



Full wwPDB X-ray Structure Validation Report ⓘ

Sep 13, 2023 – 05:10 AM EDT

PDB ID : 4PRI
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 : 4.02b-467
Xtriage (Phenix) : 1.13
EDS : 2.35.1
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0158
CCP4 : 7.0.044 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.35.1

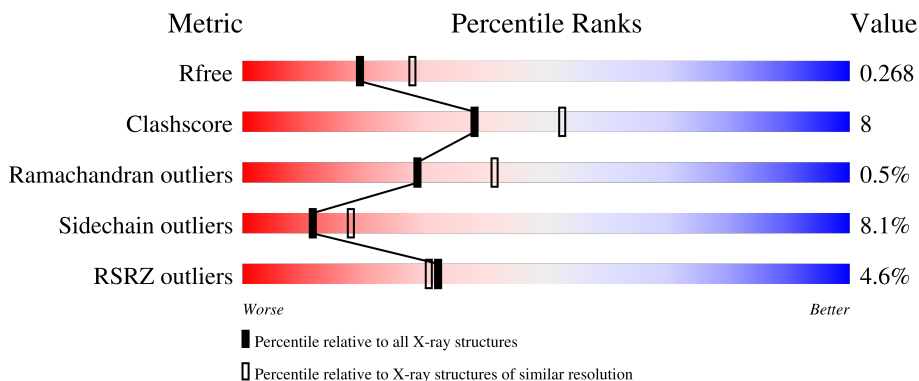
1 Overall quality at a glance

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}	130704	3907 (2.40-2.40)
Clashscore	141614	4398 (2.40-2.40)
Ramachandran outliers	138981	4318 (2.40-2.40)
Sidechain outliers	138945	4319 (2.40-2.40)
RSRZ outliers	127900	3811 (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	
2	B	99	
3	C	11	
4	D	202	
5	E	240	

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
			Total	C	N	O	S			
1	A	276	2304	1433	425	438	8	0	5	0

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

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

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

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

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

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

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

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

- Molecule 6 is CHLORIDE ION (three-letter code: 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 (three-letter code: 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

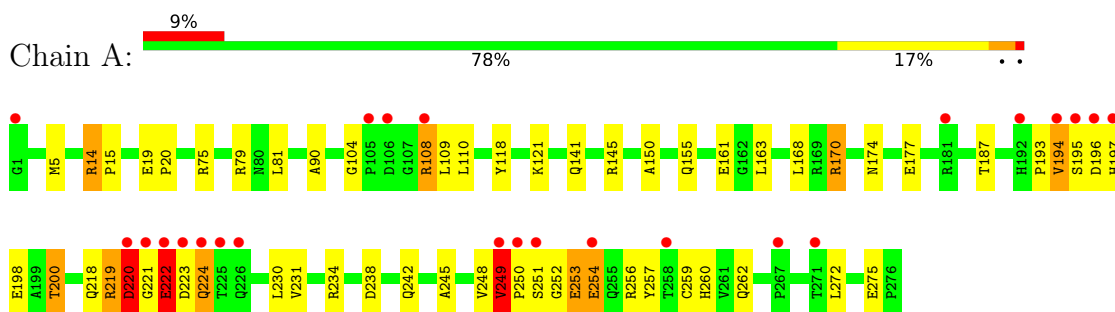
- Molecule 8 is water.

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

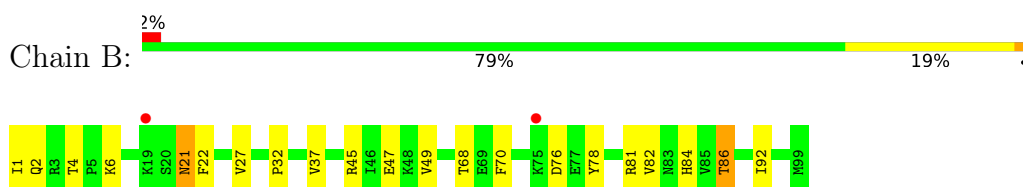
3 Residue-property plots [i](#)

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.

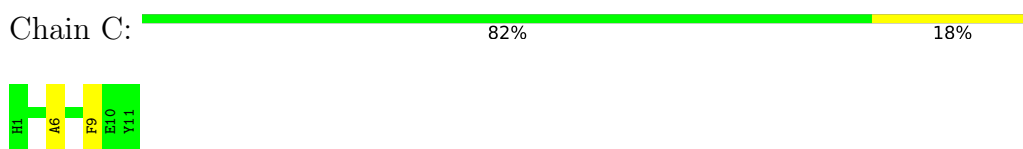
- Molecule 1: MHC class I antigen



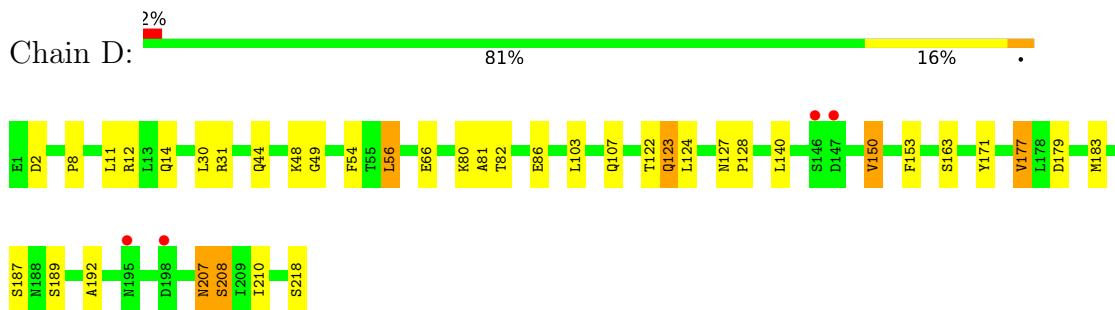
- Molecule 2: Beta-2-microglobulin



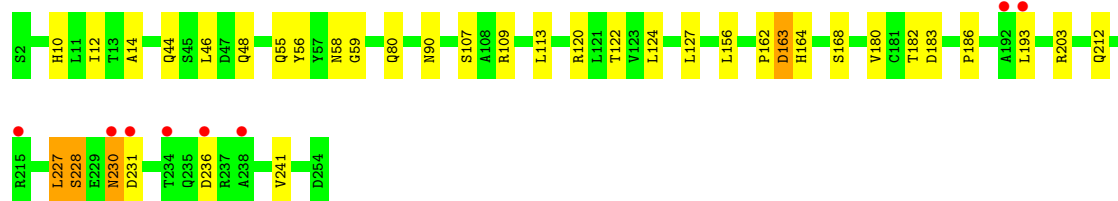
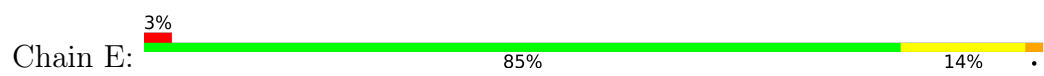
- Molecule 3: Epstein-Barr nuclear antigen 1



- 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 41.73 – 2.40	Depositor EDS
% Data completeness (in resolution range)	(Not available) (41.70-2.40) 95.4 (41.73-2.40)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.87 (at 2.39Å)	Xtrriage
Refinement program	PHENIX	Depositor
R, R_{free}	0.213 , 0.261 0.222 , 0.268	Depositor DCC
R_{free} test set	1873 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å ²)	27.3	Xtrriage
Anisotropy	0.637	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 45.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
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

Xtrriage'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 [i](#)

5.1 Standard geometry [i](#)

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

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	0.62	1/2367 (0.0%)	0.76	0/3215
2	B	0.53	0/852	0.70	0/1152
3	C	0.57	0/99	0.72	0/133
4	D	0.53	0/1626	0.71	0/2201
5	E	0.51	0/1960	0.73	1/2664 (0.0%)
All	All	0.56	1/6904 (0.0%)	0.73	1/9365 (0.0%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	90	ALA	CA-CB	-5.03	1.41	1.52

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	E	227	LEU	CA-CB-CG	5.42	127.77	115.30

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	2304	0	2167	54	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	B	829	0	794	12	0
3	C	95	0	76	1	0
4	D	1593	0	1509	20	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	100	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 (100) 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: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:220:ASP:C	1:A:220:ASP:OD1	2.30	0.69
4:D:14:GLN:HE22	4:D:127:ASN:HD22	1.40	0.69

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:250:PRO:O	1:A:251:SER:C	2.33	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: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
1:A:250:PRO:C	1:A:252:GLY:N	2.63	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
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
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
2:B:21:ASN:CG	2:B:22:PHE:H	2.17	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%)	11	15
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%)	29	41

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%)	215 (90%)	24 (10%)	7	11
2	B	94/94 (100%)	88 (94%)	6 (6%)	17	28
3	C	9/9 (100%)	9 (100%)	0	100	100
4	D	182/180 (101%)	166 (91%)	16 (9%)	10	15

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
5	E	208/208 (100%)	194 (93%)	14 (7%)	16	26
All	All	732/725 (101%)	672 (92%)	60 (8%)	11	17

All (60) 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	170	ARG
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	21	ASN
2	B	45	ARG
2	B	47	GLU
2	B	70	PHE
2	B	86	THR
4	D	2	ASP
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	123	GLN
4	D	150	VAL
4	D	177	VAL
4	D	179	ASP
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	46	LEU
5	E	48	GLN
5	E	58	ASN
5	E	90	ASN
5	E	156	LEU
5	E	163	ASP
5	E	168	SER
5	E	182	THR
5	E	193	LEU
5	E	212	GLN
5	E	228	SER
5	E	230	ASN
5	E	231	ASP
5	E	236	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (19) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	32	GLN
1	A	72	GLN
1	A	115	GLN
1	A	127	ASN
1	A	174	ASN
1	A	218	GLN
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

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
4	D	129	ASN
4	D	207	ASN
5	E	80	GLN
5	E	164	HIS
5	E	216	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 monosaccharides in this entry.

5.6 Ligand geometry [i](#)

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 [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	276/276 (100%)	0.30	24 (8%) 10 9	10, 33, 76, 115	10 (3%)
2	B	99/99 (100%)	0.07	2 (2%) 65 63	17, 39, 68, 81	1 (1%)
3	C	11/11 (100%)	-0.28	0 100 100	14, 19, 29, 34	0
4	D	202/202 (100%)	-0.19	4 (1%) 65 63	12, 25, 55, 72	2 (0%)
5	E	240/240 (100%)	-0.12	8 (3%) 46 45	9, 28, 60, 79	2 (0%)
All	All	828/828 (100%)	0.02	38 (4%) 32 31	9, 30, 68, 115	15 (1%)

All (38) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	223	ASP	7.1
1	A	197	HIS	7.1
1	A	221	GLY	6.0
1	A	194	VAL	4.3
1	A	224	GLN	4.3
1	A	250	PRO	4.2
1	A	196	ASP	4.1
1	A	222	GLU	3.8
1	A	181	ARG	3.5
1	A	1	GLY	3.5
1	A	105	PRO	3.3
4	D	146	SER	3.2
5	E	238	ALA	3.1
1	A	225	THR	3.1
1	A	251	SER	3.0
1	A	220	ASP	3.0
1	A	195	SER	2.9
5	E	230	ASN	2.9
4	D	198	ASP	2.9
2	B	19	LYS	2.9

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
5	E	234	THR	2.8
5	E	192	ALA	2.7
1	A	267	PRO	2.7
4	D	195	ASN	2.7
5	E	215	ARG	2.6
1	A	254	GLU	2.6
1	A	108	ARG	2.5
1	A	271	THR	2.4
5	E	236	ASP	2.3
4	D	147	ASP	2.3
1	A	249	VAL	2.3
1	A	226	GLN	2.3
5	E	193	LEU	2.2
1	A	192	HIS	2.2
2	B	75	LYS	2.2
1	A	258	THR	2.1
1	A	106	ASP	2.1
5	E	231	ASP	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 monosaccharides 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(Å ²)	Q<0.9
7	NA	B	101	1/1	0.82	0.15	45,45,45,45	0
7	NA	D	301	1/1	0.95	0.10	30,30,30,30	0
7	NA	E	301	1/1	0.96	0.07	29,29,29,29	0
6	CL	D	302	1/1	0.97	0.10	45,45,45,45	0
6	CL	A	301	1/1	0.97	0.10	35,35,35,35	0

6.5 Other polymers [i](#)

There are no such residues in this entry.