G:395:HOH:O	2.07	0.55
1:A:162:SER:OG	2:B:172:PRO:HD2	2.07	0.55
1:A:110:VAL:HG21	1:A:199:GLN:NE2	2.22	0.55
2:D:100:LEU:HD21	2:D:106:ASP:OD2	2.07	0.54
1:C:163:VAL:HG22	1:C:175:LEU:HD12	1.90	0.54
2:D:132:SER:H	2:D:135:SER:HB2	1.73	0.53
2:B:136:THR:HG22	2:B:141:ALA:CB	2.39	0.53
1:E:19:VAL:CG1	1:E:75:ILE:HB	2.37	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:162:SER:HB3	3:E:335:HOH:O	2.08	0.53
1:G:198:HIS:HD2	1:G:200:GLY:H	1.55	0.53
1:G:14:THR:HG22	1:G:107:LYS:HE3	1.90	0.53
1:A:123:GLU:HG3	3:A:413:HOH:O	2.10	0.52
1:A:163:VAL:HG22	1:A:175:LEU:HD12	1.92	0.52
1:E:123:GLU:HG3	3:E:410:HOH:O	2.09	0.52
1:C:33:LEU:HD22	1:C:71:PHE:CG	2.46	0.51
1:C:141:PRO:O	1:C:198:HIS:HE1	1.93	0.51
1:G:14:THR:CG2	1:G:107:LYS:HE3	2.40	0.51
1:G:36:TYR:HE1	1:G:89:HIS:HB3	1.74	0.51
2:F:206:LYS:HB2	2:F:207:PRO:HD3	1.92	0.51
1:A:4:LEU:HD23	1:A:25:ALA:HA	1.93	0.51
1:C:193:ALA:HB2	1:C:208:SER:HB3	1.92	0.50
1:E:15:PRO:O	1:E:16:LYS:HB2	2.12	0.50
2:F:124:PRO:HB3	2:F:150:TYR:HB3	1.93	0.50
2:D:91:THR:O	2:D:92:ALA:HB2	2.12	0.50
1:E:36:TYR:HE1	1:E:89:HIS:HB3	1.75	0.50
2:F:183:LEU:HD12	2:F:183:LEU:C	2.32	0.50
2:B:144:GLY:HA2	2:B:159:TRP:CH2	2.47	0.49
2:F:22:CYS:HB3	2:F:79:LEU:HB3	1.93	0.49
2:F:16:ARG:HD3	3:F:370:HOH:O	2.11	0.49
2:D:148:LYS:HE2	3:D:387:HOH:O	2.11	0.49
1:A:214:CYS:N	2:B:221:CYS:HB2	2.28	0.49
2:H:101:ARG:HG2	2:H:102:THR:HG23	1.95	0.49
1:A:19:VAL:CG1	1:A:75:ILE:HB	2.40	0.48
2:F:91:THR:O	2:F:92:ALA:HB2	2.14	0.48
1:A:24:ARG:HA	1:A:69:THR:O	2.14	0.48
2:B:217:GLU:HG2	3:B:387:HOH:O	2.14	0.48
1:E:193:ALA:HB2	1:E:208:SER:HB3	1.96	0.48
1:E:13:VAL:HB	1:E:78:LEU:HD13	1.95	0.47
2:D:16:ARG:HD2	3:D:394:HOH:O	2.14	0.47
2:F:11:VAL:HG21	2:F:152:PRO:HG3	1.97	0.47
2:H:16:ARG:HD2	3:H:406:HOH:O	2.15	0.47
2:D:124:PRO:HB3	2:D:150:TYR:HB3	1.97	0.47
1:C:59:PRO:HB2	1:C:61:ARG:HG2	1.97	0.47
1:G:193:ALA:CB	1:G:208:SER:HB3	2.46	0.46
1:E:18:LYS:HG2	1:E:19:VAL:N	2.30	0.46
1:A:94:LEU:HD13	2:B:59:TYR:CG	2.51	0.46
2:B:6:GLU:HG3	2:B:96:CYS:HB2	1.98	0.46
2:B:183:LEU:HD12	2:B:183:LEU:C	2.36	0.46
1:E:163:VAL:HG22	1:E:175:LEU:HD12	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:113:PRO:HB3	1:G:139:PHE:HB3	1.98	0.46
1:A:19:VAL:HG11	1:A:78:LEU:HD12	1.96	0.46
1:A:141:PRO:O	1:A:198:HIS:HE1	1.99	0.46
1:C:161:GLU:OE1	1:C:175:LEU:HD11	2.16	0.46
1:G:175:LEU:C	1:G:175:LEU:HD23	2.37	0.46
1:E:141:PRO:O	1:E:198:HIS:HE1	1.99	0.45
2:D:183:LEU:C	2:D:183:LEU:HD12	2.37	0.45
3:F:319:HOH:O	1:G:16:LYS:HD3	2.15	0.45
2:H:29:PHE:CD2	2:H:77:ASN:HA	2.51	0.45
1:A:36:TYR:HE1	1:A:89:HIS:HB3	1.82	0.45
1:A:214:CYS:H	2:B:221:CYS:HB2	1.81	0.44
1:A:140:TYR:CG	1:A:141:PRO:HA	2.53	0.44
1:C:123:GLU:HG3	3:C:367:HOH:O	2.17	0.44
1:G:58:VAL:HA	1:G:59:PRO:HD3	1.85	0.44
2:D:135:SER:HB3	2:D:142:ALA:O	2.18	0.44
1:C:19:VAL:HG21	1:C:75:ILE:HD12	2.00	0.44
1:C:198:HIS:HD2	1:C:200:GLY:H	1.65	0.44
2:F:12:VAL:HG22	2:F:16:ARG:HB2	2.00	0.44
1:A:145:LYS:HB3	1:A:197:THR:HB	1.99	0.44
1:G:18:LYS:HG2	1:G:19:VAL:N	2.32	0.44
2:H:11:VAL:CG1	3:H:301:HOH:O	2.66	0.43
2:D:176:GLN:HG3	3:D:318:HOH:O	2.19	0.43
2:B:12:VAL:HG11	2:B:86:LEU:HD13	2.01	0.43
1:C:58:VAL:HA	1:C:59:PRO:HD3	1.76	0.43
1:C:193:ALA:CB	1:C:208:SER:HB3	2.47	0.43
2:D:144:GLY:HA2	2:D:159:TRP:CH2	2.53	0.43
1:A:125:LEU:O	1:A:183:LYS:HD2	2.19	0.43
1:C:18:LYS:HE3	1:C:76:ASN:OD1	2.19	0.43
1:C:152:ASN:HD22	1:C:152:ASN:HA	1.72	0.43
2:D:102:THR:HG22	3:D:334:HOH:O	2.19	0.42
1:E:162:SER:OG	2:F:172:PRO:HD2	2.19	0.42
2:H:11:VAL:HG13	3:H:301:HOH:O	2.19	0.42
1:C:15:PRO:O	1:C:16:LYS:HB2	2.19	0.42
2:H:35:ASN:HD21	2:H:99:ASP:HB2	1.78	0.42
2:B:200:ILE:HD13	2:B:215:ARG:CA	2.48	0.42
2:H:124:PRO:HB3	2:H:150:TYR:HB3	2.02	0.42
1:C:184:ALA:O	1:C:188:LYS:HG3	2.20	0.42
1:E:113:PRO:HB3	1:E:139:PHE:HB3	2.01	0.42
2:F:210:THR:CG2	2:F:212:VAL:HG23	2.50	0.42
2:H:22:CYS:HB3	2:H:79:LEU:HB3	2.02	0.42
2:H:183:LEU:C	2:H:183:LEU:HD12	2.40	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:100:LEU:HD12	2:H:104:PRO:HG2	2.02	0.42
2:D:198:THR:HG23	2:D:215:ARG:HE	1.85	0.41
2:F:210:THR:HG22	2:F:212:VAL:HG23	2.02	0.41
1:G:184:ALA:O	1:G:188:LYS:HG3	2.20	0.41
2:D:12:VAL:O	2:D:116:VAL:HA	2.20	0.41
2:D:131:PRO:HA	2:D:135:SER:HB2	2.01	0.41
1:A:89:HIS:HB2	1:A:98:PHE:CD2	2.56	0.41
1:G:76:ASN:O	1:G:77:SER:C	2.59	0.41
1:A:193:ALA:HB2	1:A:208:SER:HB3	2.02	0.41
1:C:202:SER:HB3	3:C:381:HOH:O	2.20	0.41
2:B:22:CYS:HB3	2:B:79:LEU:HB3	2.03	0.41
1:C:31:SER:O	1:C:50:TYR:HA	2.20	0.40
1:A:152:ASN:HD22	1:A:152:ASN:HA	1.68	0.40
1:C:40:PRO:HB3	1:C:165:GLU:HG3	2.03	0.40
2:D:189:VAL:HB	2:D:190:PRO:HD2	2.03	0.40
1:E:24:ARG:HA	1:E:69:THR:O	2.21	0.40
2:F:167:GLY:O	2:F:187:VAL:HA	2.21	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	212/214 (99%)	206 (97%)	6 (3%)	0	100	100
1	C	212/214 (99%)	204 (96%)	8 (4%)	0	100	100
1	E	212/214 (99%)	207 (98%)	5 (2%)	0	100	100
1	G	212/214 (99%)	207 (98%)	5 (2%)	0	100	100
2	B	222/225 (99%)	216 (97%)	6 (3%)	0	100	100
2	D	220/225 (98%)	208 (94%)	12 (6%)	0	100	100
2	F	208/225 (92%)	200 (96%)	8 (4%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	H	216/225 (96%)	211 (98%)	5 (2%)	0	100	100
All	All	1714/1756 (98%)	1659 (97%)	55 (3%)	0	100	100

There are no Ramachandran outliers to report.

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	190/190 (100%)	187 (98%)	3 (2%)	62	67
1	C	190/190 (100%)	185 (97%)	5 (3%)	46	48
1	E	190/190 (100%)	187 (98%)	3 (2%)	62	67
1	G	190/190 (100%)	188 (99%)	2 (1%)	73	78
2	B	187/188 (100%)	183 (98%)	4 (2%)	53	57
2	D	185/188 (98%)	183 (99%)	2 (1%)	73	78
2	F	176/188 (94%)	173 (98%)	3 (2%)	60	65
2	H	181/188 (96%)	176 (97%)	5 (3%)	43	44
All	All	1489/1512 (98%)	1462 (98%)	27 (2%)	59	63

All (27) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	9	ASP
1	A	89	HIS
1	A	152	ASN
2	B	52	TRP
2	B	100	LEU
2	B	154	PRO
2	B	204	ASN
1	C	14	THR
1	C	61	ARG
1	C	89	HIS

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Mol	Chain	Res	Type
1	C	105	ASP
1	C	152	ASN
2	D	152	PRO
2	D	154	PRO
1	E	41	ASP
1	E	89	HIS
1	E	152	ASN
2	F	110	GLN
2	F	154	PRO
2	F	197	GLN
1	G	14	THR
1	G	89	HIS
2	H	13	GLN
2	H	52	TRP
2	H	154	PRO
2	H	197	GLN
2	H	214	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (22) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	152	ASN
1	A	198	HIS
1	A	199	GLN
2	B	77	ASN
2	B	110	GLN
1	C	152	ASN
1	C	198	HIS
2	D	77	ASN
2	D	176	GLN
1	E	152	ASN
1	E	198	HIS
2	F	77	ASN
2	F	84	ASN
2	F	110	GLN
1	G	27	GLN
1	G	152	ASN
1	G	198	HIS
2	H	13	GLN
2	H	57	ASN
2	H	77	ASN
2	H	197	GLN

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Mol	Chain	Res	Type
2	H	204	ASN

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	$\# Z > 2$
2	PCA	D	1	2	7,8,9	0.85	0	9,10,12	0.60	0
2	PCA	H	1	2	7,8,9	0.77	0	9,10,12	0.44	0
2	PCA	F	1	2	7,8,9	0.85	0	9,10,12	0.57	0
2	PCA	B	1	2	7,8,9	0.80	0	9,10,12	0.53	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
2	PCA	D	1	2	-	0/0/11/13	0/1/1/1
2	PCA	H	1	2	-	0/0/11/13	0/1/1/1
2	PCA	F	1	2	-	0/0/11/13	0/1/1/1
2	PCA	B	1	2	-	0/0/11/13	0/1/1/1

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.

5.5 Carbohydrates [i](#)

There are no monosaccharides 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	214/214 (100%)	-0.41	1 (0%) 91 90	11, 22, 34, 48	0
1	C	214/214 (100%)	-0.21	3 (1%) 75 74	14, 26, 39, 64	0
1	E	214/214 (100%)	-0.29	3 (1%) 75 74	12, 23, 41, 62	0
1	G	214/214 (100%)	-0.45	1 (0%) 91 90	10, 20, 34, 58	0
2	B	223/225 (99%)	-0.40	3 (1%) 77 76	10, 21, 38, 58	0
2	D	221/225 (98%)	-0.19	10 (4%) 33 32	11, 23, 52, 64	0
2	F	211/225 (93%)	-0.25	3 (1%) 75 74	11, 25, 47, 55	0
2	H	217/225 (96%)	-0.51	1 (0%) 91 90	11, 19, 34, 55	0
All	All	1728/1756 (98%)	-0.34	25 (1%) 75 74	10, 22, 42, 64	0

All (25) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	E	214	CYS	7.8
1	C	214	CYS	7.0
2	D	102	THR	5.9
2	D	221	CYS	5.8
2	D	222	ASP	5.5
2	H	102	THR	5.0
1	G	214	CYS	4.5
2	D	137	SER	3.9
1	C	169	LYS	3.7
1	E	152	ASN	3.6
2	D	101	ARG	3.6
1	E	41	ASP	3.3
2	B	222	ASP	3.3
2	B	138	GLY	3.1
2	F	209	ASN	3.1
2	F	195	GLY	3.0

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Mol	Chain	Res	Type	RSRZ
2	D	138	GLY	2.8
2	D	134	LYS	2.5
1	C	213	GLU	2.3
2	D	220	SER	2.3
2	F	208	SER	2.3
1	A	214	CYS	2.2
2	D	219	LYS	2.1
2	B	221	CYS	2.0
2	D	135	SER	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
2	PCA	D	1	8/9	0.76	0.21	34,42,46,49	0
2	PCA	H	1	8/9	0.76	0.28	34,42,47,50	0
2	PCA	F	1	8/9	0.91	0.15	25,35,40,44	0
2	PCA	B	1	8/9	0.92	0.13	24,30,34,41	0

6.3 Carbohydrates [i](#)

There are no monosaccharides 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.