



Full wwPDB X-ray Structure Validation Report ⓘ

Apr 5, 2026 – 02:00 AM UTC

PDB ID : 9NW6 / pdb_00009nw6
Title : CA147v24 Fab bound to HLA-E-VL9
Authors : Wrapp, D.; Hwang, J.K.; Marston, D.J.; Haynes, B.F.; Azoitei, M.L.
Deposited on : 2025-03-21
Resolution : 3.10 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

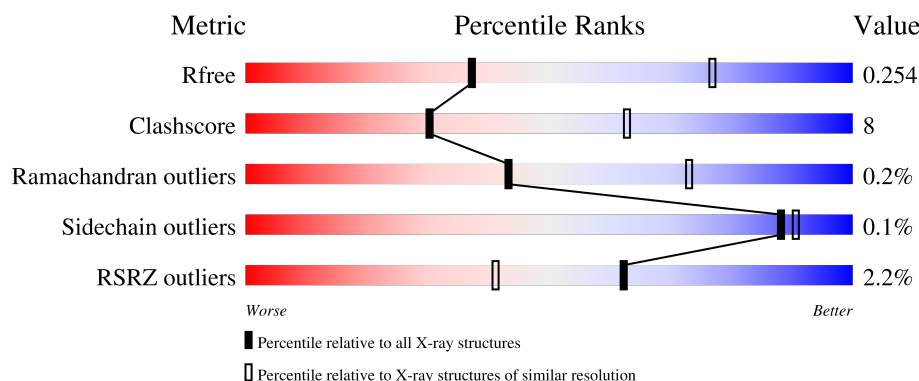
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.10 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	1456 (3.10-3.10)
Clashscore	190562	1539 (3.10-3.10)
Ramachandran outliers	187476	1467 (3.10-3.10)
Sidechain outliers	187428	1467 (3.10-3.10)
RSRZ outliers	180081	1456 (3.10-3.10)

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	275	<div> <div></div> <div>89%</div> <div>10%</div> <div>.</div> </div>
1	C	275	<div> <div>3%</div> <div>83%</div> <div>14%</div> <div>..</div> </div>
2	B	100	<div> <div></div> <div>91%</div> <div>9%</div> </div>
2	D	100	<div> <div>3%</div> <div>90%</div> <div>10%</div> </div>
3	E	234	<div> <div>5%</div> <div>78%</div> <div>16%</div> <div>..</div> </div>

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Mol	Chain	Length	Quality of chain
3	G	234	<div> <div></div> <div>77%</div> <div>16%</div> <div>7%</div> </div>
4	F	9	<div> <div>11%</div> <div>56%</div> <div>33%</div> </div>
4	P	9	<div> <div>78%</div> <div>22%</div> </div>
5	H	214	<div> <div></div> <div>91%</div> <div>9%</div> </div>
5	I	214	<div> <div>3%</div> <div>86%</div> <div>14%</div> </div>

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 12854 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 HLA class I histocompatibility antigen, alpha chain E.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	273	Total	C	N	O	S	0	0	0
			2227	1392	398	430	7			
1	C	269	Total	C	N	O	S	0	0	0
			2197	1375	391	424	7			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	0	MET	-	initiating methionine	UNP P13747
C	0	MET	-	initiating methionine	UNP P13747

- Molecule 2 is a protein called Beta-2-microglobulin.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	100	Total	C	N	O	S	0	0	0
			837	533	141	159	4			
2	D	100	Total	C	N	O	S	0	0	0
			837	533	141	159	4			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	1	MET	-	initiating methionine	UNP P61769
D	1	MET	-	initiating methionine	UNP P61769

- Molecule 3 is a protein called CA147v24 heavy chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	E	224	Total	C	N	O	S	0	0	0
			1677	1057	281	332	7			
3	G	224	Total	C	N	O	S	0	0	0
			1677	1057	281	332	7			

- Molecule 4 is a protein called VL9 peptide.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	F	9	Total	C	N	O	S	0	0	0
			70	46	12	11	1			
4	P	9	Total	C	N	O	S	0	0	0
			70	46	12	11	1			

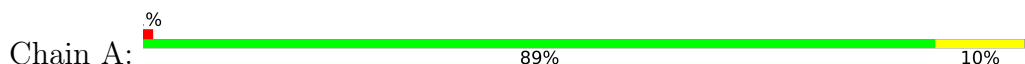
- Molecule 5 is a protein called CA147v24 light chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	H	214	Total	C	N	O	S	0	0	0
			1631	1018	276	332	5			
5	I	214	Total	C	N	O	S	0	0	0
			1631	1018	276	332	5			

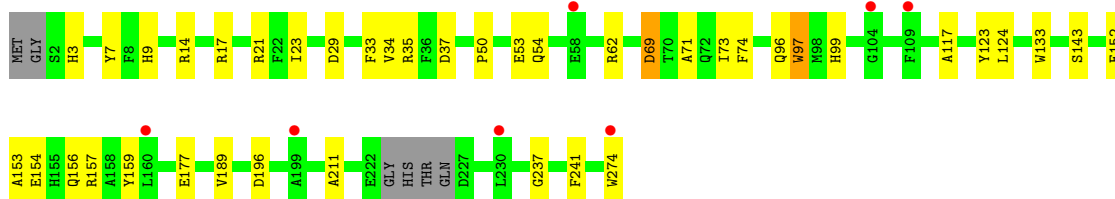
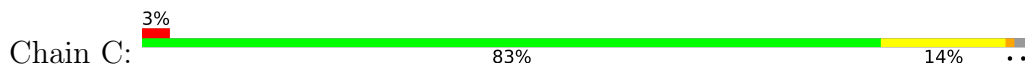
3 Residue-property plots [i](#)

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.

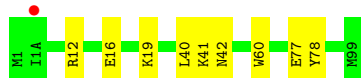
- Molecule 1: HLA class I histocompatibility antigen, alpha chain E



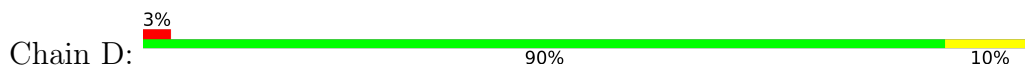
- Molecule 1: HLA class I histocompatibility antigen, alpha chain E



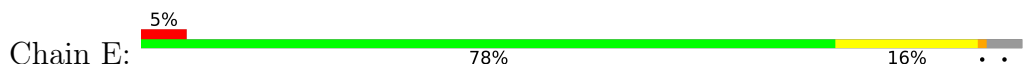
- Molecule 2: Beta-2-microglobulin

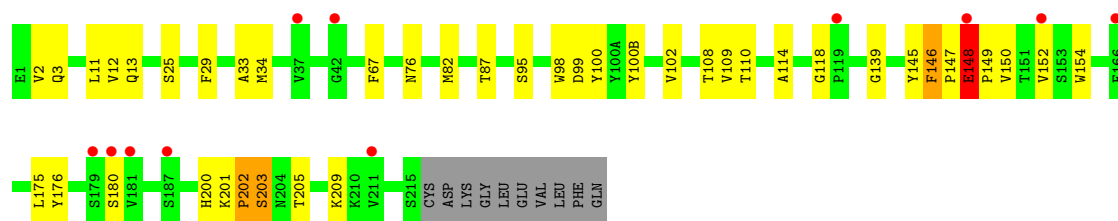


- Molecule 2: Beta-2-microglobulin

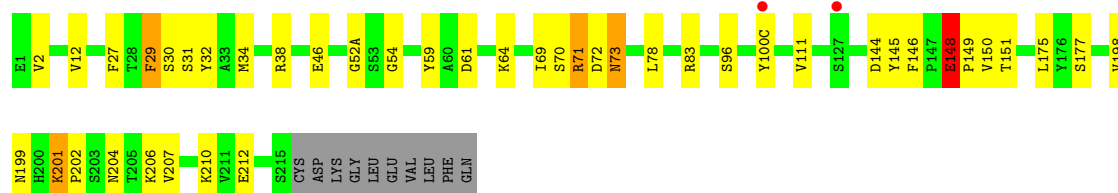
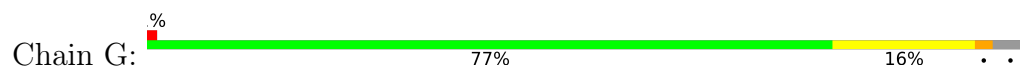


- Molecule 3: CA147v24 heavy chain

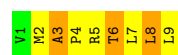
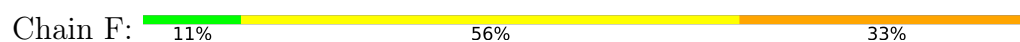




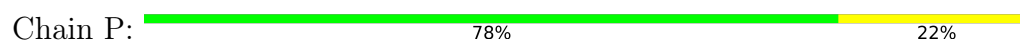
• Molecule 3: CA147v24 heavy chain



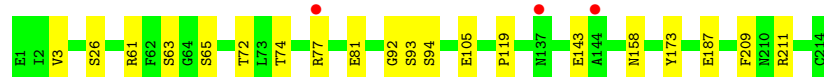
• Molecule 4: VL9 peptide



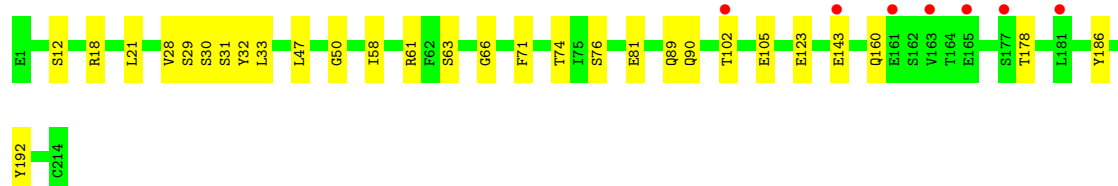
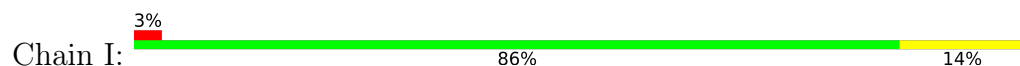
• Molecule 4: VL9 peptide



• Molecule 5: CA147v24 light chain



• Molecule 5: CA147v24 light chain



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	73.68Å 92.86Å 319.26Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	79.81 – 3.10 79.81 – 3.10	Depositor EDS
% Data completeness (in resolution range)	99.3 (79.81-3.10) 99.3 (79.81-3.10)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.82 (at 3.13Å)	Xtriage
Refinement program	PHENIX dev_3758	Depositor
R, R_{free}	0.239 , 0.258 0.236 , 0.254	Depositor DCC
R_{free} test set	2002 reflections (4.91%)	wwPDB-VP
Wilson B-factor (Å ²)	77.2	Xtriage
Anisotropy	0.829	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.28 , 50.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	12854	wwPDB-VP
Average B, all atoms (Å ²)	82.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 13.91% 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	0.44	0/2293	0.63	0/3118
1	C	0.72	6/2261 (0.3%)	0.66	0/3073
2	B	0.36	0/860	0.66	0/1162
2	D	0.35	0/860	0.66	0/1162
3	E	0.83	4/1718 (0.2%)	0.83	5/2338 (0.2%)
3	G	1.19	12/1718 (0.7%)	1.22	11/2338 (0.5%)
4	F	2.55	2/70 (2.9%)	1.92	3/93 (3.2%)
4	P	0.43	0/70	0.92	0/93
5	H	0.31	0/1665	0.61	0/2259
5	I	0.49	0/1665	0.70	1/2259 (0.0%)
All	All	0.70	24/13180 (0.2%)	0.78	20/17895 (0.1%)

All (24) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	G	29	PHE	C-O	-6.91	1.16	1.24
1	C	71	ALA	CA-C	-6.79	1.44	1.52
3	G	29	PHE	CA-C	-6.73	1.44	1.52
3	G	148	GLU	CA-C	-6.60	1.45	1.52
1	C	97	TRP	C-O	-6.07	1.16	1.23
4	F	3	ALA	CA-C	-6.06	1.45	1.52
1	C	71	ALA	C-O	-5.96	1.17	1.24
3	G	177	SER	C-O	-5.95	1.16	1.23
3	E	109	VAL	CA-CB	-5.92	1.46	1.54
1	C	96	GLN	C-O	-5.78	1.16	1.23
3	G	32	TYR	C-O	-5.65	1.16	1.23
1	C	157	ARG	C-O	-5.50	1.17	1.24
3	E	100(B)	TYR	C-O	-5.32	1.17	1.24
3	G	73	ASN	C-O	-5.30	1.18	1.24
3	G	175	LEU	C-O	-5.26	1.17	1.24
3	G	72	ASP	CA-C	-5.16	1.46	1.53
3	E	114	ALA	CA-C	-5.14	1.46	1.52
1	C	69	ASP	CA-C	-5.13	1.46	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	G	70	SER	C-O	-5.12	1.17	1.23
3	G	71	ARG	C-O	-5.10	1.17	1.23
3	G	12	VAL	C-O	-5.09	1.17	1.23
4	F	8	LEU	CA-C	-5.07	1.46	1.52
3	G	207	VAL	C-O	-5.06	1.19	1.24
3	E	100(B)	TYR	CA-C	-5.04	1.45	1.52

All (20) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	G	148	GLU	CA-C-N	27.47	154.18	119.84
3	G	148	GLU	C-N-CA	27.47	154.18	119.84
3	G	148	GLU	C-N-CD	-11.59	77.49	125.00
4	F	3	ALA	CA-C-N	7.91	128.39	119.93
4	F	3	ALA	C-N-CA	7.91	128.39	119.93
3	G	201	LYS	CA-C-N	7.82	129.61	119.84
3	G	201	LYS	C-N-CA	7.82	129.61	119.84
3	G	54	GLY	N-CA-C	-7.72	104.39	115.27
3	E	148	GLU	N-CA-C	7.15	125.61	109.81
5	I	66	GLY	N-CA-C	6.60	118.84	111.85
3	E	146	PHE	N-CA-C	6.09	123.27	109.81
3	G	30	SER	N-CA-C	6.08	119.79	112.38
3	E	203	SER	N-CA-C	-6.00	103.72	113.19
4	F	6	THR	N-CA-C	5.71	118.12	110.35
3	E	118	GLY	CA-C-N	-5.64	114.79	120.31
3	E	118	GLY	C-N-CA	-5.64	114.79	120.31
3	G	148	GLU	N-CA-C	5.63	119.44	108.85
3	G	198	VAL	N-CA-C	5.59	115.94	108.11
3	G	144	ASP	N-CA-C	5.39	117.76	111.02
3	G	31	SER	N-CA-C	5.03	119.10	112.92

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	2227	0	2062	24	0
1	C	2197	0	2036	58	0
2	B	837	0	803	7	0
2	D	837	0	803	7	0
3	E	1677	0	1635	49	0
3	G	1677	0	1635	33	0
4	F	70	0	85	44	0
4	P	70	0	85	4	0
5	H	1631	0	1586	12	1
5	I	1631	0	1586	25	1
All	All	12854	0	12316	211	1

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 8.

All (211) 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:9:HIS:CE1	4:F:2:MET:HE3	1.63	1.34
1:C:152:GLU:CD	4:F:7:LEU:CD2	2.02	1.31
3:G:52(A):GLY:HA2	3:G:71:ARG:NH1	1.50	1.24
1:C:152:GLU:CB	4:F:7:LEU:HD21	1.68	1.23
3:G:201:LYS:HB2	3:G:202:PRO:CD	1.70	1.20
1:C:152:GLU:CG	4:F:7:LEU:CD2	2.28	1.12
1:C:143:SER:HB3	4:F:9:LEU:HD22	1.27	1.10
3:G:201:LYS:HB2	3:G:202:PRO:HD3	1.29	1.09
1:C:152:GLU:CD	4:F:7:LEU:HD23	1.76	1.08
1:A:222:GLU:OE1	1:A:224:HIS:HD2	1.37	1.07
3:G:52(A):GLY:HA2	3:G:71:ARG:HH12	0.92	1.07
1:C:143:SER:HB3	4:F:9:LEU:CD2	1.86	1.05
3:E:100:TYR:CZ	4:F:4:PRO:HD3	1.92	1.03
1:C:9:HIS:HE1	4:F:2:MET:HE3	0.92	1.03
4:F:8:LEU:HD12	4:F:8:LEU:O	1.58	1.03
1:C:152:GLU:HB3	4:F:7:LEU:HD21	1.02	1.01
1:C:143:SER:CB	4:F:9:LEU:HD22	1.94	0.96
1:C:152:GLU:HB3	4:F:7:LEU:CD2	1.94	0.96
1:C:152:GLU:CG	4:F:7:LEU:HD22	1.95	0.95
1:C:152:GLU:CG	4:F:7:LEU:HD21	1.96	0.94
1:C:9:HIS:CE1	4:F:2:MET:CE	2.50	0.93
1:C:152:GLU:HG3	4:F:7:LEU:HD22	1.51	0.90
3:E:201:LYS:HB2	3:E:202:PRO:HD3	1.54	0.90
1:C:152:GLU:CB	4:F:7:LEU:CD2	2.48	0.89

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:16:GLU:OE1	2:B:19:LYS:NZ	2.04	0.89
3:E:100:TYR:CE1	4:F:4:PRO:HD3	2.06	0.88
3:E:146:PHE:HB3	3:E:147:PRO:HD3	1.53	0.88
3:E:203:SER:OG	3:E:205:THR:OG1	1.91	0.88
1:C:35:ARG:NH1	2:D:53:ASP:OD1	2.05	0.88
3:G:204:ASN:O	3:G:204:ASN:ND2	2.08	0.87
3:G:201:LYS:HB2	3:G:202:PRO:HD2	1.56	0.86
5:I:33:LEU:O	5:I:50:GLY:O	1.92	0.86
5:I:33:LEU:HD12	5:I:89:GLN:O	1.75	0.85
1:A:222:GLU:OE1	1:A:224:HIS:CD2	2.29	0.85
1:C:123:TYR:HE2	4:F:9:LEU:HD13	1.43	0.83
3:G:201:LYS:CB	3:G:202:PRO:CD	2.42	0.81
5:H:105:GLU:OE2	5:H:173:TYR:OH	1.98	0.81
1:C:152:GLU:CD	4:F:7:LEU:HD21	1.95	0.81
4:F:8:LEU:HD12	4:F:8:LEU:C	2.04	0.80
1:C:123:TYR:CE2	4:F:9:LEU:HD13	2.16	0.80
3:E:201:LYS:HD3	3:E:201:LYS:H	1.44	0.80
3:E:11:LEU:C	3:E:11:LEU:HD12	2.06	0.80
1:C:152:GLU:OE1	4:F:7:LEU:CD2	2.30	0.79
3:G:201:LYS:CB	3:G:202:PRO:HD3	2.09	0.78
1:A:35:ARG:HG2	1:A:48:ARG:HD2	1.64	0.78
1:C:69:ASP:HB3	4:F:5:ARG:HH11	1.49	0.76
1:C:189:VAL:HG11	1:C:274:TRP:HB2	1.68	0.75
3:G:52(A):GLY:CA	3:G:71:ARG:NH1	2.42	0.75
3:G:71:ARG:HD3	3:G:73:ASN:OD1	1.87	0.74
1:C:152:GLU:CD	4:F:7:LEU:HD22	2.08	0.73
3:E:201:LYS:H	3:E:201:LYS:CD	1.99	0.73
3:G:38:ARG:HD2	3:G:46:GLU:OE2	1.90	0.72
3:E:146:PHE:CB	3:E:147:PRO:HD3	2.21	0.69
1:C:152:GLU:OE1	4:F:7:LEU:HD23	1.91	0.69
4:F:8:LEU:O	4:F:8:LEU:CD1	2.40	0.69
3:E:201:LYS:CB	3:E:202:PRO:HD3	2.23	0.69
1:A:224:HIS:O	1:A:224:HIS:ND1	2.27	0.68
3:E:148:GLU:HB3	3:E:176:TYR:CE2	2.29	0.68
3:E:11:LEU:HD12	3:E:11:LEU:O	1.93	0.68
3:G:151:THR:OG1	3:G:199:ASN:ND2	2.27	0.67
1:C:143:SER:HB3	4:F:9:LEU:HD23	1.78	0.66
3:E:201:LYS:HB2	3:E:202:PRO:CD	2.26	0.65
1:C:154:GLU:OE1	1:C:154:GLU:N	2.31	0.63
4:F:5:ARG:HH21	5:I:31:SER:HB2	1.63	0.63
3:G:199:ASN:HB3	3:G:206:LYS:HE3	1.81	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:152:GLU:OE1	4:F:7:LEU:HD21	1.96	0.62
3:G:201:LYS:N	3:G:202:PRO:HD2	2.16	0.61
3:G:148:GLU:O	3:G:148:GLU:HG3	2.00	0.60
3:E:201:LYS:HD3	3:E:201:LYS:N	2.15	0.60
1:A:117:ALA:HB2	2:B:60:TRP:CE2	2.38	0.59
5:I:28:VAL:HG22	5:I:29:SER:H	1.67	0.59
1:A:133:TRP:CZ2	4:P:7:LEU:HD11	2.38	0.58
3:G:34:MET:HB2	3:G:71:ARG:HH21	1.69	0.57
5:I:61:ARG:NH2	5:I:81:GLU:OE2	2.38	0.57
3:E:11:LEU:C	3:E:11:LEU:CD1	2.78	0.57
2:D:77:GLU:OE1	2:D:94:LYS:HD3	2.05	0.56
5:I:63:SER:HB3	5:I:74:THR:HG23	1.87	0.56
1:A:85:TYR:O	1:A:86:ASN:HB2	2.04	0.56
1:C:50:PRO:HA	1:C:53:GLU:OE1	2.06	0.56
5:I:21:LEU:HD23	5:I:102:THR:HB	1.88	0.56
5:I:33:LEU:CD1	5:I:89:GLN:O	2.52	0.56
1:A:133:TRP:CE2	4:P:7:LEU:HD11	2.41	0.56
1:A:173:GLU:O	1:A:176:LYS:HD3	2.06	0.56
3:E:87:THR:HG23	3:E:110:THR:HA	1.87	0.55
1:C:21:ARG:HD3	1:C:23:ILE:HD11	1.89	0.55
3:G:210:LYS:NZ	3:G:212:GLU:OE2	2.38	0.55
3:E:201:LYS:CB	3:E:202:PRO:CD	2.84	0.54
1:C:62:ARG:HG2	1:C:62:ARG:HH11	1.73	0.54
3:E:145:TYR:C	3:E:145:TYR:CD1	2.85	0.54
3:E:33:ALA:HB2	3:E:99:ASP:HA	1.90	0.54
4:F:5:ARG:NH2	5:I:31:SER:HB2	2.22	0.54
3:G:145:TYR:CZ	3:G:150:VAL:HG21	2.42	0.54
2:B:42:ASN:HA	2:B:77:GLU:HB3	1.89	0.54
5:I:32:TYR:HB2	5:I:90:GLN:OE1	2.08	0.53
3:G:146:PHE:CD2	3:G:146:PHE:C	2.85	0.53
3:E:95:SER:OG	3:E:98:TRP:O	2.22	0.53
3:G:145:TYR:C	3:G:145:TYR:CD2	2.86	0.53
5:I:33:LEU:CD2	5:I:71:PHE:CG	2.91	0.53
5:H:187:GLU:HG2	5:H:211:ARG:HD2	1.90	0.53
3:E:100:TYR:CZ	4:F:4:PRO:CD	2.81	0.52
5:H:92:GLY:C	5:H:94:SER:H	2.17	0.52
3:G:100(C):TYR:HA	4:P:5:ARG:HH22	1.75	0.52
1:C:14:ARG:HB3	1:C:17:ARG:HB2	1.92	0.52
3:E:11:LEU:C	3:E:12:VAL:HG23	2.35	0.51
3:E:147:PRO:HD2	3:E:200:HIS:CE1	2.46	0.51
1:C:159:TYR:CE2	4:F:3:ALA:HB2	2.46	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:36:PHE:HZ	1:A:68:ARG:HD3	1.75	0.51
1:C:21:ARG:NH2	1:C:37:ASP:OD2	2.43	0.51
5:H:77:ARG:HH11	5:H:77:ARG:HB3	1.76	0.51
1:C:152:GLU:OE2	4:F:7:LEU:HD23	2.06	0.51
5:H:61:ARG:NH2	5:H:81:GLU:OE2	2.44	0.51
1:C:196:ASP:N	1:C:196:ASP:OD1	2.43	0.51
3:E:12:VAL:HG12	3:E:13:GLN:N	2.25	0.50
1:C:54:GLN:O	1:C:54:GLN:HG2	2.12	0.50
5:I:63:SER:HB3	5:I:74:THR:CG2	2.41	0.49
3:G:83:ARG:O	3:G:111:VAL:HG11	2.12	0.49
3:E:11:LEU:O	3:E:12:VAL:CG2	2.61	0.49
5:H:65:SER:HB3	5:H:72:THR:HG23	1.94	0.49
3:G:2:VAL:HG13	3:G:27:PHE:CD1	2.47	0.48
1:C:14:ARG:NH1	1:C:21:ARG:HB2	2.28	0.48
5:H:92:GLY:O	5:H:93:SER:OG	2.24	0.48
3:E:152:VAL:HG11	3:E:180:SER:CB	2.43	0.48
1:C:3:HIS:HA	1:C:29:ASP:OD1	2.14	0.48
5:I:12:SER:OG	5:I:105:GLU:OE1	2.22	0.48
5:H:158:ASN:OD1	5:H:158:ASN:N	2.47	0.48
5:I:18:ARG:HG3	5:I:76:SER:HA	1.96	0.48
3:E:100:TYR:OH	4:F:4:PRO:HD3	2.14	0.47
3:E:201:LYS:H	3:E:201:LYS:CE	2.27	0.47
2:D:73:THR:OG1	2:D:76:ASP:OD2	2.22	0.47
3:G:71:ARG:CD	3:G:73:ASN:OD1	2.61	0.47
1:A:68:ARG:HA	1:A:68:ARG:HD2	1.63	0.47
1:C:143:SER:OG	4:F:9:LEU:HB3	2.14	0.47
5:I:29:SER:C	5:I:30:SER:HG	2.21	0.47
3:E:2:VAL:HG11	3:E:102:VAL:HG21	1.96	0.47
1:A:151:SER:OG	1:A:154:GLU:OE2	2.27	0.46
1:C:21:ARG:CD	1:C:23:ILE:HD11	2.45	0.46
1:C:7:TYR:HB2	1:C:99:HIS:CE1	2.50	0.46
3:E:3:GLN:HB2	3:E:25:SER:HB3	1.97	0.46
1:A:226:GLN:N	1:A:226:GLN:CD	2.73	0.45
5:I:33:LEU:HD12	5:I:33:LEU:HA	1.45	0.45
2:B:40:LEU:O	2:B:78:TYR:HA	2.16	0.45
1:C:62:ARG:HH11	1:C:62:ARG:CG	2.30	0.45
2:D:7:ILE:HG12	2:D:82:VAL:HG21	1.98	0.45
5:H:77:ARG:HB3	5:H:77:ARG:NH1	2.32	0.45
3:E:145:TYR:CD1	3:E:145:TYR:O	2.70	0.45
3:E:146:PHE:CD1	3:E:146:PHE:O	2.70	0.45
1:C:211:ALA:HB2	1:C:241:PHE:CE2	2.52	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:74:PHE:CE1	4:F:6:THR:HG21	2.52	0.45
1:C:133:TRP:HE1	1:C:153:ALA:HB2	1.82	0.45
1:C:74:PHE:HE1	4:F:6:THR:HG21	1.82	0.45
3:E:11:LEU:HD22	3:E:146:PHE:HE2	1.82	0.44
3:E:29:PHE:CD2	3:E:76:ASN:HA	2.52	0.44
3:G:59:TYR:OH	3:G:69:ILE:HG22	2.17	0.44
3:G:145:TYR:CE1	3:G:150:VAL:HG21	2.53	0.44
3:E:11:LEU:O	3:E:12:VAL:HG23	2.17	0.44
3:E:209:LYS:NZ	5:I:123:GLU:OE1	2.49	0.44
1:C:117:ALA:HB2	2:D:60:TRP:CE2	2.53	0.44
3:E:12:VAL:CG1	3:E:13:GLN:N	2.81	0.43
5:I:160:GLN:CG	5:I:178:THR:HB	2.48	0.43
3:G:61:ASP:O	3:G:64:LYS:HB2	2.17	0.43
1:A:19:GLU:OE1	1:A:75:ARG:NH1	2.51	0.43
1:A:224:HIS:O	1:A:224:HIS:CG	2.70	0.43
5:H:63:SER:HB3	5:H:74:THR:HG23	2.00	0.43
1:C:133:TRP:NE1	1:C:153:ALA:HB2	2.33	0.43
5:I:28:VAL:HG22	5:I:29:SER:N	2.33	0.43
1:A:103:LEU:HD13	1:A:107:GLY:HA2	2.01	0.43
2:D:42:ASN:HA	2:D:77:GLU:HB2	2.00	0.43
3:E:29:PHE:CE1	3:E:34:MET:HE3	2.53	0.43
3:E:108:THR:HG22	3:E:110:THR:HG23	2.00	0.43
3:E:147:PRO:HG2	3:E:202:PRO:HB2	2.01	0.43
1:A:215:LEU:HD22	1:A:261:VAL:HG22	2.01	0.43
1:C:97:TRP:CZ3	4:F:6:THR:HB	2.53	0.43
1:A:111:ARG:HB3	1:A:111:ARG:NH1	2.34	0.43
3:G:34:MET:HB2	3:G:71:ARG:NH2	2.33	0.42
1:A:237:GLY:HA3	2:B:12:ARG:HH11	1.83	0.42
1:A:237:GLY:HA3	2:B:12:ARG:NH1	2.34	0.42
1:C:97:TRP:CH2	4:F:6:THR:HB	2.55	0.42
3:E:67:PHE:CD2	3:E:82:MET:HG2	2.55	0.42
5:I:89:GLN:HG2	5:I:90:GLN:N	2.33	0.42
1:C:124:LEU:HD22	4:F:9:LEU:CD2	2.50	0.42
3:E:139:GLY:HA2	3:E:154:TRP:CH2	2.55	0.42
5:H:119:PRO:HB3	5:H:209:PHE:CE2	2.54	0.42
1:A:62:ARG:NH1	3:G:96:SER:O	2.52	0.42
1:C:177:GLU:OE2	1:C:177:GLU:HA	2.20	0.42
3:E:67:PHE:HE2	3:E:82:MET:CE	2.33	0.41
5:I:33:LEU:HA	5:I:89:GLN:O	2.20	0.41
3:E:145:TYR:CE2	3:E:150:VAL:HG21	2.56	0.41
3:E:145:TYR:CE1	3:E:176:TYR:HB2	2.55	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:G:38:ARG:NH1	3:G:46:GLU:OE2	2.37	0.41
1:C:73:ILE:HD12	1:C:73:ILE:HG23	1.62	0.41
3:G:210:LYS:HZ2	3:G:212:GLU:CD	2.27	0.41
1:A:133:TRP:CH2	4:P:7:LEU:HD11	2.56	0.41
2:B:41:LYS:HA	2:B:77:GLU:O	2.20	0.41
3:G:29:PHE:CE1	3:G:34:MET:HE3	2.55	0.41
5:I:33:LEU:HD22	5:I:71:PHE:CG	2.56	0.41
1:C:33:PHE:CD2	1:C:34:VAL:HG13	2.56	0.41
3:E:146:PHE:CB	3:E:147:PRO:CD	2.93	0.41
4:F:3:ALA:HB1	4:F:4:PRO:HD2	2.03	0.41
5:H:3:VAL:H	5:H:26:SER:HB3	1.86	0.41
3:E:146:PHE:O	3:E:146:PHE:CG	2.70	0.41
3:G:34:MET:HG3	3:G:78:LEU:HD22	2.02	0.41
5:I:29:SER:C	5:I:31:SER:N	2.78	0.41
1:C:237:GLY:HA3	2:D:12:ARG:NH1	2.35	0.40
5:I:47:LEU:HA	5:I:58:ILE:HG12	2.04	0.40
5:I:186:TYR:HA	5:I:192:TYR:OH	2.21	0.40
1:A:108:ARG:NE	1:A:108:ARG:HA	2.37	0.40
1:A:204:TRP:CZ3	1:A:244:TRP:HD1	2.39	0.40
3:E:11:LEU:C	3:E:12:VAL:CG2	2.94	0.40
1:C:124:LEU:CD2	4:F:9:LEU:HD21	2.51	0.40
3:E:175:LEU:N	3:E:175:LEU:HD12	2.36	0.40
1:C:156:GLN:O	1:C:159:TYR:HB3	2.22	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:H:143:GLU:OE2	5:I:143:GLU:OE2[3_654]	2.11	0.09

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	271/275 (98%)	262 (97%)	9 (3%)	0	100	100
1	C	265/275 (96%)	257 (97%)	8 (3%)	0	100	100
2	B	98/100 (98%)	95 (97%)	3 (3%)	0	100	100
2	D	98/100 (98%)	96 (98%)	2 (2%)	0	100	100
3	E	222/234 (95%)	207 (93%)	12 (5%)	3 (1%)	9	34
3	G	222/234 (95%)	210 (95%)	11 (5%)	1 (0%)	24	57
4	F	7/9 (78%)	7 (100%)	0	0	100	100
4	P	7/9 (78%)	5 (71%)	2 (29%)	0	100	100
5	H	212/214 (99%)	203 (96%)	9 (4%)	0	100	100
5	I	212/214 (99%)	204 (96%)	8 (4%)	0	100	100
All	All	1614/1664 (97%)	1546 (96%)	64 (4%)	4 (0%)	43	73

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	E	149	PRO
3	G	149	PRO
3	E	202	PRO
3	E	148	GLU

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	235/236 (100%)	235 (100%)	0	100	100
1	C	232/236 (98%)	232 (100%)	0	100	100
2	B	95/95 (100%)	95 (100%)	0	100	100
2	D	95/95 (100%)	95 (100%)	0	100	100
3	E	187/196 (95%)	187 (100%)	0	100	100
3	G	187/196 (95%)	186 (100%)	1 (0%)	81	85
4	F	8/8 (100%)	8 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
4	P	8/8 (100%)	8 (100%)	0	100	100
5	H	184/184 (100%)	184 (100%)	0	100	100
5	I	184/184 (100%)	184 (100%)	0	100	100
All	All	1415/1438 (98%)	1414 (100%)	1 (0%)	88	90

All (1) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	G	148	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (13) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	197	HIS
1	A	224	HIS
2	B	17	ASN
2	B	31	HIS
1	C	96	GLN
1	C	127	ASN
1	C	255	GLN
2	D	2	GLN
3	E	204	ASN
5	H	42	GLN
5	H	124	GLN
5	I	42	GLN
5	I	147	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry

There are no ligands in this entry.

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q < 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	273/275 (99%)	0.12	2 (0%) 84 68	48, 77, 107, 142	0
1	C	269/275 (97%)	0.19	7 (2%) 57 36	50, 79, 106, 125	0
2	B	100/100 (100%)	-0.07	1 (1%) 79 61	46, 64, 91, 106	0
2	D	100/100 (100%)	0.23	3 (3%) 52 31	52, 76, 106, 115	0
3	E	224/234 (95%)	0.47	11 (4%) 35 18	68, 95, 124, 134	0
3	G	224/234 (95%)	0.06	2 (0%) 81 63	54, 74, 124, 142	0
4	F	9/9 (100%)	0.59	0 100 100	72, 76, 84, 87	0
4	P	9/9 (100%)	0.65	0 100 100	59, 72, 79, 87	0
5	H	214/214 (100%)	0.35	3 (1%) 73 53	53, 83, 107, 122	0
5	I	214/214 (100%)	0.19	7 (3%) 49 29	64, 82, 102, 118	0
All	All	1636/1664 (98%)	0.21	36 (2%) 62 41	46, 80, 116, 142	0

All (36) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	E	179	SER	4.1
3	E	119	PRO	3.9
1	C	109	PHE	3.8
5	I	161	GLU	3.7
3	E	148	GLU	3.6
1	C	199	ALA	3.6
2	D	99	MET	3.3
5	I	143	GLU	3.1
3	E	181	VAL	3.0
3	E	42	GLY	3.0
3	E	211	VAL	3.0
1	C	274	TRP	2.9
1	C	230	LEU	2.7

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Mol	Chain	Res	Type	RSRZ
2	D	45	ARG	2.6
3	E	37	VAL	2.6
3	G	100(C)	TYR	2.6
1	C	104	GLY	2.5
3	E	187	SER	2.5
2	B	1(A)	ILE	2.4
1	C	58	GLU	2.4
3	E	152	VAL	2.3
3	E	166	PHE	2.3
2	D	77	GLU	2.3
3	E	180	SER	2.3
1	A	162	ASP	2.3
5	H	77	ARG	2.2
1	C	160	LEU	2.2
5	I	163	VAL	2.2
5	H	137	ASN	2.1
5	H	144	ALA	2.1
3	G	127	SER	2.1
5	I	165	GLU	2.1
5	I	177	SER	2.1
5	I	102	THR	2.1
5	I	181	LEU	2.0
1	A	232	GLU	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.