



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 09:16 PM UTC

PDB ID : 3VXT / pdb_00003vxt
Title : T36-5 TCR specific for HLA-A24-Nef134-10
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Deposited on : 2012-09-20
Resolution : 2.50 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
Xtrriage (Phenix) : 2.0
EDS : 3.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

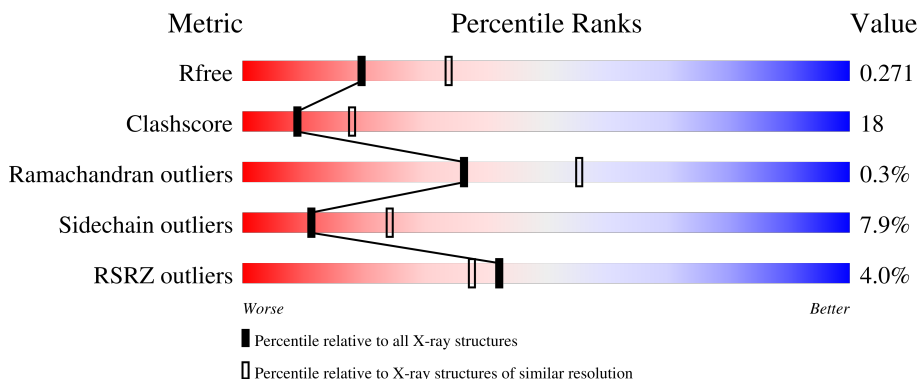
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.50 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	5829 (2.50-2.50)
Clashscore	190562	6492 (2.50-2.50)
Ramachandran outliers	187476	6378 (2.50-2.50)
Sidechain outliers	187428	6380 (2.50-2.50)
RSRZ outliers	180081	5833 (2.50-2.50)

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	205	
1	C	205	
2	B	242	
2	D	242	

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 7080 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 T36-5 TCR alpha chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	C	199	1553	968	257	321	7	0	0	0
1	A	199	1553	968	257	321	7	0	0	0

- Molecule 2 is a protein called T36-5 TCR beta chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	D	241	1933	1217	336	372	8	0	0	0
2	B	241	1933	1217	336	372	8	0	0	0

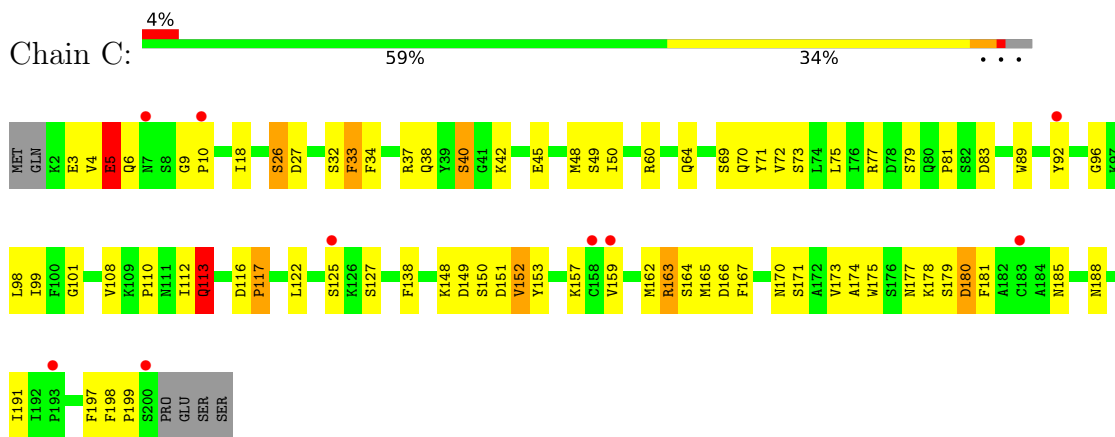
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	C	15	Total 15	O 15	0	0
3	D	50	Total 50	O 50	0	0
3	A	12	Total 12	O 12	0	0
3	B	31	Total 31	O 31	0	0

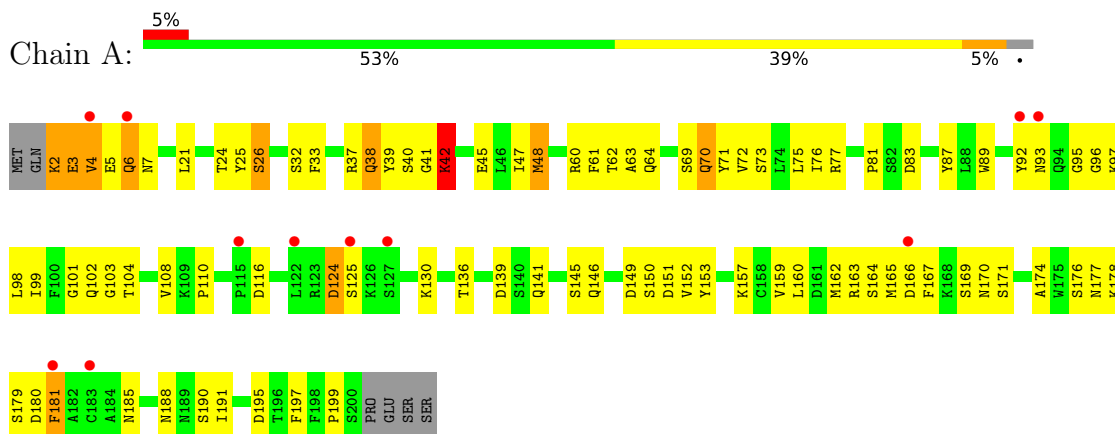
3 Residue-property plots [i](#)

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.

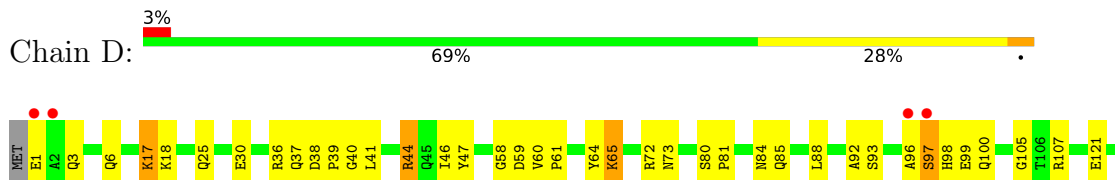
- Molecule 1: T36-5 TCR alpha chain

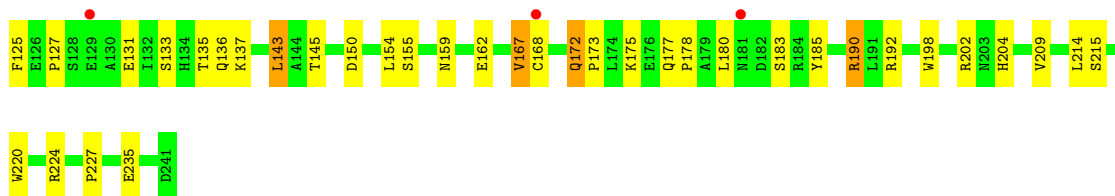


- Molecule 1: T36-5 TCR alpha chain

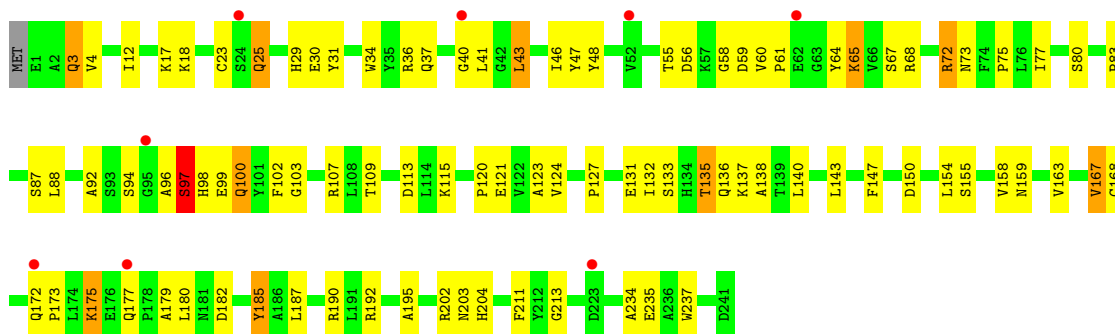


- Molecule 2: T36-5 TCR beta chain





• Molecule 2: T36-5 TCR beta chain



4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	45.77Å 65.04Å 92.28Å 91.30° 94.19° 105.93°	Depositor
Resolution (Å)	50.00 – 2.50 50.00 – 2.50	Depositor EDS
% Data completeness (in resolution range)	91.5 (50.00-2.50) 91.8 (50.00-2.50)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.04	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.08 (at 2.51Å)	Xtrriage
Refinement program	CNS 1.3	Depositor
R, R_{free}	0.230 , 0.271 0.231 , 0.271	Depositor DCC
R_{free} test set	3220 reflections (9.99%)	wwPDB-VP
Wilson B-factor (Å ²)	57.3	Xtrriage
Anisotropy	0.298	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 58.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	7080	wwPDB-VP
Average B, all atoms (Å ²)	69.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.03% 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 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	0.68	4/1587 (0.3%)	1.03	9/2149 (0.4%)
1	C	0.47	0/1587	1.10	9/2149 (0.4%)
2	B	0.50	0/1986	1.07	14/2705 (0.5%)
2	D	0.53	0/1986	1.01	11/2705 (0.4%)
All	All	0.55	4/7146 (0.1%)	1.05	43/9708 (0.4%)

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	38	GLN	C-O	-6.63	1.16	1.24
1	A	39	TYR	C-O	-6.27	1.15	1.23
1	A	41	GLY	C-O	-5.92	1.17	1.23
1	A	42	LYS	C-O	-5.58	1.16	1.23

All (43) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	6	GLN	N-CA-C	-15.34	88.88	110.50
1	A	40	SER	N-CA-C	12.03	124.40	111.28
2	B	3	GLN	N-CA-C	9.60	123.60	110.35
2	B	97	SER	N-CA-C	-9.59	94.59	109.25
1	A	181	PHE	N-CA-C	7.39	121.38	110.30
2	B	235	GLU	N-CA-C	7.24	119.08	108.86
1	C	181	PHE	N-CA-C	7.16	121.05	110.30
2	B	59	ASP	N-CA-C	6.81	119.28	111.11
2	D	80	SER	CA-C-N	6.80	126.82	119.89
2	D	80	SER	C-N-CA	6.80	126.82	119.89
2	B	80	SER	CA-C-N	6.68	126.72	119.90
2	B	80	SER	C-N-CA	6.68	126.72	119.90
1	A	116	ASP	CA-C-N	6.59	126.98	119.93
1	A	116	ASP	C-N-CA	6.59	126.98	119.93
2	D	121	GLU	N-CA-C	-6.51	98.58	109.07
2	D	72	ARG	N-CA-C	6.46	118.32	111.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	60	VAL	CA-C-N	6.20	126.73	120.04
2	B	60	VAL	C-N-CA	6.20	126.73	120.04
2	D	59	ASP	N-CA-C	5.88	118.19	111.02
1	C	113	GLN	N-CA-C	5.85	118.16	111.02
1	A	3	GLU	CB-CA-C	-5.83	108.85	115.79
1	A	130	LYS	N-CA-C	5.79	118.02	110.43
1	C	40	SER	N-CA-C	5.77	123.10	110.80
1	C	79	SER	N-CA-C	5.71	118.64	110.24
1	C	179	SER	N-CA-C	-5.58	105.59	112.90
2	D	235	GLU	N-CA-C	5.52	117.02	109.18
2	B	121	GLU	N-CA-C	-5.52	100.71	109.76
1	A	26	SER	N-CA-C	5.43	119.57	112.13
2	B	73	ASN	N-CA-C	5.38	118.84	110.17
2	D	145	THR	N-CA-C	5.37	117.57	109.41
1	C	33	PHE	N-CA-C	5.34	118.10	109.40
1	A	136	THR	N-CA-C	5.32	117.06	109.14
2	D	215	SER	N-CA-C	-5.32	102.59	110.46
2	D	97	SER	CB-CA-C	-5.27	110.48	116.54
2	B	175	LYS	N-CA-C	-5.27	101.85	109.59
2	B	72	ARG	N-CA-C	5.23	116.66	111.07
2	D	209	VAL	N-CA-C	5.09	115.37	107.28
2	D	85	GLN	N-CA-C	-5.08	106.92	113.02
1	C	26	SER	N-CA-C	5.07	119.08	112.13
2	B	55	THR	N-CA-C	5.07	116.84	108.13
2	B	185	TYR	N-CA-C	5.06	117.58	110.14
1	C	5	GLU	N-CA-C	5.04	118.54	111.74
1	A	179	SER	N-CA-C	-5.03	105.89	112.23

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	1553	0	1461	82	0
1	C	1553	0	1461	59	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	B	1933	0	1845	74	0
2	D	1933	0	1845	57	0
3	A	12	0	0	6	0
3	B	31	0	0	1	0
3	C	15	0	0	2	0
3	D	50	0	0	8	0
All	All	7080	0	6612	250	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 18.

All (250) 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:D:177:GLN:HB3	2:D:180:LEU:HD13	1.21	1.18
2:D:177:GLN:CB	2:D:180:LEU:HD13	1.85	1.07
1:C:110:PRO:HG3	1:C:159:VAL:HG21	1.43	1.00
2:B:3:GLN:HG2	2:B:4:VAL:H	1.31	0.95
2:D:177:GLN:HB3	2:D:180:LEU:CD1	1.97	0.94
2:B:92:ALA:HB1	2:B:100:GLN:HG3	1.52	0.91
1:A:6:GLN:CD	1:A:7:ASN:H	1.85	0.82
1:C:110:PRO:HG3	1:C:159:VAL:CG2	2.14	0.78
1:A:6:GLN:NE2	1:A:7:ASN:H	1.80	0.78
1:C:178:LYS:HG2	1:C:180:ASP:HB2	1.66	0.77
2:D:98:HIS:HD2	3:D:345:HOH:O	1.66	0.76
1:A:97:LYS:HE2	2:B:48:TYR:OH	1.88	0.74
1:C:166:ASP:HB2	3:C:314:HOH:O	1.89	0.73
2:D:73:ASN:HB3	3:D:311:HOH:O	1.88	0.73
2:B:31:TYR:HB3	2:B:94:SER:HB3	1.70	0.72
2:B:3:GLN:HG2	2:B:4:VAL:N	2.05	0.72
1:A:42:LYS:HD2	1:A:42:LYS:N	2.04	0.72
1:C:77:ARG:HG3	1:C:77:ARG:HH11	1.55	0.71
1:A:178:LYS:HG2	1:A:180:ASP:HB2	1.71	0.71
2:B:3:GLN:CG	2:B:4:VAL:H	2.03	0.71
1:C:197:PHE:CZ	1:C:199:PRO:HG3	2.26	0.70
1:A:4:VAL:HG22	1:A:5:GLU:HG2	1.72	0.69
2:D:202:ARG:HG3	2:D:202:ARG:HH11	1.55	0.69
1:A:38:GLN:NE2	2:B:37:GLN:HE22	1.92	0.68
2:B:135:THR:O	2:B:136:GLN:HB2	1.93	0.68
2:B:58:GLY:O	2:B:61:PRO:HD3	1.94	0.68
1:C:3:GLU:HG3	1:C:4:VAL:H	1.58	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2:LYS:HZ3	1:A:2:LYS:HB2	1.59	0.67
2:D:180:LEU:N	2:D:180:LEU:HD12	2.09	0.67
1:C:113:GLN:HE21	1:C:113:GLN:HA	1.59	0.67
1:A:2:LYS:NZ	1:A:3:GLU:H	1.93	0.66
1:C:191:ILE:O	1:C:191:ILE:HG13	1.94	0.66
1:C:5:GLU:OE2	1:C:5:GLU:HA	1.95	0.66
2:D:98:HIS:CD2	3:D:345:HOH:O	2.46	0.66
1:A:62:THR:OG1	1:A:77:ARG:NH2	2.30	0.65
1:C:42:LYS:N	1:C:42:LYS:HD2	2.11	0.65
2:B:88:LEU:HD13	2:B:107:ARG:HG3	1.79	0.65
1:C:113:GLN:HG2	3:C:311:HOH:O	1.96	0.64
2:D:167:VAL:HA	2:D:190:ARG:O	1.98	0.64
1:C:33:PHE:O	1:C:50:ILE:HG22	1.98	0.63
2:D:60:VAL:HG23	2:D:60:VAL:O	1.98	0.63
2:B:202:ARG:HG3	2:B:202:ARG:HH11	1.64	0.63
2:D:159:ASN:ND2	2:D:204:HIS:H	1.97	0.62
2:D:177:GLN:HB2	2:D:180:LEU:HD13	1.79	0.62
1:A:176:SER:HA	3:A:305:HOH:O	1.99	0.62
1:C:77:ARG:HG3	1:C:77:ARG:NH1	2.14	0.62
1:A:6:GLN:HB2	1:A:102:GLN:HB2	1.82	0.62
2:B:127:PRO:HG2	2:B:138:ALA:HB1	1.82	0.62
2:B:100:GLN:HB3	2:B:102:PHE:CE2	2.34	0.61
2:B:167:VAL:HA	2:B:190:ARG:O	2.00	0.61
2:D:92:ALA:HB1	2:D:100:GLN:HG3	1.83	0.61
1:A:81:PRO:HA	1:A:108:VAL:HB	1.83	0.61
2:D:58:GLY:O	2:D:61:PRO:HD3	2.01	0.60
1:A:159:VAL:O	2:B:168:CYS:SG	2.60	0.59
1:C:64:GLN:HB2	1:C:73:SER:OG	2.02	0.59
1:C:89:TRP:CZ2	1:C:101:GLY:HA3	2.37	0.59
1:A:110:PRO:HG3	1:A:159:VAL:HG21	1.84	0.59
1:A:6:GLN:CD	1:A:7:ASN:N	2.57	0.59
1:C:113:GLN:HE21	1:C:113:GLN:CA	2.16	0.58
1:A:152:VAL:HG13	1:A:152:VAL:O	2.03	0.58
1:A:89:TRP:CZ2	1:A:101:GLY:HA3	2.39	0.58
1:C:149:ASP:HB3	1:C:152:VAL:HG12	1.84	0.57
1:C:197:PHE:CD1	1:C:198:PHE:N	2.73	0.57
1:C:197:PHE:CE2	1:C:199:PRO:HG3	2.39	0.57
1:A:64:GLN:HB2	1:A:73:SER:OG	2.05	0.57
1:C:113:GLN:HA	1:C:113:GLN:NE2	2.19	0.57
2:D:159:ASN:HD21	2:D:204:HIS:H	1.51	0.57
1:C:34:PHE:HD1	1:C:49:SER:HG	1.52	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:60:ARG:NH2	1:C:83:ASP:OD2	2.37	0.57
1:A:97:LYS:HE2	2:B:48:TYR:CZ	2.39	0.57
2:B:97:SER:O	2:B:99:GLU:HG2	2.05	0.56
2:B:154:LEU:HD23	2:B:155:SER:N	2.19	0.56
1:C:185:ASN:HA	1:C:188:ASN:ND2	2.20	0.56
1:A:60:ARG:HA	1:A:77:ARG:NH1	2.21	0.56
1:A:160:LEU:HB3	2:B:168:CYS:HB2	1.87	0.56
1:A:6:GLN:N	1:A:6:GLN:HE21	2.04	0.56
2:B:135:THR:HG21	2:B:192:ARG:NH2	2.20	0.56
1:C:173:VAL:HG12	1:C:174:ALA:N	2.21	0.56
1:C:153:TYR:O	1:C:174:ALA:HA	2.06	0.56
2:B:4:VAL:HB	2:B:103:GLY:HA2	1.88	0.55
1:C:98:LEU:HD13	2:D:100:GLN:OE1	2.07	0.55
2:B:120:PRO:HB3	2:B:147:PHE:HB3	1.88	0.55
2:D:135:THR:HG21	2:D:192:ARG:NH2	2.22	0.55
1:C:185:ASN:HA	1:C:188:ASN:HD21	1.72	0.55
1:C:175:TRP:CD2	2:D:143:LEU:HD21	2.41	0.54
2:D:36:ARG:HB3	2:D:46:ILE:HD11	1.90	0.54
1:A:180:ASP:HB3	3:A:312:HOH:O	2.06	0.54
2:D:220:TRP:CZ2	2:D:227:PRO:HD3	2.44	0.53
1:A:6:GLN:CG	1:A:7:ASN:N	2.71	0.53
1:A:33:PHE:CD1	1:A:72:VAL:HG21	2.42	0.53
2:D:202:ARG:HG3	2:D:202:ARG:NH1	2.20	0.53
1:A:2:LYS:HB2	1:A:2:LYS:NZ	2.24	0.53
1:A:38:GLN:HE22	2:B:37:GLN:HE22	1.55	0.53
2:B:177:GLN:HB3	2:B:180:LEU:HD13	1.91	0.53
2:B:12:ILE:CD1	2:B:213:GLY:HA2	2.38	0.53
2:B:150:ASP:HB3	2:B:185:TYR:CD2	2.42	0.53
2:D:88:LEU:HD13	2:D:107:ARG:HG3	1.91	0.53
2:B:113:ASP:C	2:B:115:LYS:H	2.18	0.53
1:C:117:PRO:HG3	1:C:138:PHE:HA	1.91	0.52
2:B:127:PRO:CG	2:B:138:ALA:HB1	2.38	0.52
2:B:135:THR:HG21	2:B:192:ARG:HH21	1.74	0.52
1:A:69:SER:O	1:A:70:GLN:HB2	2.09	0.51
1:A:149:ASP:HB3	1:A:152:VAL:HG12	1.91	0.51
2:B:36:ARG:HB3	2:B:46:ILE:HD11	1.93	0.51
1:C:149:ASP:HB3	1:C:152:VAL:CG1	2.41	0.51
1:A:157:LYS:HA	1:A:171:SER:O	2.11	0.50
1:A:162:MET:HE1	2:B:137:LYS:HD3	1.94	0.50
1:A:98:LEU:HD13	2:B:100:GLN:OE1	2.12	0.50
2:B:23:CYS:HB2	2:B:34:TRP:CZ2	2.46	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:96:ALA:O	2:D:97:SER:C	2.55	0.50
1:A:60:ARG:NH2	1:A:83:ASP:OD2	2.45	0.50
1:A:110:PRO:HG3	1:A:159:VAL:CG2	2.42	0.50
1:A:153:TYR:O	1:A:174:ALA:HA	2.11	0.50
1:A:149:ASP:HB3	1:A:152:VAL:CG1	2.42	0.50
2:B:25:GLN:OE1	2:B:29:HIS:N	2.28	0.50
1:A:159:VAL:HG22	1:A:170:ASN:OD1	2.12	0.49
2:D:162:GLU:HB2	3:D:339:HOH:O	2.12	0.49
1:A:185:ASN:HA	1:A:188:ASN:ND2	2.28	0.49
1:C:4:VAL:HG22	1:C:5:GLU:N	2.27	0.49
1:C:69:SER:O	1:C:70:GLN:HB2	2.11	0.49
2:B:40:GLY:C	2:B:41:LEU:HD22	2.37	0.49
2:B:173:PRO:HG3	2:B:187:LEU:HD13	1.95	0.49
2:B:127:PRO:HD3	2:B:140:LEU:HG	1.93	0.49
1:A:181:PHE:HA	3:A:306:HOH:O	2.12	0.49
2:D:214:LEU:CD1	2:D:227:PRO:HG2	2.43	0.48
1:A:124:ASP:OD1	1:A:124:ASP:N	2.44	0.48
2:B:154:LEU:HD23	2:B:154:LEU:C	2.38	0.48
1:C:5:GLU:OE2	1:C:5:GLU:CA	2.60	0.48
1:A:21:LEU:HD21	1:A:104:THR:HG21	1.94	0.48
2:B:202:ARG:HG3	2:B:202:ARG:NH1	2.28	0.48
2:B:64:TYR:O	2:B:65:LYS:HD2	2.14	0.48
1:C:71:TYR:CD1	1:C:71:TYR:C	2.92	0.48
1:A:92:TYR:OH	1:A:96:GLY:HA2	2.13	0.48
1:C:38:GLN:NE2	2:D:37:GLN:HE22	2.12	0.48
1:C:38:GLN:HE22	2:D:37:GLN:HE22	1.60	0.48
2:B:72:ARG:HG3	2:B:72:ARG:HH11	1.79	0.48
1:A:97:LYS:O	1:A:99:ILE:HD12	2.14	0.48
1:C:157:LYS:HA	1:C:171:SER:O	2.14	0.47
1:A:103:GLY:N	3:A:304:HOH:O	2.48	0.47
1:C:33:PHE:CD1	1:C:72:VAL:HG21	2.50	0.47
2:B:131:GLU:O	2:B:131:GLU:HG2	2.15	0.47
2:B:25:GLN:HE21	2:B:25:GLN:HB3	1.56	0.47
2:B:123:ALA:HB2	3:B:322:HOH:O	2.15	0.47
2:D:172:GLN:NE2	2:D:173:PRO:CD	2.78	0.47
1:A:97:LYS:CE	2:B:48:TYR:OH	2.61	0.47
2:B:135:THR:CG2	2:B:137:LYS:HB2	2.44	0.47
2:D:135:THR:HG22	2:D:137:LYS:HG3	1.97	0.47
1:A:37:ARG:HB2	1:A:47:ILE:HD13	1.97	0.47
1:C:4:VAL:HG22	1:C:5:GLU:CD	2.40	0.46
2:D:64:TYR:O	2:D:65:LYS:HD2	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:25:TYR:CZ	1:A:70:GLN:HG2	2.50	0.46
1:C:159:VAL:O	2:D:168:CYS:SG	2.74	0.46
1:A:61:PHE:CD1	1:A:76:ILE:HG12	2.50	0.46
1:A:97:LYS:HB2	1:A:97:LYS:HE3	1.63	0.46
2:B:87:SER:OG	2:B:88:LEU:N	2.49	0.46
1:A:71:TYR:CD1	1:A:71:TYR:C	2.94	0.46
1:A:159:VAL:N	2:B:168:CYS:SG	2.89	0.46
2:B:31:TYR:HB3	2:B:94:SER:CB	2.45	0.46
2:B:68:ARG:HG2	2:B:68:ARG:HH11	1.81	0.46
2:D:131:GLU:O	2:D:135:THR:HB	2.16	0.46
2:D:177:GLN:HB2	2:D:183:SER:HB2	1.98	0.45
1:A:101:GLY:O	1:A:102:GLN:C	2.59	0.45
2:D:177:GLN:OE1	2:D:177:GLN:HA	2.16	0.45
2:D:127:PRO:HD2	2:D:198:TRP:CZ2	2.51	0.45
2:D:150:ASP:HB3	2:D:185:TYR:CD2	2.51	0.45
1:A:92:TYR:CZ	1:A:96:GLY:HA2	2.51	0.45
2:B:97:SER:HB3	2:B:99:GLU:HG2	1.98	0.45
2:B:204:HIS:HB2	2:B:237:TRP:CZ3	2.51	0.45
2:D:154:LEU:HD23	2:D:155:SER:N	2.31	0.45
2:D:135:THR:O	2:D:136:GLN:HB2	2.15	0.45
2:B:12:ILE:HD11	2:B:213:GLY:HA2	1.98	0.45
2:D:224:ARG:NH1	3:D:340:HOH:O	2.50	0.45
1:A:2:LYS:HZ2	1:A:3:GLU:H	1.63	0.45
2:B:67:SER:O	2:B:75:PRO:HD2	2.17	0.45
1:A:159:VAL:C	2:B:168:CYS:SG	3.00	0.45
1:C:26:SER:OG	1:C:27:ASP:N	2.50	0.44
1:C:122:LEU:N	1:C:122:LEU:HD12	2.31	0.44
1:A:97:LYS:HE2	2:B:48:TYR:CE2	2.52	0.44
1:A:160:LEU:C	1:A:160:LEU:HD12	2.42	0.44
1:A:162:MET:HE3	1:A:167:PHE:HD2	1.81	0.44
1:A:191:ILE:HG13	1:A:191:ILE:O	2.17	0.44
1:C:9:GLY:HA2	1:C:10:PRO:HD3	1.70	0.44
2:B:120:PRO:HD3	2:B:211:PHE:CD1	2.52	0.44
1:C:162:MET:CE	2:D:192:ARG:HD3	2.48	0.44
1:A:4:VAL:HG22	1:A:5:GLU:N	2.33	0.44
2:B:147:PHE:CE1	2:B:185:TYR:HB2	2.53	0.44
2:D:175:LYS:HE2	2:D:178:PRO:O	2.18	0.44
2:B:12:ILE:HD12	2:B:213:GLY:C	2.42	0.44
1:C:162:MET:HE1	2:D:192:ARG:HD3	2.00	0.44
2:D:17:LYS:O	2:D:81:PRO:HG2	2.18	0.44
1:A:165:MET:O	1:A:166:ASP:C	2.61	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:60:ARG:HA	1:A:77:ARG:HH12	1.82	0.43
2:D:172:GLN:NE2	2:D:173:PRO:HD2	2.33	0.43
1:A:102:GLN:NE2	3:A:308:HOH:O	2.39	0.43
2:D:131:GLU:O	2:D:131:GLU:HG2	2.17	0.43
1:C:162:MET:HE3	1:C:167:PHE:HD2	1.83	0.43
1:A:2:LYS:N	1:A:3:GLU:OE2	2.52	0.43
1:A:38:GLN:HE22	2:B:37:GLN:NE2	2.16	0.43
1:A:71:TYR:CD1	1:A:71:TYR:O	2.71	0.43
2:D:46:ILE:HG22	2:D:47:TYR:HD2	1.83	0.43
1:A:48:MET:HG2	1:A:63:ALA:HB2	2.00	0.43
1:C:37:ARG:HE	1:C:37:ARG:HB3	1.54	0.43
1:C:81:PRO:HA	1:C:108:VAL:HB	2.00	0.43
1:C:92:TYR:OH	1:C:96:GLY:HA2	2.19	0.42
2:B:179:ALA:C	2:B:180:LEU:HD12	2.44	0.42
1:C:4:VAL:HG22	1:C:5:GLU:H	1.83	0.42
1:C:112:ILE:HD11	1:C:170:ASN:ND2	2.34	0.42
1:A:21:LEU:O	1:A:73:SER:HB2	2.19	0.42
2:B:37:GLN:HB2	2:B:43:LEU:HD12	2.01	0.42
2:D:39:PRO:HD2	3:D:332:HOH:O	2.18	0.42
2:D:84:ASN:H	2:D:84:ASN:ND2	2.16	0.42
1:A:171:SER:OG	2:B:190:ARG:HD2	2.19	0.42
2:B:96:ALA:O	2:B:98:HIS:CE1	2.72	0.42
2:B:158:VAL:CG2	2:B:163:VAL:HG21	2.50	0.42
1:A:37:ARG:HG3	1:A:87:TYR:CE1	2.55	0.42
2:B:124:VAL:HG23	2:B:234:ALA:HB3	2.01	0.42
1:C:163:ARG:H	1:C:163:ARG:HG2	1.53	0.42
2:D:6:GLN:HE22	2:D:105:GLY:HA2	1.84	0.42
1:A:169:SER:HA	3:A:303:HOH:O	2.18	0.42
1:A:93:ASN:CG	1:A:95:GLY:H	2.28	0.42
1:A:177:ASN:OD1	1:A:177:ASN:N	2.53	0.42
1:A:197:PHE:CZ	1:A:199:PRO:HG3	2.55	0.42
1:C:175:TRP:CG	2:D:143:LEU:HD21	2.55	0.42
2:D:172:GLN:NE2	2:D:173:PRO:HD3	2.35	0.42
1:A:139:ASP:C	1:A:141:GLN:H	2.27	0.42
2:D:40:GLY:C	2:D:41:LEU:HD22	2.45	0.41
2:D:64:TYR:C	2:D:65:LYS:HD2	2.45	0.41
2:B:77:ILE:HD12	2:B:77:ILE:H	1.84	0.41
1:A:24:THR:HG22	1:A:71:TYR:HB3	2.03	0.41
2:D:125:PHE:HE2	2:D:143:LEU:HB2	1.84	0.41
1:A:188:ASN:C	1:A:190:SER:H	2.27	0.41
1:C:116:ASP:N	1:C:117:PRO:HD3	2.35	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:127:SER:HB3	3:D:341:HOH:O	2.20	0.41
1:C:177:ASN:OD1	1:C:177:ASN:N	2.52	0.41
2:B:41:LEU:HD13	2:B:41:LEU:HA	1.93	0.41
1:C:159:VAL:HG22	1:C:170:ASN:OD1	2.21	0.41
2:D:38:ASP:HB3	3:D:332:HOH:O	2.20	0.41
1:A:145:SER:O	1:A:146:GLN:C	2.64	0.41
2:B:46:ILE:HG22	2:B:47:TYR:HD2	1.84	0.41
2:B:159:ASN:HD21	2:B:203:ASN:HA	1.86	0.41
2:B:172:GLN:HA	2:B:173:PRO:HD3	1.85	0.41
1:C:99:ILE:N	1:C:99:ILE:HD12	2.36	0.41
2:D:41:LEU:HB3	2:D:44:ARG:HD3	2.03	0.41
1:A:24:THR:HA	1:A:71:TYR:HA	2.03	0.41
2:D:1:GLU:OE2	2:D:1:GLU:O	2.39	0.40
2:B:132:ILE:HG23	2:B:195:ALA:HB1	2.03	0.40
1:A:195:ASP:OD2	1:A:195:ASP:O	2.39	0.40
2:B:124:VAL:HG23	2:B:234:ALA:CB	2.52	0.40
1:A:2:LYS:HZ3	1:A:3:GLU:H	1.65	0.40
2:B:135:THR:HG22	2:B:137:LYS:HB2	2.03	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	197/205 (96%)	178 (90%)	17 (9%)	2 (1%)	12	24
1	C	197/205 (96%)	178 (90%)	18 (9%)	1 (0%)	24	43
2	B	239/242 (99%)	227 (95%)	12 (5%)	0	100	100
2	D	239/242 (99%)	230 (96%)	9 (4%)	0	100	100
All	All	872/894 (98%)	813 (93%)	56 (6%)	3 (0%)	36	55

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	40	SER
1	A	70	GLN
1	A	4	VAL

5.3.2 Protein sidechains [i](#)

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	177/183 (97%)	163 (92%)	14 (8%)	11 24
1	C	177/183 (97%)	160 (90%)	17 (10%)	8 17
2	B	214/215 (100%)	197 (92%)	17 (8%)	11 24
2	D	214/215 (100%)	200 (94%)	14 (6%)	15 32
All	All	782/796 (98%)	720 (92%)	62 (8%)	11 24

All (62) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	5	GLU
1	C	18	ILE
1	C	32	SER
1	C	45	GLU
1	C	48	MET
1	C	75	LEU
1	C	113	GLN
1	C	117	PRO
1	C	125	SER
1	C	148	LYS
1	C	150	SER
1	C	151	ASP
1	C	152	VAL
1	C	163	ARG
1	C	164	SER
1	C	165	MET
1	C	180	ASP
2	D	3	GLN
2	D	17	LYS

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Mol	Chain	Res	Type
2	D	18	LYS
2	D	25	GLN
2	D	30	GLU
2	D	44	ARG
2	D	65	LYS
2	D	93	SER
2	D	99	GLU
2	D	133	SER
2	D	143	LEU
2	D	167	VAL
2	D	172	GLN
2	D	190	ARG
1	A	2	LYS
1	A	6	GLN
1	A	26	SER
1	A	32	SER
1	A	42	LYS
1	A	45	GLU
1	A	48	MET
1	A	75	LEU
1	A	124	ASP
1	A	125	SER
1	A	150	SER
1	A	151	ASP
1	A	163	ARG
1	A	164	SER
2	B	17	LYS
2	B	18	LYS
2	B	25	GLN
2	B	30	GLU
2	B	43	LEU
2	B	56	ASP
2	B	65	LYS
2	B	83	PRO
2	B	97	SER
2	B	100	GLN
2	B	109	THR
2	B	133	SER
2	B	135	THR
2	B	143	LEU
2	B	167	VAL
2	B	175	LYS

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Mol	Chain	Res	Type
2	B	182	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (28) such sidechains are listed below:

Mol	Chain	Res	Type
1	C	6	GLN
1	C	22	ASN
1	C	64	GLN
1	C	113	GLN
1	C	114	ASN
1	C	188	ASN
1	C	189	ASN
2	D	37	GLN
2	D	84	ASN
2	D	151	HIS
2	D	159	ASN
2	D	172	GLN
2	D	203	ASN
2	D	217	ASN
1	A	6	GLN
1	A	22	ASN
1	A	38	GLN
1	A	113	GLN
1	A	146	GLN
1	A	188	ASN
1	A	189	ASN
2	B	45	GLN
2	B	84	ASN
2	B	159	ASN
2	B	172	GLN
2	B	203	ASN
2	B	210	GLN
2	B	217	ASN

5.3.3 RNA

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	199/205 (97%)	0.79	11 (5%) 30 27	50, 78, 106, 143	0
1	C	199/205 (97%)	0.58	9 (4%) 38 33	41, 71, 95, 131	0
2	B	241/242 (99%)	0.36	8 (3%) 49 45	38, 67, 90, 97	0
2	D	241/242 (99%)	0.30	7 (2%) 53 49	33, 60, 83, 97	0
All	All	880/894 (98%)	0.49	35 (3%) 42 38	33, 69, 96, 143	0

All (35) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	125	SER	3.8
1	A	4	VAL	3.8
2	B	40	GLY	3.5
2	B	177	GLN	3.3
1	C	92	TYR	2.8
1	A	166	ASP	2.8
2	B	95	GLY	2.8
1	A	92	TYR	2.8
1	C	183	CYS	2.8
2	D	97	SER	2.7
1	C	158	CYS	2.7
2	D	181	ASN	2.6
2	B	172	GLN	2.6
1	A	183	CYS	2.5
2	D	2	ALA	2.5
1	C	10	PRO	2.5
2	D	1	GLU	2.4
2	B	62	GLU	2.4
1	C	159	VAL	2.4
1	A	93	ASN	2.3
2	B	24	SER	2.3

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Mol	Chain	Res	Type	RSRZ
1	C	7	ASN	2.3
2	B	223	ASP	2.2
1	A	6	GLN	2.2
2	D	168	CYS	2.2
1	A	115	PRO	2.2
1	A	181	PHE	2.2
1	A	127	SER	2.2
2	B	52	VAL	2.1
1	C	125	SER	2.1
1	C	193	PRO	2.1
2	D	129	GLU	2.1
1	C	200	SER	2.1
2	D	96	ALA	2.0
1	A	122	LEU	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.