



Full wwPDB X-ray Structure Validation Report ⓘ

Apr 25, 2026 – 08:15 PM EDT

PDB ID : 4PRI / pdb_00004pri
Title : Crystal structure of TK3 TCR-HLA-B*35:08-HPVG complex
Authors : Yu Chih, L.; Rossjohn, J.; Gras, S.
Deposited on : 2014-03-05
Resolution : 2.40 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

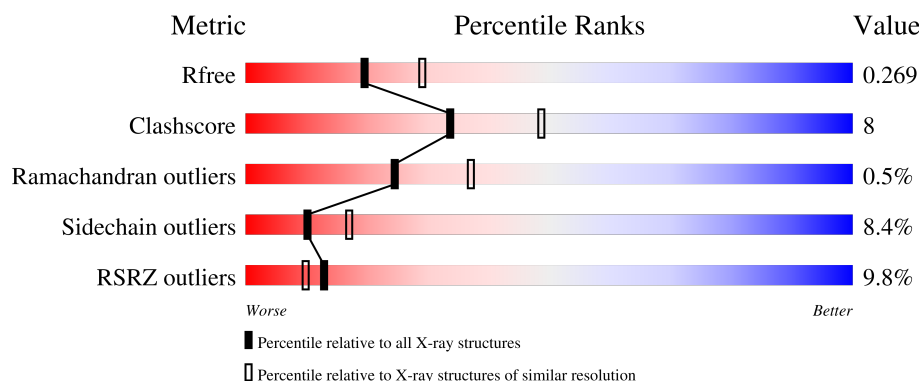
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.40 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	4912 (2.40-2.40)
Clashscore	190562	5391 (2.40-2.40)
Ramachandran outliers	187476	5320 (2.40-2.40)
Sidechain outliers	187428	5321 (2.40-2.40)
RSRZ outliers	180081	4916 (2.40-2.40)

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	276	17% 75% 19% • •
2	B	99	8% 77% 20% •
3	C	11	73% 27%
4	D	202	6% 75% 22% •
5	E	240	6% 82% 15% •

2 Entry composition [i](#)

There are 8 unique types of molecules in this entry. The entry contains 6792 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 MHC class I antigen.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	276	Total	C	N	O	S	0	5	0
			2304	1433	425	438	8			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	99	Total	C	N	O	S	0	0	0
			829	528	140	158	3			

- Molecule 3 is a protein called Epstein-Barr nuclear antigen 1.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
3	C	11	Total	C	N	O	0	0	0
			95	62	13	20			

- Molecule 4 is a protein called TK3 TCR alpha chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	D	202	Total	C	N	O	S	0	2	0
			1593	990	265	331	7			

- Molecule 5 is a protein called TK3 TCR beta chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	E	240	Total	C	N	O	S	0	0	0
			1911	1203	333	370	5			

- Molecule 6 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	1	Total	Cl	0	0
			1	1		

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	D	1	Total Cl 1 1	0	0

- Molecule 7 is SODIUM ION (CCD ID: NA) (formula: Na).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	B	1	Total Na 1 1	0	0
7	D	1	Total Na 1 1	0	0
7	E	1	Total Na 1 1	0	0

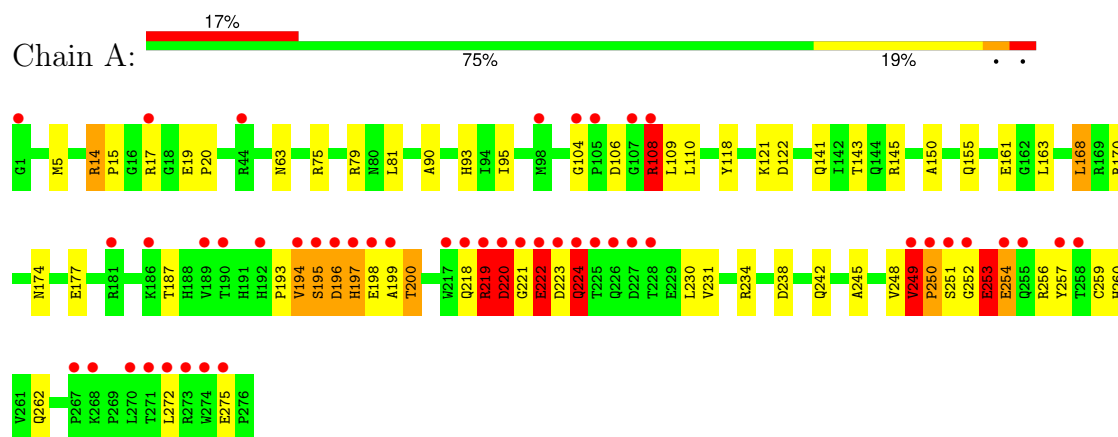
- Molecule 8 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
8	A	21	Total O 21 21	0	0
8	B	4	Total O 4 4	0	0
8	C	2	Total O 2 2	0	0
8	D	12	Total O 12 12	0	0
8	E	16	Total O 16 16	0	0

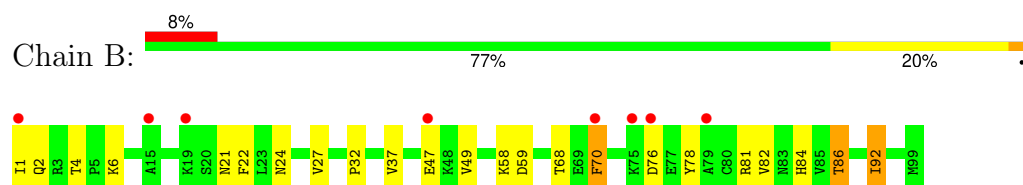
3 Residue-property plots

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

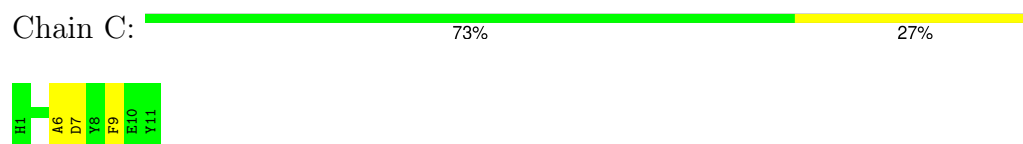
• Molecule 1: MHC class I antigen



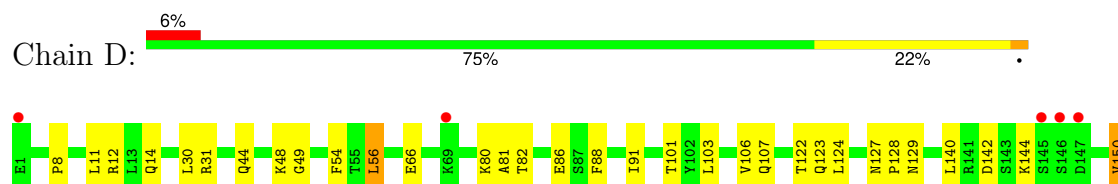
• Molecule 2: Beta-2-microglobulin

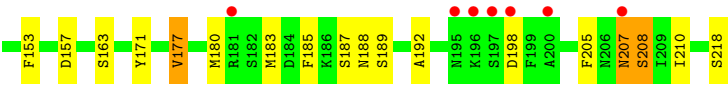


• Molecule 3: Epstein-Barr nuclear antigen 1

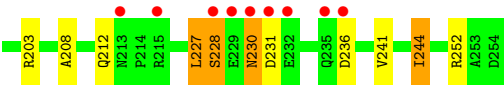
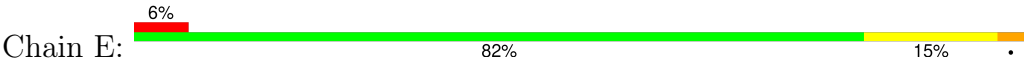


• Molecule 4: TK3 TCR alpha chain





• Molecule 5: TK3 TCR beta chain



4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	44.58Å 62.38Å 100.46Å 98.17° 94.59° 109.12°	Depositor
Resolution (Å)	41.70 – 2.40 41.70 – 2.40	Depositor EDS
% Data completeness (in resolution range)	(Not available) (41.70-2.40) 95.3 (41.70-2.40)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.87 (at 2.39Å)	Xtriage
Refinement program	PHENIX	Depositor
R, R_{free}	0.213 , 0.261 0.223 , 0.269	Depositor DCC
R_{free} test set	1873 reflections (4.78%)	wwPDB-VP
Wilson B-factor (Å ²)	27.3	Xtriage
Anisotropy	0.637	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 45.1	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	0.91	EDS
Total number of atoms	6792	wwPDB-VP
Average B, all atoms (Å ²)	34.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.22% 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

Bond lengths and bond angles in the following residue types are not validated in this section: NA, CL

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	0.94	2/2367 (0.1%)	1.35	21/3215 (0.7%)
2	B	0.83	0/852	1.21	4/1152 (0.3%)
3	C	0.84	0/99	1.24	1/133 (0.8%)
4	D	0.88	2/1626 (0.1%)	1.17	7/2201 (0.3%)
5	E	0.82	2/1960 (0.1%)	1.23	8/2664 (0.3%)
All	All	0.88	6/6904 (0.1%)	1.26	41/9365 (0.4%)

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	90	ALA	CA-CB	-7.32	1.41	1.53
5	E	227	LEU	CA-C	-5.93	1.45	1.52
4	D	88	PHE	CA-C	-5.57	1.46	1.52
4	D	101	THR	C-O	-5.38	1.17	1.24
5	E	227	LEU	C-O	-5.26	1.17	1.24
1	A	93	HIS	C-O	-5.25	1.17	1.23

All (41) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	196	ASP	N-CA-C	12.05	124.15	111.14
1	A	197	HIS	N-CA-C	-7.90	103.21	113.17
1	A	106	ASP	N-CA-C	7.63	119.67	111.36
1	A	219	ARG	N-CA-C	-7.57	103.77	113.16
2	B	70	PHE	CA-CB-CG	7.54	121.34	113.80
1	A	224	GLN	CA-C-N	7.24	130.95	120.38
1	A	224	GLN	C-N-CA	7.24	130.95	120.38
5	E	162	PRO	CA-C-N	7.12	131.99	120.60
5	E	162	PRO	C-N-CA	7.12	131.99	120.60
1	A	195	SER	N-CA-C	6.73	118.69	111.36

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	E	76	PHE	CA-CB-CG	6.56	120.36	113.80
4	D	157	ASP	CA-CB-CG	6.41	119.00	112.60
1	A	108	ARG	N-CA-C	-6.15	100.13	109.85
1	A	199	ALA	N-CA-C	6.05	117.69	110.19
5	E	208	ALA	CA-C-N	5.88	128.48	120.54
5	E	208	ALA	C-N-CA	5.88	128.48	120.54
1	A	253	GLU	N-CA-C	5.83	118.05	109.24
4	D	129	ASN	CA-CB-CG	5.82	118.42	112.60
2	B	92	ILE	N-CA-CB	5.75	116.99	110.72
1	A	63	ASN	CA-C-N	5.70	128.19	120.38
1	A	63	ASN	C-N-CA	5.70	128.19	120.38
2	B	59	ASP	CA-CB-CG	5.69	118.29	112.60
1	A	250	PRO	N-CA-C	-5.51	106.02	113.40
4	D	198	ASP	CA-CB-CG	5.50	118.10	112.60
1	A	95	ILE	N-CA-CB	5.50	117.64	111.21
5	E	252	ARG	CA-C-N	5.39	127.51	120.28
5	E	252	ARG	C-N-CA	5.39	127.51	120.28
5	E	244	ILE	N-CA-CB	5.22	117.26	110.99
3	C	7	ASP	CA-CB-CG	5.18	117.78	112.60
4	D	188	ASN	CA-CB-CG	5.17	117.77	112.60
2	B	24	ASN	CA-CB-CG	5.08	117.68	112.60
1	A	143	THR	CA-C-N	5.06	127.02	120.44
1	A	143	THR	C-N-CA	5.06	127.02	120.44
1	A	122	ASP	CA-CB-CG	5.05	117.65	112.60
4	D	142	ASP	CA-CB-CG	5.04	117.64	112.60
4	D	205	PHE	CA-C-N	5.03	127.52	120.28
4	D	205	PHE	C-N-CA	5.03	127.52	120.28
1	A	17	ARG	CA-C-N	5.03	124.87	120.10
1	A	17	ARG	C-N-CA	5.03	124.87	120.10
1	A	168	LEU	CA-C-N	5.01	127.00	120.28
1	A	168	LEU	C-N-CA	5.01	127.00	120.28

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	2304	0	2167	54	0
2	B	829	0	794	12	0
3	C	95	0	76	1	0
4	D	1593	0	1509	21	0
5	E	1911	0	1815	16	0
6	A	1	0	0	0	0
6	D	1	0	0	0	0
7	B	1	0	0	0	0
7	D	1	0	0	0	0
7	E	1	0	0	0	0
8	A	21	0	0	0	0
8	B	4	0	0	0	0
8	C	2	0	0	0	0
8	D	12	0	0	1	0
8	E	16	0	0	0	0
All	All	6792	0	6361	101	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 8.

All (101) 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:A:219:ARG:CD	1:A:224:GLN:HE22	1.63	1.12
1:A:219:ARG:HD2	1:A:224:GLN:HE22	1.15	1.07
2:B:4:THR:HA	2:B:86:THR:HG21	1.46	0.97
1:A:248:VAL:O	1:A:249:VAL:HG12	1.63	0.97
2:B:21:ASN:ND2	2:B:22:PHE:H	1.63	0.96
1:A:218:GLN:NE2	1:A:260:HIS:NE2	2.24	0.86
1:A:249:VAL:HG13	1:A:249:VAL:O	1.76	0.85
1:A:200:THR:OG1	1:A:248:VAL:HG22	1.77	0.85
1:A:219:ARG:HD2	1:A:224:GLN:NE2	1.92	0.85
1:A:249:VAL:O	1:A:249:VAL:CG1	2.29	0.80
1:A:253:GLU:HG3	1:A:254:GLU:H	1.47	0.80
1:A:248:VAL:O	1:A:249:VAL:CG1	2.29	0.80
4:D:48:LYS:HD3	4:D:49:GLY:H	1.50	0.77
2:B:21:ASN:ND2	2:B:22:PHE:N	2.34	0.75
1:A:220:ASP:C	1:A:220:ASP:OD1	2.30	0.74
1:A:219:ARG:HD3	1:A:224:GLN:HE22	1.48	0.74
1:A:248:VAL:O	1:A:249:VAL:CB	2.36	0.73
4:D:128:PRO:HG3	4:D:177:VAL:HG21	1.71	0.73
1:A:250:PRO:O	1:A:251:SER:C	2.33	0.70

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:14:GLN:HE22	4:D:127:ASN:HD22	1.40	0.69
4:D:12:ARG:HH12	4:D:123:GLN:HE22	1.37	0.69
4:D:48:LYS:CD	4:D:49:GLY:H	2.08	0.67
2:B:21:ASN:HD22	2:B:22:PHE:N	1.91	0.66
1:A:253:GLU:HG3	1:A:254:GLU:N	2.10	0.65
1:A:104:GLY:N	1:A:108:ARG:O	2.27	0.65
4:D:207:ASN:ND2	8:D:405:HOH:O	2.29	0.65
2:B:81:ARG:HG3	2:B:92:ILE:HG12	1.78	0.64
4:D:12:ARG:HH12	4:D:123:GLN:NE2	1.97	0.63
1:A:234:ARG:HE	1:A:242:GLN:HE21	1.46	0.63
5:E:227:LEU:O	5:E:241:VAL:HA	1.98	0.63
4:D:44:GLN:HE22	5:E:44:GLN:HE22	1.46	0.63
1:A:252:GLY:HA3	1:A:256:ARG:HH11	1.65	0.61
1:A:219:ARG:CB	1:A:257:TYR:CE1	2.85	0.60
5:E:12:ILE:HG12	5:E:162:PRO:HG2	1.84	0.59
5:E:10:HIS:ND1	5:E:164:HIS:HD2	2.01	0.59
1:A:219:ARG:HB3	1:A:257:TYR:CE1	2.39	0.58
4:D:31:ARG:HB3	4:D:107:GLN:HB3	1.86	0.57
4:D:12:ARG:NH1	4:D:123:GLN:HE22	2.02	0.56
1:A:219:ARG:CD	1:A:224:GLN:NE2	2.49	0.56
5:E:107:SER:HB3	5:E:113:LEU:HD22	1.88	0.56
4:D:66:GLU:HG2	4:D:82:THR:HG22	1.86	0.56
1:A:250:PRO:C	1:A:252:GLY:N	2.63	0.55
1:A:248:VAL:O	1:A:249:VAL:HB	2.07	0.54
4:D:44:GLN:HE21	4:D:103:LEU:HD11	1.73	0.54
2:B:84:HIS:HB3	2:B:86:THR:HG22	1.90	0.53
1:A:250:PRO:HB2	1:A:252:GLY:O	2.07	0.53
5:E:59:GLY:H	5:E:80:GLN:NE2	2.07	0.53
1:A:198:GLU:HB2	1:A:250:PRO:HD2	1.91	0.52
1:A:20:PRO:HD2	1:A:75[B]:ARG:HG2	1.93	0.51
4:D:153:PHE:O	4:D:189:SER:HA	2.11	0.51
1:A:219:ARG:O	1:A:220:ASP:HB3	2.10	0.51
1:A:219:ARG:HB2	1:A:257:TYR:CE1	2.46	0.51
1:A:220:ASP:OD1	1:A:220:ASP:O	2.29	0.50
1:A:221:GLY:O	1:A:222:GLU:HB2	2.11	0.50
1:A:81:LEU:HD23	1:A:118:TYR:CD1	2.46	0.50
5:E:228:SER:O	5:E:230:ASN:OD1	2.30	0.50
1:A:221:GLY:O	1:A:222:GLU:OE2	2.30	0.50
1:A:5:MET:HB2	1:A:168:LEU:HD13	1.94	0.50
1:A:218:GLN:NE2	1:A:260:HIS:CE1	2.79	0.50
1:A:150:ALA:HA	5:E:109:ARG:O	2.12	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:55:GLN:HG2	5:E:56:TYR:N	2.27	0.49
4:D:163:SER:H	4:D:208:SER:HB3	1.76	0.49
4:D:171:TYR:O	4:D:192:ALA:HA	2.13	0.49
1:A:219:ARG:HB2	1:A:257:TYR:CD1	2.48	0.48
1:A:219:ARG:CB	1:A:257:TYR:CD1	2.97	0.48
3:C:6:ALA:HB3	3:C:9:PHE:CE1	2.49	0.47
5:E:14:ALA:HA	5:E:124:LEU:O	2.14	0.47
2:B:21:ASN:CG	2:B:22:PHE:H	2.17	0.47
1:A:222:GLU:O	1:A:224:GLN:HG2	2.15	0.46
1:A:230:LEU:HD12	1:A:245:ALA:HB2	1.98	0.46
5:E:120:ARG:HH12	5:E:163:ASP:HB3	1.80	0.46
1:A:197:HIS:NE2	1:A:249:VAL:HG23	2.31	0.46
1:A:170:ARG:HH11	1:A:174:ASN:HD21	1.63	0.46
2:B:2:GLN:HG2	2:B:32:PRO:HD3	1.98	0.46
5:E:163:ASP:OD1	5:E:186:PRO:HG2	2.16	0.45
4:D:8:PRO:O	4:D:122:THR:HG23	2.17	0.45
1:A:219:ARG:HD3	1:A:224:GLN:NE2	2.23	0.44
1:A:193:PRO:O	1:A:194:VAL:HG22	2.18	0.44
1:A:14:ARG:HD3	1:A:19[A]:GLU:O	2.17	0.44
5:E:122:THR:OG1	5:E:164:HIS:HE1	2.00	0.44
1:A:141:GLN:O	1:A:145:ARG:HD2	2.18	0.44
4:D:140:LEU:HB2	4:D:150:VAL:HG12	1.99	0.44
5:E:127:LEU:HB3	5:E:227:LEU:HD11	2.00	0.44
1:A:219:ARG:O	1:A:220:ASP:CB	2.66	0.43
1:A:249:VAL:HG22	1:A:251:SER:OG	2.19	0.43
4:D:180:MET:HE2	4:D:185:PHE:CD1	2.54	0.43
1:A:109:LEU:HD22	1:A:161:GLU:HA	2.01	0.42
2:B:37:VAL:HG22	2:B:82:VAL:HG22	2.00	0.42
1:A:75[A]:ARG:NH1	1:A:79:ARG:HH22	2.18	0.42
1:A:250:PRO:HB3	1:A:253:GLU:HA	2.01	0.42
1:A:14:ARG:HD3	1:A:19[B]:GLU:O	2.20	0.42
5:E:183:ASP:OD2	5:E:203:ARG:NH1	2.47	0.42
4:D:11:LEU:HD23	4:D:124:LEU:HD13	2.01	0.41
2:B:76:ASP:HB3	2:B:78:TYR:CE2	2.55	0.41
1:A:155:GLN:OE1	4:D:31:ARG:HD2	2.20	0.41
1:A:259:CYS:HB3	1:A:272:LEU:HB3	2.03	0.41
2:B:49:VAL:HG22	2:B:68:THR:HB	2.02	0.41
5:E:180:VAL:HA	5:E:203:ARG:O	2.21	0.41
2:B:6:LYS:O	2:B:27:VAL:HA	2.21	0.40
1:A:187:THR:HB	1:A:272:LEU:HD22	2.04	0.40
4:D:56:LEU:HD11	4:D:81:ALA:HB1	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	279/276 (101%)	262 (94%)	13 (5%)	4 (1%)	9	13
2	B	97/99 (98%)	94 (97%)	3 (3%)	0	100	100
3	C	9/11 (82%)	9 (100%)	0	0	100	100
4	D	202/202 (100%)	194 (96%)	8 (4%)	0	100	100
5	E	238/240 (99%)	227 (95%)	11 (5%)	0	100	100
All	All	825/828 (100%)	786 (95%)	35 (4%)	4 (0%)	24	37

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	222	GLU
1	A	220	ASP
1	A	249	VAL
1	A	15	PRO

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	239/234 (102%)	216 (90%)	23 (10%)	8	12
2	B	94/94 (100%)	89 (95%)	5 (5%)	20	36

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
3	C	9/9 (100%)	9 (100%)	0	100	100
4	D	182/180 (101%)	166 (91%)	16 (9%)	9	15
5	E	208/208 (100%)	190 (91%)	18 (9%)	9	16
All	All	732/725 (101%)	670 (92%)	62 (8%)	10	16

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

Mol	Chain	Res	Type
1	A	14	ARG
1	A	108	ARG
1	A	110[A]	LEU
1	A	110[B]	LEU
1	A	121	LYS
1	A	163	LEU
1	A	177	GLU
1	A	194	VAL
1	A	195	SER
1	A	196	ASP
1	A	200	THR
1	A	219	ARG
1	A	220	ASP
1	A	222	GLU
1	A	223	ASP
1	A	224	GLN
1	A	231	VAL
1	A	238	ASP
1	A	249	VAL
1	A	253	GLU
1	A	254	GLU
1	A	262	GLN
1	A	275	GLU
2	B	1	ILE
2	B	47	GLU
2	B	58	LYS
2	B	70	PHE
2	B	86	THR
4	D	30	LEU
4	D	54	PHE
4	D	56	LEU
4	D	80	LYS
4	D	86	GLU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
4	D	91	ILE
4	D	106	VAL
4	D	144	LYS
4	D	150	VAL
4	D	177	VAL
4	D	183	MET
4	D	187	SER
4	D	207	ASN
4	D	208	SER
4	D	210	ILE
4	D	218	SER
5	E	9	LYS
5	E	46	LEU
5	E	48	GLN
5	E	90	ASN
5	E	125	GLU
5	E	156	LEU
5	E	163	ASP
5	E	168	SER
5	E	180	VAL
5	E	182	THR
5	E	193	LEU
5	E	194	ASN
5	E	212	GLN
5	E	228	SER
5	E	230	ASN
5	E	231	ASP
5	E	236	ASP
5	E	244	ILE

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

Mol	Chain	Res	Type
1	A	54	GLN
1	A	63	ASN
1	A	65	GLN
1	A	115	GLN
1	A	127	ASN
1	A	141	GLN
1	A	174	ASN
1	A	188	HIS
1	A	218	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	224	GLN
1	A	242	GLN
1	A	262	GLN
2	B	21	ASN
2	B	42	ASN
4	D	14	GLN
4	D	44	GLN
4	D	123	GLN
4	D	129	ASN
5	E	80	GLN
5	E	164	HIS
5	E	216	ASN
5	E	217	HIS

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 ⓘ

Of 5 ligands modelled in this entry, 5 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 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	276/276 (100%)	0.77	47 (17%) 4 3	10, 32, 74, 115	15 (5%)
2	B	99/99 (100%)	0.84	8 (8%) 18 14	17, 39, 68, 81	1 (1%)
3	C	11/11 (100%)	0.06	0 100 100	14, 19, 29, 34	0
4	D	202/202 (100%)	0.25	12 (5%) 28 24	7, 25, 55, 72	4 (1%)
5	E	240/240 (100%)	0.30	14 (5%) 29 25	9, 28, 60, 79	2 (0%)
All	All	828/828 (100%)	0.51	81 (9%) 13 10	7, 30, 67, 115	22 (2%)

All (81) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	195	SER	8.5
1	A	197	HIS	8.2
1	A	196	ASP	6.9
1	A	194	VAL	5.6
1	A	250	PRO	5.4
1	A	220	ASP	4.7
1	A	255	GLN	4.5
1	A	225	THR	4.4
1	A	224	GLN	4.2
1	A	105	PRO	4.0
5	E	230	ASN	3.9
1	A	223	ASP	3.8
1	A	222	GLU	3.8
2	B	19	LYS	3.7
1	A	221	GLY	3.7
5	E	193	LEU	3.6
1	A	219	ARG	3.4
1	A	108	ARG	3.4
4	D	181	ARG	3.4
5	E	231	ASP	3.3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
5	E	46	LEU	3.3
4	D	146	SER	3.3
5	E	229	GLU	3.3
1	A	227	ASP	3.2
1	A	251	SER	3.1
1	A	254	GLU	3.1
1	A	1	GLY	3.0
5	E	215	ARG	3.0
5	E	192	ALA	3.0
1	A	226	GLN	3.0
1	A	258	THR	2.9
1	A	198	GLU	2.9
1	A	189	VAL	2.9
4	D	198	ASP	2.9
1	A	273[A]	ARG	2.8
4	D	195	ASN	2.8
1	A	272	LEU	2.8
5	E	194	ASN	2.7
1	A	271	THR	2.7
4	D	200	ALA	2.7
1	A	249	VAL	2.7
1	A	190	THR	2.7
2	B	75	LYS	2.6
1	A	270	LEU	2.6
4	D	145	SER	2.6
5	E	228	SER	2.6
1	A	192	HIS	2.6
2	B	79	ALA	2.6
1	A	104	GLY	2.5
1	A	275	GLU	2.5
4	D	197	SER	2.5
1	A	17	ARG	2.5
1	A	268	LYS	2.5
4	D	207	ASN	2.4
4	D	196	LYS	2.4
1	A	199	ALA	2.4
1	A	252	GLY	2.4
1	A	44	ARG	2.4
1	A	274	TRP	2.4
4	D	69	LYS	2.4
1	A	98[A]	MET	2.4
4	D	1	GLU	2.4

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	228	THR	2.3
1	A	218	GLN	2.3
1	A	217	TRP	2.3
1	A	107	GLY	2.2
2	B	1	ILE	2.2
2	B	47	GLU	2.2
5	E	236	ASP	2.2
1	A	181	ARG	2.2
1	A	267	PRO	2.2
5	E	213	ASN	2.2
5	E	232	GLU	2.2
1	A	257	TYR	2.1
5	E	235	GLN	2.1
2	B	15	ALA	2.1
4	D	147	ASP	2.1
2	B	70	PHE	2.0
5	E	128	LYS	2.0
2	B	76	ASP	2.0
1	A	186	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](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
7	NA	B	101	1/1	0.78	0.16	45,45,45,45	0
6	CL	A	301	1/1	0.92	0.16	35,35,35,35	0
7	NA	E	301	1/1	0.92	0.06	29,29,29,29	0
6	CL	D	302	1/1	0.93	0.11	45,45,45,45	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
7	NA	D	301	1/1	0.94	0.08	30,30,30,30	0

6.5 Other polymers [i](#)

There are no such residues in this entry.