



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 10, 2026 – 03:34 PM UTC

PDB ID : 4HH9 / pdb_00004hh9
Title : Anti-Human Cytomegalovirus (HCMV) Fab KE5
Authors : Bryson, S.; Risnes, L.; Damgupta, S.; Thomson, C.A.; Pfoh, R.; Schrader, J.W.; Pai, E.F.
Deposited on : 2012-10-09
Resolution : 1.70 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
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

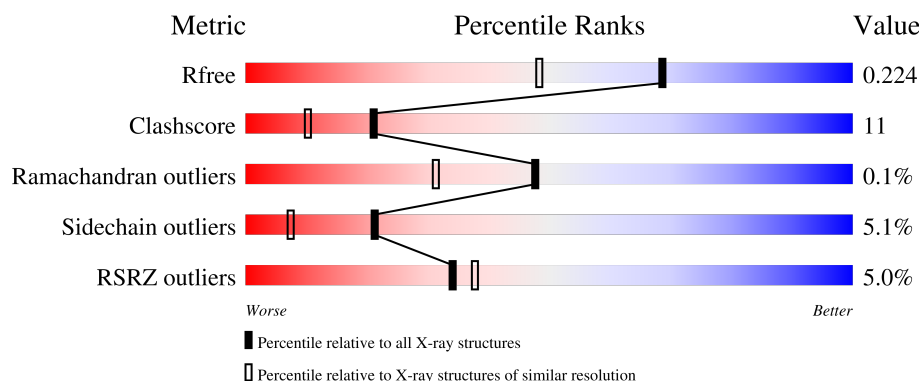
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.70 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	5551 (1.70-1.70)
Clashscore	190562	5924 (1.70-1.70)
Ramachandran outliers	187476	5846 (1.70-1.70)
Sidechain outliers	187428	5846 (1.70-1.70)
RSRZ outliers	180081	5554 (1.70-1.70)

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	215	4% 78% 20% .
1	C	215	4% 73% 24% .
2	B	236	5% 74% 22% ..
2	D	236	6% 72% 21% ..

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 7431 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 Fab KE5, light chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	214	Total	C	N	O	S	0	0	0
			1646	1030	282	329	5			
1	C	214	Total	C	N	O	S	0	0	0
			1646	1030	282	329	5			

- Molecule 2 is a protein called Fab KE5, heavy chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	229	Total	C	N	O	S	0	0	0
			1730	1082	306	334	8			
2	D	228	Total	C	N	O	S	0	0	0
			1722	1078	305	331	8			

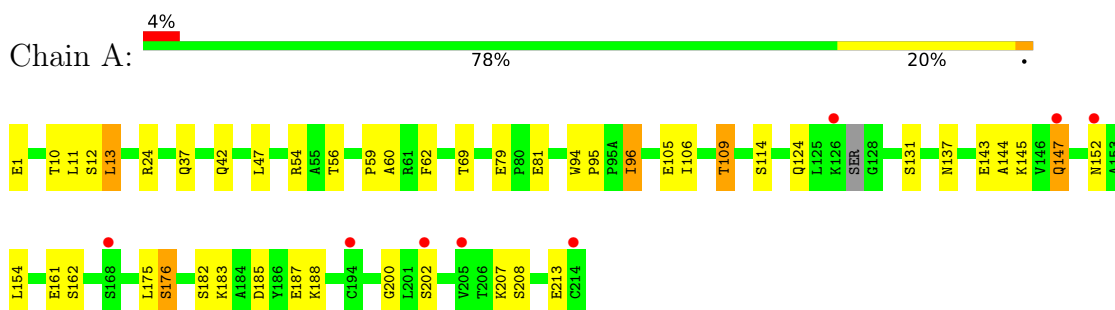
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	177	Total	O	0	0
			177	177		
3	B	192	Total	O	0	0
			192	192		
3	C	183	Total	O	0	0
			183	183		
3	D	135	Total	O	0	0
			135	135		

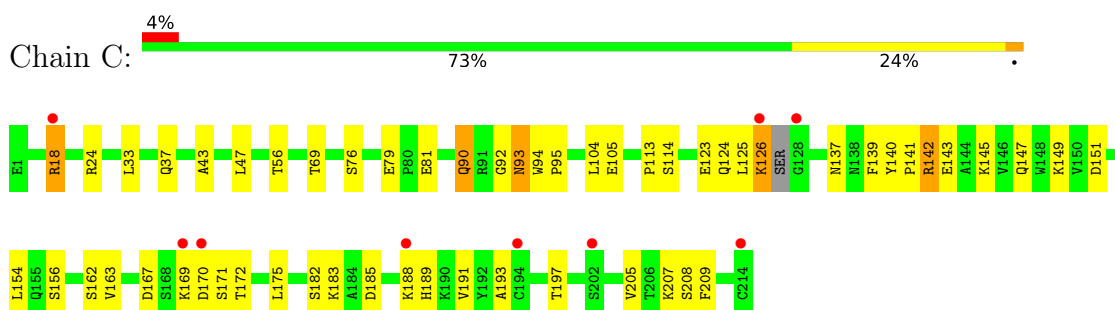
3 Residue-property plots [i](#)

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.

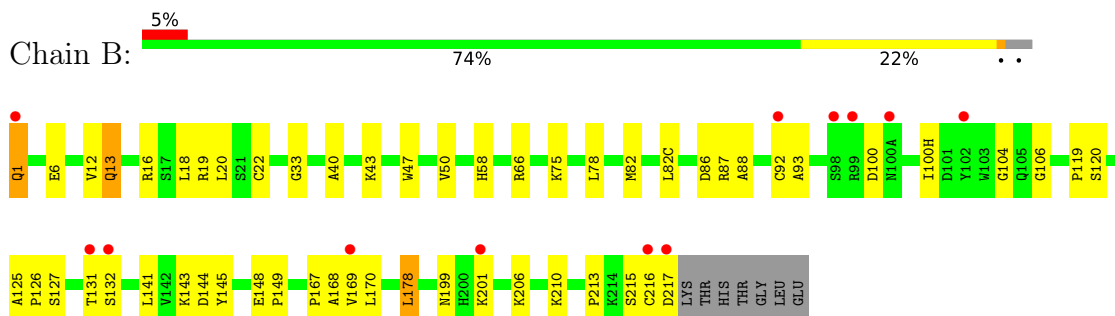
- Molecule 1: Fab KE5, light chain



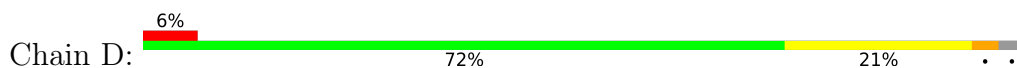
- Molecule 1: Fab KE5, light chain

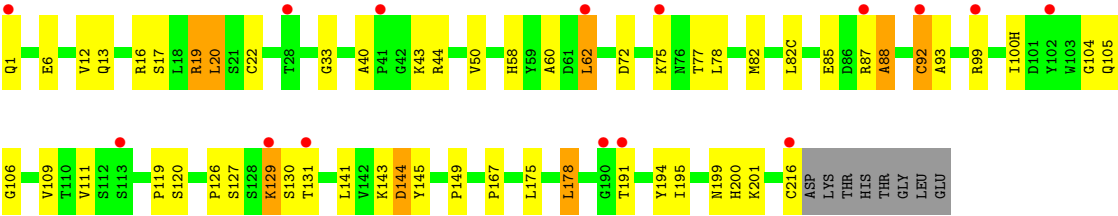


- Molecule 2: Fab KE5, heavy chain



- Molecule 2: Fab KE5, 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	73.86Å 79.47Å 86.27Å 90.00° 113.25° 90.00°	Depositor
Resolution (Å)	43.00 – 1.70 43.00 – 1.70	Depositor EDS
% Data completeness (in resolution range)	(Not available) (43.00-1.70) 95.1 (43.00-1.70)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.63 (at 1.60Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.217 , 0.224 0.217 , 0.224	Depositor DCC
R_{free} test set	5835 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	14.2	Xtriage
Anisotropy	0.259	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 29.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	0.022 for h,-k,-h-l	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	7431	wwPDB-VP
Average B, all atoms (Å ²)	16.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.55% 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 ⓘ

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	0.29	0/1682	0.87	6/2284 (0.3%)
1	C	0.28	0/1682	0.87	4/2284 (0.2%)
2	B	0.29	0/1770	0.93	9/2403 (0.4%)
2	D	0.30	0/1762	0.95	9/2392 (0.4%)
All	All	0.29	0/6896	0.90	28/9363 (0.3%)

There are no bond length outliers.

All (28) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	33	GLY	N-CA-C	-7.75	101.53	112.37
2	D	33	GLY	N-CA-C	-7.74	101.54	112.37
2	B	100	ASP	N-CA-C	6.65	121.10	112.92
1	C	182	SER	N-CA-C	-6.49	100.88	110.48
2	B	104	GLY	N-CA-C	-6.38	102.57	112.85
2	D	104	GLY	N-CA-C	-6.28	102.99	112.60
2	D	106	GLY	N-CA-C	6.18	120.69	112.65
1	A	182	SER	N-CA-C	-6.03	101.56	110.48
1	A	137	ASN	N-CA-C	6.00	119.25	109.59
2	B	106	GLY	N-CA-C	6.00	120.45	112.65
2	D	120	SER	N-CA-C	-5.96	99.98	109.76
1	C	114	SER	N-CA-C	-5.95	99.58	109.46
2	D	143	LYS	N-CA-C	5.94	119.22	109.72
1	A	114	SER	N-CA-C	-5.93	99.53	108.96
2	B	125	ALA	N-CA-C	5.74	116.93	109.64
2	D	144	ASP	N-CA-C	5.62	118.99	111.24
2	B	143	LYS	N-CA-C	5.51	118.71	109.95
2	B	120	SER	N-CA-C	-5.47	100.32	109.24
1	A	200	GLY	N-CA-C	-5.39	108.26	115.32
2	D	92	CYS	N-CA-C	-5.34	101.00	109.76
1	A	96	ILE	N-CA-C	-5.22	102.77	109.30
2	B	144	ASP	N-CA-C	5.22	118.44	111.24
1	C	191	VAL	N-CA-C	5.19	116.06	108.58

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	215	SER	N-CA-C	-5.19	103.06	110.59
1	C	137	ASN	N-CA-C	5.14	117.86	109.59
2	D	60	ALA	N-CA-C	-5.10	102.73	110.28
2	D	44	ARG	N-CA-C	5.03	117.17	110.53
1	A	208	SER	N-CA-C	5.02	116.62	109.14

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	33	0
1	C	1646	0	1598	47	0
2	B	1730	0	1693	36	0
2	D	1722	0	1689	41	0
3	A	177	0	0	7	0
3	B	192	0	0	3	0
3	C	183	0	0	6	0
3	D	135	0	0	6	0
All	All	7431	0	6578	146	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 11.

All (146) 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:C:142:ARG:HG2	1:C:142:ARG:HH21	0.97	1.12
1:C:142:ARG:HG2	1:C:142:ARG:NH2	1.77	0.92
1:C:56:THR:HB	3:C:467:HOH:O	1.72	0.89
2:D:62:LEU:HD22	3:D:369:HOH:O	1.74	0.86
2:B:216:CYS:O	2:B:217:ASP:HB2	1.76	0.85
1:A:106:ILE:HD12	3:A:437:HOH:O	1.78	0.82
1:A:187:GLU:HG3	3:A:471:HOH:O	1.80	0.81

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:72:ASP:OD2	2:D:75:LYS:HG3	1.81	0.81
2:B:1:GLN:NE2	2:B:1:GLN:HA	1.96	0.80
1:C:149:LYS:HG2	1:C:154:LEU:HD12	1.65	0.77
1:C:149:LYS:HE2	1:C:154:LEU:HD11	1.71	0.73
2:D:6:GLU:HG3	2:D:92:CYS:SG	2.30	0.71
2:B:40:ALA:HB3	2:B:43:LYS:HG3	1.73	0.70
1:A:60:ALA:H	2:D:99:ARG:NH1	1.89	0.70
2:D:127:SER:O	2:D:131:THR:HG23	1.92	0.70
1:A:147:GLN:OE1	1:A:154:LEU:HD11	1.92	0.69
2:D:119:PRO:HB3	2:D:145:TYR:HB3	1.75	0.69
1:A:54:ARG:HD2	3:A:422:HOH:O	1.92	0.69
1:C:142:ARG:HH21	1:C:142:ARG:CG	1.88	0.68
2:B:6:GLU:HG3	2:B:92:CYS:SG	2.33	0.68
2:B:1:GLN:HA	2:B:1:GLN:HE21	1.59	0.67
2:B:199:ASN:OD1	2:B:206:LYS:HE2	1.95	0.66
1:C:193:ALA:HB2	1:C:208:SER:HB3	1.77	0.66
2:D:82:MET:HE1	2:D:109:VAL:HG21	1.79	0.64
2:B:119:PRO:HB3	2:B:145:TYR:HB3	1.78	0.64
2:D:87:ARG:O	2:D:88:ALA:HB2	1.98	0.64
1:C:170:ASP:O	1:C:171:SER:HB2	1.96	0.64
1:A:11:LEU:HG	1:A:13:LEU:HD22	1.79	0.64
1:A:59:PRO:HA	2:D:99:ARG:HH11	1.64	0.63
1:A:144:ALA:O	1:A:145:LYS:HD2	1.98	0.62
1:C:125:LEU:O	1:C:183:LYS:HE2	2.00	0.62
2:B:20:LEU:HG	2:B:82:MET:HE2	1.82	0.61
2:B:178:LEU:HD12	2:B:178:LEU:C	2.26	0.61
1:A:94:TRP:HB2	1:A:95:PRO:HA	1.82	0.61
2:D:99:ARG:HD2	3:D:332:HOH:O	2.00	0.60
2:D:178:LEU:C	2:D:178:LEU:HD12	2.25	0.60
2:B:199:ASN:ND2	2:B:201:LYS:HG3	2.17	0.60
1:C:90:GLN:HE22	1:C:93:ASN:H	1.50	0.60
1:A:162:SER:OG	2:B:167:PRO:HD2	2.01	0.60
1:C:185:ASP:HA	1:C:188:LYS:HD3	1.84	0.60
1:C:162:SER:OG	2:D:167:PRO:HD2	2.02	0.59
1:C:37:GLN:HB2	1:C:47:LEU:HD11	1.83	0.59
1:A:60:ALA:H	2:D:99:ARG:HH11	1.51	0.59
1:C:94:TRP:HB2	1:C:95:PRO:HA	1.84	0.59
1:A:109:THR:HG23	3:A:306:HOH:O	2.03	0.59
2:B:213:PRO:HD3	3:B:381:HOH:O	2.03	0.58
2:B:12:VAL:CG2	2:B:18:LEU:HD22	2.34	0.58
2:B:13:GLN:HB2	2:B:16:ARG:HD2	1.84	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:13:GLN:O	2:D:16:ARG:HG2	2.03	0.57
2:D:127:SER:HB2	2:D:216:CYS:SG	2.45	0.57
2:B:127:SER:O	2:B:131:THR:HG23	2.05	0.56
1:C:43:ALA:H	2:D:105:GLN:HE22	1.53	0.56
2:B:66:ARG:NH2	2:B:86:ASP:OD2	2.34	0.56
2:B:199:ASN:HD22	2:B:201:LYS:HG3	1.72	0.55
2:B:12:VAL:HG21	2:B:18:LEU:HD22	1.88	0.55
2:D:85:GLU:H	2:D:85:GLU:CD	2.15	0.54
2:D:87:ARG:HG2	2:D:111:VAL:H	1.73	0.54
1:C:193:ALA:CB	1:C:208:SER:HB3	2.37	0.54
1:C:140:TYR:CD1	1:C:141:PRO:HA	2.43	0.54
2:D:12:VAL:HG11	2:D:82(C):LEU:HD13	1.91	0.53
2:D:19:ARG:HH11	2:D:19:ARG:HG3	1.74	0.53
2:D:19:ARG:HG3	2:D:19:ARG:NH1	2.24	0.53
2:D:131:THR:HG21	3:D:381:HOH:O	2.10	0.52
1:C:90:GLN:NE2	1:C:92:GLY:H	2.06	0.52
1:C:113:PRO:HB3	1:C:139:PHE:HB3	1.91	0.52
1:A:213:GLU:HG2	2:B:216:CYS:SG	2.49	0.52
1:A:183:LYS:O	1:A:187:GLU:HG2	2.11	0.51
2:B:178:LEU:HA	3:B:331:HOH:O	2.08	0.51
1:C:142:ARG:HD2	3:C:482:HOH:O	2.10	0.51
1:A:143:GLU:CD	1:A:143:GLU:H	2.19	0.50
2:B:199:ASN:ND2	2:B:201:LYS:CG	2.74	0.50
1:C:205:VAL:CG1	1:C:207:LYS:HE2	2.41	0.50
2:B:40:ALA:HB3	2:B:43:LYS:CG	2.41	0.50
1:C:154:LEU:HD13	3:C:412:HOH:O	2.12	0.50
1:C:151:ASP:OD2	1:C:189:HIS:HD2	1.94	0.50
2:D:17:SER:HA	2:D:82:MET:O	2.12	0.50
1:A:175:LEU:C	1:A:175:LEU:HD23	2.37	0.49
2:B:87:ARG:O	2:B:88:ALA:HB2	2.11	0.49
1:C:24:ARG:HA	1:C:69:THR:O	2.12	0.49
1:C:167:ASP:HB3	1:C:170:ASP:HB2	1.95	0.49
1:C:209:PHE:HB3	2:D:129:LYS:HD3	1.94	0.49
2:D:75:LYS:O	2:D:77:THR:HG23	2.13	0.48
2:D:12:VAL:HG22	2:D:16:ARG:HB2	1.94	0.48
2:B:43:LYS:HZ3	2:B:43:LYS:HB3	1.78	0.48
2:D:40:ALA:HB3	2:D:43:LYS:HD3	1.96	0.48
1:A:24:ARG:HA	1:A:69:THR:O	2.13	0.48
1:C:142:ARG:HG2	1:C:142:ARG:O	2.14	0.48
2:D:99:ARG:NH2	3:D:376:HOH:O	2.47	0.48
1:C:142:ARG:CZ	1:C:163:VAL:HG21	2.44	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:12:SER:O	1:A:13:LEU:HD13	2.14	0.47
1:A:54:ARG:CD	3:A:422:HOH:O	2.55	0.47
1:A:124:GLN:NE2	3:A:421:HOH:O	2.47	0.47
2:B:22:CYS:HB3	2:B:78:LEU:HB3	1.97	0.47
2:D:199:ASN:HD22	2:D:200:HIS:N	2.13	0.47
1:A:79:GLU:OE1	1:A:81:GLU:OE1	2.33	0.47
2:B:13:GLN:HE21	2:B:13:GLN:HB3	1.54	0.47
2:D:131:THR:CG2	3:D:381:HOH:O	2.62	0.47
1:A:144:ALA:C	1:A:145:LYS:HD2	2.41	0.46
2:B:93:ALA:HB1	2:B:100(H):ILE:HG23	1.97	0.46
1:C:151:ASP:OD2	1:C:189:HIS:CD2	2.68	0.46
1:C:175:LEU:HD23	1:C:175:LEU:C	2.40	0.46
1:A:10:THR:HG22	3:A:365:HOH:O	2.16	0.46
1:C:90:GLN:HE21	1:C:92:GLY:H	1.64	0.46
2:D:93:ALA:HB1	2:D:100(H):ILE:HG23	1.97	0.46
2:D:12:VAL:CG2	2:D:16:ARG:HB2	2.46	0.46
1:A:56:THR:OG1	1:C:56:THR:CG2	2.64	0.45
2:B:13:GLN:HB2	2:B:16:ARG:CD	2.47	0.45
2:D:126:PRO:HA	2:D:130:SER:OG	2.17	0.45
2:D:201:LYS:HE3	3:D:364:HOH:O	2.16	0.45
1:A:42:GLN:HE21	1:A:42:GLN:HB2	1.58	0.45
1:A:185:ASP:O	1:A:188:LYS:HB3	2.17	0.44
1:C:142:ARG:NH2	1:C:142:ARG:CG	2.58	0.44
1:C:145:LYS:CE	1:C:147:GLN:HG2	2.47	0.44
2:B:178:LEU:C	2:B:178:LEU:CD1	2.91	0.44
2:D:6:GLU:CG	2:D:92:CYS:SG	3.03	0.44
1:A:37:GLN:HB2	1:A:47:LEU:HD11	2.00	0.44
1:A:59:PRO:HG2	1:A:62:PHE:CD1	2.53	0.44
1:C:123:GLU:CD	3:C:345:HOH:O	2.61	0.44
2:D:20:LEU:HD13	2:D:82:MET:HE2	1.99	0.43
1:C:145:LYS:HB3	1:C:197:THR:HB	2.00	0.43
1:A:56:THR:OG1	1:C:56:THR:HG22	2.18	0.43
1:C:79:GLU:OE1	1:C:81:GLU:OE1	2.37	0.43
2:D:194:TYR:O	2:D:195:ILE:HD13	2.18	0.43
2:B:50:VAL:HG12	2:B:58:HIS:HB2	2.00	0.43
1:C:188:LYS:HG3	3:C:413:HOH:O	2.19	0.43
2:D:50:VAL:HG12	2:D:58:HIS:HB2	2.00	0.42
1:C:93:ASN:ND2	3:C:441:HOH:O	2.52	0.42
1:C:142:ARG:NH1	1:C:163:VAL:HG21	2.33	0.42
1:A:96:ILE:HB	2:B:47:TRP:CG	2.55	0.42
2:B:12:VAL:HG11	2:B:82(C):LEU:HD12	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:12:VAL:HG11	2:D:82(C):LEU:CD1	2.50	0.42
2:B:19:ARG:NH2	3:B:443:HOH:O	2.53	0.42
1:A:175:LEU:HD23	1:A:176:SER:N	2.34	0.42
2:B:6:GLU:CG	2:B:92:CYS:SG	3.06	0.42
1:C:143:GLU:H	1:C:143:GLU:CD	2.28	0.41
2:B:148:GLU:OE2	2:B:168:ALA:HB3	2.19	0.41
1:C:170:ASP:HB3	1:C:172:THR:HG23	2.01	0.41
1:C:18:ARG:CB	1:C:76:SER:HA	2.50	0.41
2:B:126:PRO:HG2	2:B:213:PRO:HA	2.02	0.41
1:A:207:LYS:HA	1:A:207:LYS:HD3	1.67	0.41
2:D:22:CYS:HB3	2:D:78:LEU:HB3	2.03	0.40
1:C:140:TYR:CG	1:C:141:PRO:HA	2.55	0.40
1:C:90:GLN:HE21	1:C:90:GLN:HB2	1.69	0.40
2:D:144:ASP:HB3	2:D:175:LEU:HD13	2.03	0.40
1:A:124:GLN:HE22	1:A:131:SER:HB2	1.86	0.40
1:C:124:GLN:C	1:C:126:LYS:H	2.29	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	210/215 (98%)	203 (97%)	7 (3%)	0	100	100
1	C	210/215 (98%)	203 (97%)	7 (3%)	0	100	100
2	B	227/236 (96%)	219 (96%)	8 (4%)	0	100	100
2	D	226/236 (96%)	221 (98%)	4 (2%)	1 (0%)	30	16
All	All	873/902 (97%)	846 (97%)	26 (3%)	1 (0%)	48	31

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	D	88	ALA

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	183/184 (100%)	174 (95%)	9 (5%)	22	8
1	C	183/184 (100%)	173 (94%)	10 (6%)	19	6
2	B	193/199 (97%)	183 (95%)	10 (5%)	21	7
2	D	192/199 (96%)	183 (95%)	9 (5%)	23	9
All	All	751/766 (98%)	713 (95%)	38 (5%)	21	7

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

Mol	Chain	Res	Type
1	A	1	GLU
1	A	13	LEU
1	A	105	GLU
1	A	109	THR
1	A	147	GLN
1	A	152	ASN
1	A	161	GLU
1	A	176	SER
1	A	202	SER
2	B	1	GLN
2	B	13	GLN
2	B	75	LYS
2	B	132	SER
2	B	141	LEU
2	B	149	PRO
2	B	169	VAL
2	B	170	LEU
2	B	178	LEU
2	B	210	LYS
1	C	18	ARG
1	C	33	LEU

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Mol	Chain	Res	Type
1	C	90	GLN
1	C	93	ASN
1	C	104	LEU
1	C	105	GLU
1	C	126	LYS
1	C	142	ARG
1	C	156	SER
1	C	169	LYS
2	D	1	GLN
2	D	19	ARG
2	D	20	LEU
2	D	62	LEU
2	D	129	LYS
2	D	141	LEU
2	D	149	PRO
2	D	178	LEU
2	D	191	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (26) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	42	GLN
1	A	124	GLN
1	A	137	ASN
1	A	152	ASN
1	A	189	HIS
1	A	199	GLN
2	B	1	GLN
2	B	13	GLN
2	B	58	HIS
2	B	82(A)	ASN
2	B	164	HIS
1	C	90	GLN
1	C	93	ASN
1	C	124	GLN
1	C	137	ASN
1	C	138	ASN
1	C	189	HIS
1	C	199	GLN
1	C	210	ASN
2	D	32	HIS
2	D	56	HIS

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Mol	Chain	Res	Type
2	D	58	HIS
2	D	76	ASN
2	D	105	GLN
2	D	164	HIS
2	D	199	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](#)

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 [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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	214/215 (99%)	0.24	8 (3%) 45 49	7, 13, 24, 33	0
1	C	214/215 (99%)	0.19	9 (4%) 40 45	8, 13, 23, 29	0
2	B	229/236 (97%)	0.32	12 (5%) 33 36	7, 14, 23, 36	0
2	D	228/236 (96%)	0.53	15 (6%) 24 26	9, 17, 28, 36	0
All	All	885/902 (98%)	0.32	44 (4%) 34 38	7, 14, 24, 36	0

All (44) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	216	CYS	5.0
1	A	214	CYS	4.3
1	C	170	ASP	4.1
2	B	102	TYR	3.9
2	B	99	ARG	3.6
2	D	99	ARG	3.3
2	B	92	CYS	3.2
2	B	217	ASP	3.2
2	D	191	THR	3.1
2	D	62	LEU	2.9
2	D	87	ARG	2.9
2	D	28	THR	2.8
2	D	190	GLY	2.8
2	B	169	VAL	2.6
1	C	214	CYS	2.6
2	B	131	THR	2.5
1	C	169	LYS	2.5
2	D	41	PRO	2.5
2	B	132	SER	2.5
2	B	201	LYS	2.5
2	D	216	CYS	2.4

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Mol	Chain	Res	Type	RSRZ
1	C	128	GLY	2.4
1	A	168	SER	2.4
1	A	202	SER	2.4
1	C	194	CYS	2.4
2	B	1	GLN	2.4
1	C	18	ARG	2.3
1	C	188	LYS	2.3
2	D	131	THR	2.3
2	D	113	SER	2.3
1	A	126	LYS	2.3
2	D	1	GLN	2.3
1	C	202	SER	2.3
2	D	102	TYR	2.2
1	A	205	VAL	2.2
2	D	92	CYS	2.2
1	C	126	LYS	2.2
2	D	75	LYS	2.2
2	B	100(A)	ASN	2.1
1	A	152	ASN	2.1
1	A	194	CYS	2.1
2	B	98	SER	2.0
1	A	147	GLN	2.0
2	D	129	LYS	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](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.