



Full wwPDB X-ray Structure Validation Report ⓘ

Jul 23, 2026 – 02:07 PM EDT

PDB ID : 9NW2 / pdb_00009nw2
Title : Crystal structure of NP204 TCR in complex with NP366-H-2Db
Authors : Tan, K.; Reinherz, E.L.; Mallis, R.J.
Deposited on : 2025-03-21
Resolution : 4.44 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	:	9.0.015 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.50

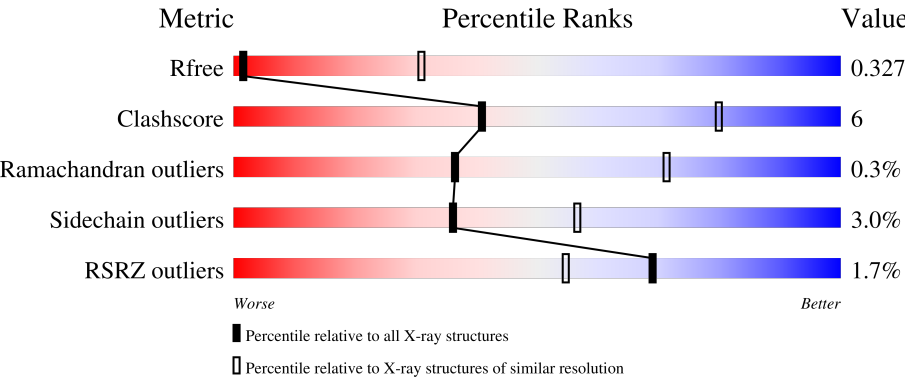
1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 4.44 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	1093 (4.98-3.90)
Clashscore	190562	1140 (4.98-3.90)
Ramachandran outliers	187476	1029 (4.98-3.90)
Sidechain outliers	187428	1013 (4.98-3.90)
RSRZ outliers	180081	1089 (4.98-3.90)

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	43% 10% • 47%
1	F	214	2% 42% 10% • 48%
2	B	253	2% 68% 19% • 10%
2	G	253	2% 68% 19% • 11%
3	C	281	2% 91% 7% •

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Mol	Chain	Length	Quality of chain
3	H	281	% 90% 8% •
4	D	100	3% 81% 17% •
4	I	100	2% 82% 15% ••
5	E	9	78% 22%
5	J	9	89% 11%

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 10901 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 NP204 TCR alpha-chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	114	Total	C	N	O	S	0	0	0
			822	509	144	166	3			
1	F	112	Total	C	N	O	S	0	0	0
			827	515	145	164	3			

- Molecule 2 is a protein called NP204 TCR beta-chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	227	Total	C	N	O	S	0	0	0
			1760	1101	326	325	8			
2	G	224	Total	C	N	O	S	0	0	0
			1734	1083	317	327	7			

- Molecule 3 is a protein called H-2 class I histocompatibility antigen, D-B alpha chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	278	Total	C	N	O	S	0	0	0
			2035	1278	356	392	9			
3	H	277	Total	C	N	O	S	0	0	0
			2043	1283	361	390	9			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	0	MET	-	initiating methionine	UNP P01899
H	0	MET	-	initiating methionine	UNP P01899

- Molecule 4 is a protein called Beta-2-microglobulin.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	D	98	Total	C	N	O	S	0	0	0
			769	493	124	146	6			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	I	98	Total	C	N	O	S	0	0	0
			773	496	125	146	6			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
D	0	MET	-	initiating methionine	UNP P01887
D	85	ASP	ALA	variant	UNP P01887
I	0	MET	-	initiating methionine	UNP P01887
I	85	ASP	ALA	variant	UNP P01887

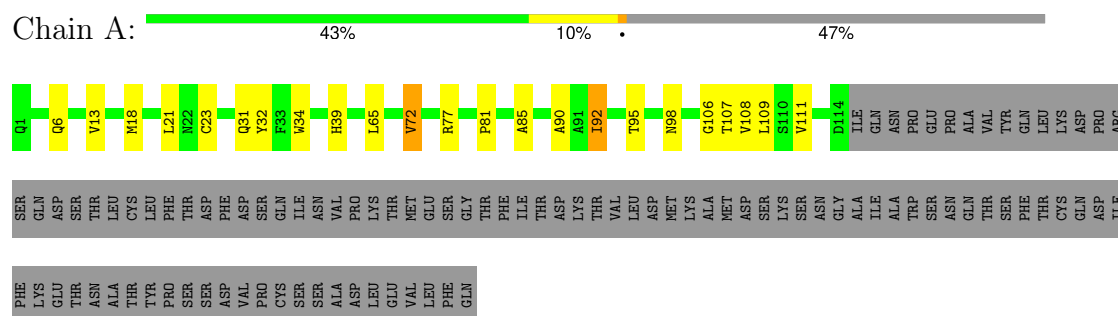
- Molecule 5 is a protein called Nucleoprotein peptide.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	E	9	Total	C	N	O	S	0	0	0
			69	38	11	18	2			
5	J	9	Total	C	N	O	S	0	0	0
			69	38	11	18	2			

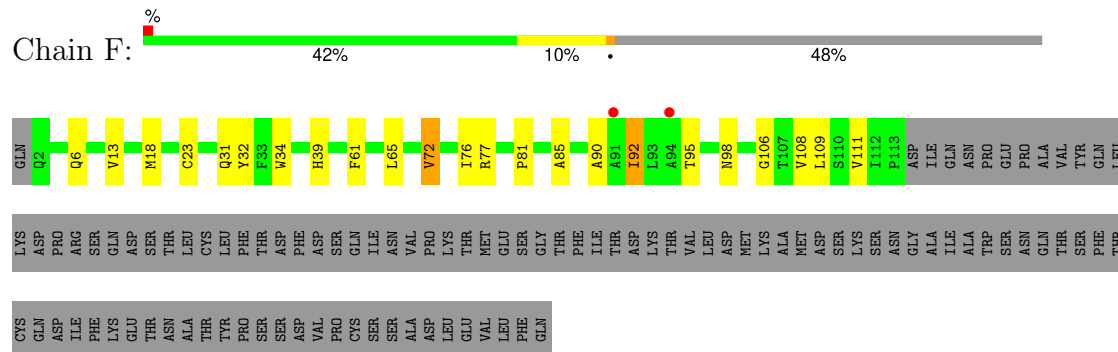
3 Residue-property plots [i](#)

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.

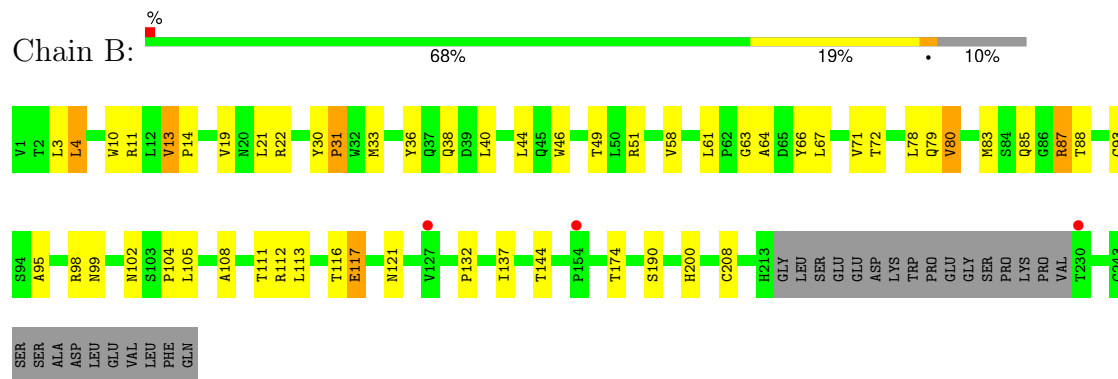
- Molecule 1: NP204 TCR alpha-chain



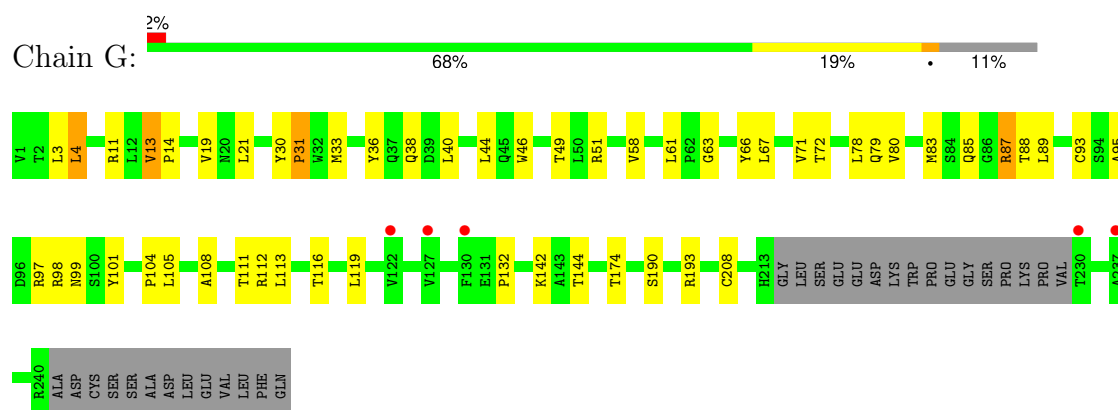
- Molecule 1: NP204 TCR alpha-chain



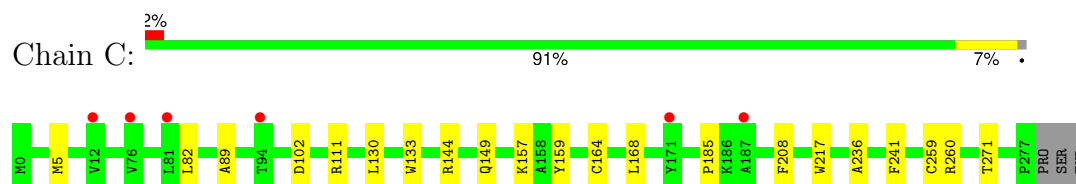
- Molecule 2: NP204 TCR beta-chain



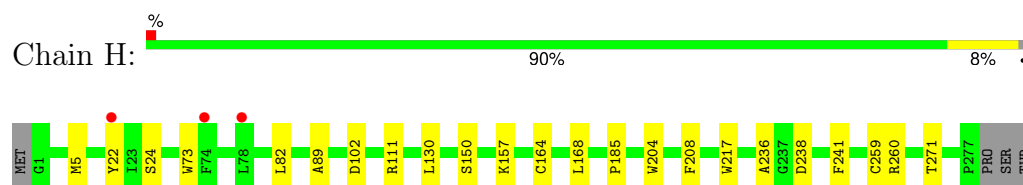
- Molecule 2: NP204 TCR beta-chain



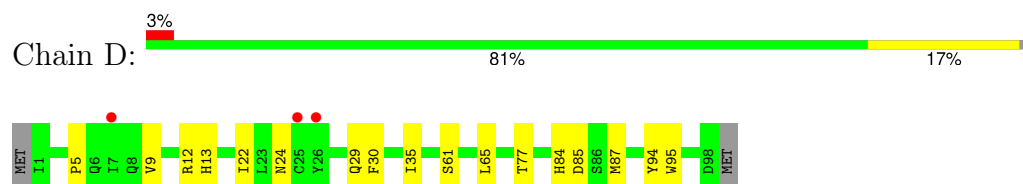
- Molecule 3: H-2 class I histocompatibility antigen, D-B alpha chain



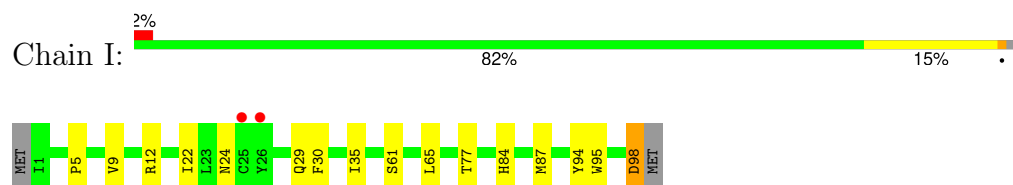
- Molecule 3: H-2 class I histocompatibility antigen, D-B alpha chain



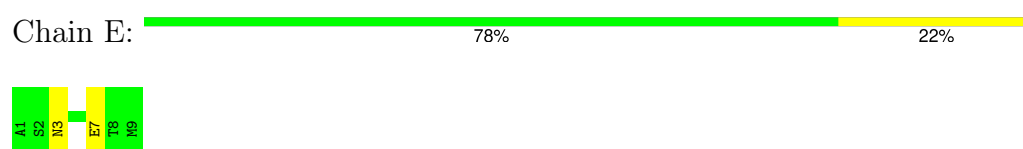
- Molecule 4: Beta-2-microglobulin



- Molecule 4: Beta-2-microglobulin



- Molecule 5: Nucleoprotein peptide



- Molecule 5: Nucleoprotein peptide

Chain J:

89%

11%



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	91.09Å 146.42Å 153.98Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	43.67 – 4.44 43.67 – 4.44	Depositor EDS
% Data completeness (in resolution range)	97.5 (43.67-4.44) 97.4 (43.67-4.44)	Depositor EDS
R_{merge}	0.17	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.57 (at 4.45Å)	Xtriage
Refinement program	PHENIX 1.21.2_5419	Depositor
R, R_{free}	0.294 , 0.328 0.295 , 0.327	Depositor DCC
R_{free} test set	562 reflections (4.24%)	wwPDB-VP
Wilson B-factor (Å ²)	171.3	Xtriage
Anisotropy	0.329	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.23 , 230.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.41$, $\langle L^2 \rangle = 0.24$	Xtriage
Estimated twinning fraction	0.000 for -h,l,k	Xtriage
F_o, F_c correlation	0.89	EDS
Total number of atoms	10901	wwPDB-VP
Average B, all atoms (Å ²)	240.0	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 46.05 % 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 1.2100e-04. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

¹ Intensities estimated from amplitudes.

² Theoretical 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 [i](#)

5.1 Standard geometry [i](#)

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	0.08	0/841	0.22	0/1146
1	F	0.08	0/847	0.21	0/1150
2	B	0.10	0/1804	0.26	0/2459
2	G	0.11	0/1778	0.27	0/2426
3	C	0.08	0/2090	0.22	0/2859
3	H	0.08	0/2098	0.22	0/2867
4	D	0.09	0/795	0.25	0/1091
4	I	0.10	0/799	0.25	0/1095
5	E	0.12	0/68	0.29	0/88
5	J	0.09	0/68	0.27	0/88
All	All	0.09	0/11188	0.24	0/15269

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

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	822	0	733	13	0
1	F	827	0	751	12	0
2	B	1760	0	1639	33	0
2	G	1734	0	1599	35	0
3	C	2035	0	1690	12	0
3	H	2043	0	1714	15	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	D	769	0	687	10	0
4	I	773	0	698	11	0
5	E	69	0	61	1	0
5	J	69	0	61	0	0
All	All	10901	0	9633	133	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 (133) 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)
4:D:12:ARG:HH21	4:D:22:ILE:HG21	1.49	0.78
1:A:32:TYR:H	1:A:92:ILE:HG12	1.52	0.75
4:I:12:ARG:HH21	4:I:22:ILE:HG21	1.54	0.73
4:D:24:ASN:HB3	4:D:65:LEU:HD11	1.72	0.71
4:I:29:GLN:HA	4:I:61:SER:HB2	1.73	0.70
1:F:32:TYR:H	1:F:92:ILE:HG12	1.57	0.70
4:I:24:ASN:HB3	4:I:65:LEU:HD11	1.72	0.69
2:G:95:ALA:H	2:G:99:ASN:HD21	1.40	0.67
2:B:95:ALA:H	2:B:99:ASN:HD21	1.40	0.67
4:D:29:GLN:HA	4:D:61:SER:HB2	1.74	0.67
2:G:132:PRO:HG3	2:G:144:THR:H	1.60	0.67
2:G:67:LEU:HB3	2:G:79:GLN:HB2	1.77	0.66
2:B:67:LEU:HB3	2:B:79:GLN:HB2	1.76	0.65
1:A:13:VAL:HG22	1:A:109:LEU:HD11	1.79	0.65
2:B:38:GLN:HB3	2:B:88:THR:HG23	1.79	0.65
2:B:132:PRO:HG3	2:B:144:THR:H	1.61	0.65
2:G:142:LYS:HG2	2:G:193:ARG:HG2	1.81	0.62
1:F:13:VAL:HG22	1:F:109:LEU:HD11	1.82	0.61
2:B:61:LEU:HD23	2:B:63:GLY:H	1.66	0.61
2:G:61:LEU:HD23	2:G:63:GLY:H	1.67	0.59
2:G:36:TYR:HB3	2:G:44:LEU:HD11	1.86	0.58
3:H:5:MET:HB2	3:H:168:LEU:HD13	1.86	0.58
2:G:46:TRP:HZ2	2:G:49:THR:HG22	1.70	0.57
2:B:46:TRP:HZ2	2:B:49:THR:HG22	1.70	0.56
2:G:97:ARG:HH21	3:H:73:TRP:HB2	1.70	0.56
2:B:66:TYR:HB3	2:B:78:LEU:HD11	1.88	0.56
2:G:38:GLN:HB3	2:G:88:THR:HG23	1.87	0.56
1:A:21:LEU:HD22	1:A:107:THR:HG21	1.87	0.55
4:D:5:PRO:HB3	4:D:30:PHE:HB3	1.89	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:11:ARG:HG2	2:B:19:VAL:HG21	1.89	0.54
4:D:30:PHE:HB2	4:D:84:HIS:CE1	2.41	0.54
4:I:30:PHE:HB2	4:I:84:HIS:CE1	2.43	0.54
2:B:174:THR:HG23	2:B:190:SER:HB2	1.89	0.54
2:G:66:TYR:HB3	2:G:78:LEU:HD11	1.88	0.54
2:B:36:TYR:HB3	2:B:44:LEU:HD11	1.89	0.54
3:H:82:LEU:HD11	3:H:89:ALA:HA	1.90	0.53
3:C:5:MET:HB2	3:C:168:LEU:HD13	1.89	0.53
3:C:82:LEU:HD11	3:C:89:ALA:HA	1.91	0.53
3:C:133:TRP:HB2	3:C:144:ARG:HG3	1.91	0.53
2:G:40:LEU:HD11	2:G:85:GLN:HB3	1.90	0.52
2:B:40:LEU:HD11	2:B:85:GLN:HB3	1.90	0.52
3:H:260:ARG:HA	3:H:271:THR:HA	1.91	0.52
4:I:5:PRO:HB3	4:I:30:PHE:HB3	1.91	0.52
1:A:23:CYS:HB3	1:A:72:VAL:HG13	1.91	0.52
2:G:63:GLY:HA3	2:G:87:ARG:NH2	2.24	0.52
3:H:102:ASP:HB2	3:H:111:ARG:HB3	1.92	0.52
3:C:102:ASP:HB2	3:C:111:ARG:HB3	1.91	0.51
2:G:11:ARG:HG2	2:G:19:VAL:HG21	1.92	0.51
1:A:95:THR:HG23	1:A:98:ASN:H	1.74	0.51
2:B:3:LEU:HD12	2:B:4:LEU:HB2	1.93	0.50
2:B:21:LEU:HD13	2:B:111:THR:HG21	1.93	0.50
2:G:98:ARG:HG2	2:G:99:ASN:H	1.76	0.50
2:B:71:VAL:HG12	2:B:72:THR:HG23	1.93	0.50
1:F:23:CYS:HB3	1:F:72:VAL:HG13	1.94	0.50
2:B:58:VAL:HG12	2:B:67:LEU:HD13	1.93	0.49
2:G:3:LEU:HD12	2:G:4:LEU:HB2	1.94	0.49
3:C:260:ARG:HA	3:C:271:THR:HA	1.93	0.49
2:B:117:GLU:O	2:B:121:ASN:HA	2.12	0.49
2:B:63:GLY:HA3	2:B:87:ARG:NH2	2.28	0.49
1:F:18:MET:HE2	1:F:77:ARG:HA	1.95	0.48
3:H:238:ASP:N	4:I:12:ARG:HD3	2.29	0.48
4:I:5:PRO:HD2	4:I:87:MET:HE2	1.95	0.48
2:G:30:TYR:CB	2:G:95:ALA:HA	2.44	0.48
2:G:4:LEU:HD12	2:G:108:ALA:HB2	1.96	0.47
2:G:71:VAL:HG12	2:G:72:THR:HG23	1.95	0.47
2:B:46:TRP:CZ2	2:B:49:THR:HG22	2.49	0.47
4:D:5:PRO:HD2	4:D:87:MET:HE2	1.97	0.47
2:G:46:TRP:CZ2	2:G:49:THR:HG22	2.48	0.47
1:F:65:LEU:HD13	1:F:72:VAL:HB	1.95	0.47
2:G:40:LEU:HD12	2:G:40:LEU:H	1.80	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:102:ASN:HB3	3:C:149:GLN:O	2.15	0.46
2:G:174:THR:HG23	2:G:190:SER:HB2	1.96	0.46
2:G:97:ARG:NH2	3:H:73:TRP:HB2	2.30	0.46
2:B:31:PRO:HG2	2:B:51:ARG:HE	1.80	0.46
2:G:95:ALA:H	2:G:99:ASN:ND2	2.10	0.46
1:F:81:PRO:HA	1:F:111:VAL:HB	1.97	0.46
2:B:30:TYR:CB	2:B:95:ALA:HA	2.45	0.46
4:I:77:THR:HB	4:I:94:TYR:HE2	1.81	0.46
2:B:33:MET:HA	2:B:93:CYS:HA	1.97	0.46
2:G:58:VAL:HG12	2:G:67:LEU:HD13	1.98	0.46
3:H:130:LEU:HB2	3:H:157:LYS:HE2	1.98	0.46
2:B:98:ARG:HG2	2:B:99:ASN:H	1.81	0.45
2:B:137:ILE:HG21	2:B:200:HIS:CE1	2.52	0.45
2:G:101:TYR:HB3	3:H:150:SER:O	2.16	0.45
1:A:65:LEU:HD13	1:A:72:VAL:HB	1.97	0.45
2:B:95:ALA:H	2:B:99:ASN:ND2	2.11	0.45
1:A:18:MET:HE2	1:A:77:ARG:HA	1.98	0.45
2:G:83:MET:HE2	2:G:83:MET:HB3	1.83	0.45
3:H:208:PHE:CE1	3:H:241:PHE:HB2	2.52	0.45
2:B:40:LEU:H	2:B:40:LEU:HD12	1.81	0.44
3:C:208:PHE:CE1	3:C:241:PHE:HB2	2.52	0.44
1:F:95:THR:HG23	1:F:98:ASN:H	1.82	0.44
3:H:217:TRP:CD2	3:H:259:CYS:HB2	2.52	0.44
1:A:81:PRO:HA	1:A:111:VAL:HB	1.99	0.44
2:B:4:LEU:HD12	2:B:108:ALA:HB2	2.00	0.44
2:G:21:LEU:HD13	2:G:111:THR:HG21	1.99	0.44
4:D:77:THR:HB	4:D:94:TYR:HE2	1.82	0.44
2:G:31:PRO:HG2	2:G:51:ARG:HE	1.82	0.44
2:B:83:MET:HE2	2:B:83:MET:HB3	1.84	0.44
1:F:34:TRP:HB2	1:F:90:ALA:HB3	1.99	0.44
1:F:98:ASN:O	2:G:98:ARG:HG3	2.17	0.43
3:H:236:ALA:H	3:H:241:PHE:HA	1.83	0.43
2:G:13:VAL:HG22	2:G:14:PRO:HD2	1.99	0.43
2:B:13:VAL:HG22	2:B:14:PRO:HD2	2.01	0.43
3:C:185:PRO:HB3	3:C:208:PHE:HB3	2.01	0.43
2:G:11:ARG:O	2:G:113:LEU:HA	2.19	0.43
1:F:61:PHE:HD2	1:F:76:ILE:HG12	1.83	0.43
3:C:217:TRP:CD2	3:C:259:CYS:HB2	2.54	0.43
1:F:39:HIS:CD2	1:F:85:ALA:HB2	2.54	0.43
3:H:185:PRO:HB3	3:H:208:PHE:HB3	2.00	0.43
1:A:34:TRP:HB2	1:A:90:ALA:HB3	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:H:22:TYR:CZ	3:H:24:SER:HB2	2.54	0.43
4:I:9:VAL:HG12	4:I:95:TRP:HD1	1.84	0.42
4:D:9:VAL:HG12	4:D:95:TRP:HD1	1.85	0.42
1:F:6:GLN:CD	1:F:106:GLY:H	2.27	0.42
3:C:236:ALA:H	3:C:241:PHE:HA	1.84	0.42
3:H:204:TRP:CH2	4:I:98:ASP:HB2	2.55	0.42
1:A:92:ILE:HB	2:B:98:ARG:CZ	2.50	0.41
2:G:30:TYR:HB2	2:G:95:ALA:HA	2.02	0.41
2:G:33:MET:HA	2:G:93:CYS:HA	2.02	0.41
1:A:6:GLN:CD	1:A:106:GLY:H	2.28	0.41
3:C:159:TYR:CD1	5:E:3:ASN:HB2	2.56	0.41
1:A:39:HIS:CD2	1:A:85:ALA:HB2	2.56	0.41
2:B:64:ALA:HB1	2:B:80:VAL:HG23	2.03	0.41
3:C:130:LEU:HB2	3:C:157:LYS:HE2	2.02	0.41
2:B:10:TRP:HE3	2:B:112:ARG:HB3	1.85	0.41
4:D:84:HIS:CD2	4:D:85:ASP:H	2.39	0.41
4:D:12:ARG:HG2	4:D:13:HIS:ND1	2.36	0.41
2:G:66:TYR:CE1	2:G:89:LEU:HD21	2.56	0.40
2:B:11:ARG:O	2:B:113:LEU:HA	2.21	0.40
1:A:13:VAL:O	1:A:111:VAL:HA	2.21	0.40
2:G:88:THR:HA	2:G:112:ARG:HA	2.03	0.40
4:I:9:VAL:HG12	4:I:95:TRP:CD1	2.57	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	112/214 (52%)	106 (95%)	6 (5%)	0	100	100
1	F	110/214 (51%)	106 (96%)	4 (4%)	0	100	100
2	B	223/253 (88%)	198 (89%)	23 (10%)	2 (1%)	14	49

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	G	220/253 (87%)	197 (90%)	21 (10%)	2 (1%)	14	49
3	C	276/281 (98%)	253 (92%)	23 (8%)	0	100	100
3	H	275/281 (98%)	252 (92%)	23 (8%)	0	100	100
4	D	96/100 (96%)	88 (92%)	8 (8%)	0	100	100
4	I	96/100 (96%)	88 (92%)	8 (8%)	0	100	100
5	E	7/9 (78%)	6 (86%)	1 (14%)	0	100	100
5	J	7/9 (78%)	6 (86%)	1 (14%)	0	100	100
All	All	1422/1714 (83%)	1300 (91%)	118 (8%)	4 (0%)	36	71

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	31	PRO
2	G	31	PRO
2	B	104	PRO
2	G	104	PRO

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	83/188 (44%)	79 (95%)	4 (5%)	23	45
1	F	85/188 (45%)	81 (95%)	4 (5%)	23	45
2	B	180/225 (80%)	171 (95%)	9 (5%)	22	43
2	G	178/225 (79%)	170 (96%)	8 (4%)	24	46
3	C	173/239 (72%)	172 (99%)	1 (1%)	78	80
3	H	175/239 (73%)	174 (99%)	1 (1%)	78	80
4	D	81/95 (85%)	80 (99%)	1 (1%)	63	73
4	I	82/95 (86%)	80 (98%)	2 (2%)	43	63
5	E	8/8 (100%)	7 (88%)	1 (12%)	4	17

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
5	J	8/8 (100%)	7 (88%)	1 (12%)	4 17
All	All	1053/1510 (70%)	1021 (97%)	32 (3%)	36 56

All (32) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	31	GLN
1	A	72	VAL
1	A	92	ILE
1	A	108	VAL
2	B	4	LEU
2	B	13	VAL
2	B	22	ARG
2	B	80	VAL
2	B	87	ARG
2	B	105	LEU
2	B	116	THR
2	B	117	GLU
2	B	208	CYS
3	C	164	CYS
4	D	35	ILE
5	E	7	GLU
1	F	31	GLN
1	F	72	VAL
1	F	92	ILE
1	F	108	VAL
2	G	4	LEU
2	G	13	VAL
2	G	80	VAL
2	G	87	ARG
2	G	105	LEU
2	G	116	THR
2	G	119	LEU
2	G	208	CYS
3	H	164	CYS
4	I	35	ILE
4	I	98	ASP
5	J	7	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (12) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	22	ASN
3	C	42	ASN
3	C	97	GLN
4	D	6	GLN
5	E	3	ASN
5	E	5	ASN
1	F	22	ASN
1	F	75	HIS
3	H	42	ASN
3	H	127	ASN
4	I	6	GLN
5	J	3	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

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	114/214 (53%)	-0.01	0 100 100	183, 250, 301, 326	0
1	F	112/214 (52%)	0.15	2 (1%) 67 53	182, 267, 340, 351	0
2	B	227/253 (89%)	0.06	3 (1%) 75 60	179, 250, 360, 440	0
2	G	224/253 (88%)	0.13	5 (2%) 62 49	186, 248, 351, 395	0
3	C	278/281 (98%)	0.04	6 (2%) 62 49	158, 221, 279, 321	0
3	H	277/281 (98%)	0.02	3 (1%) 78 63	167, 227, 281, 296	0
4	D	98/100 (98%)	0.19	3 (3%) 51 40	173, 210, 283, 326	0
4	I	98/100 (98%)	0.08	2 (2%) 65 51	169, 216, 301, 339	0
5	E	9/9 (100%)	0.36	0 100 100	186, 221, 268, 290	0
5	J	9/9 (100%)	0.51	0 100 100	193, 222, 262, 298	0
All	All	1446/1714 (84%)	0.07	24 (1%) 69 55	158, 236, 330, 440	0

All (24) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	C	187	ALA	4.7
2	B	127	VAL	4.0
2	B	230	THR	3.3
2	B	154	PRO	3.3
2	G	130	PHE	3.2
4	D	25	CYS	3.2
4	I	26	TYR	3.0
2	G	237	ALA	2.6
2	G	127	VAL	2.5
3	H	74	PHE	2.5
1	F	91	ALA	2.4
3	C	76	VAL	2.4
4	D	26	TYR	2.3

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Mol	Chain	Res	Type	RSRZ
2	G	230	THR	2.2
4	D	7	ILE	2.2
1	F	94	ALA	2.2
3	C	94	THR	2.2
3	C	81	LEU	2.2
3	H	78	LEU	2.2
3	C	12	VAL	2.2
3	C	171	TYR	2.1
3	H	22	TYR	2.1
4	I	25	CYS	2.1
2	G	122	VAL	2.1

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.