



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 11:48 AM UTC

PDB ID : 3MV8 / pdb_00003mv8
Title : Crystal Structure of the TK3-Gln55His TCR in complex with HLA-B*3501/HPVG
Authors : Gras, S.; Chen, Z.; Miles, J.J.; Liu, Y.C.; Bell, M.J.; Sullivan, L.C.; Kjer-Nielsen, L.; Brennan, R.M.; Burrows, J.M.; Neller, M.A.; Khanna, R.; Purcell, A.W.; Brooks, A.G.; McCluskey, J.; Rossjohn, J.; Burrows, S.R.
Deposited on : 2010-05-03
Resolution : 2.10 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
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

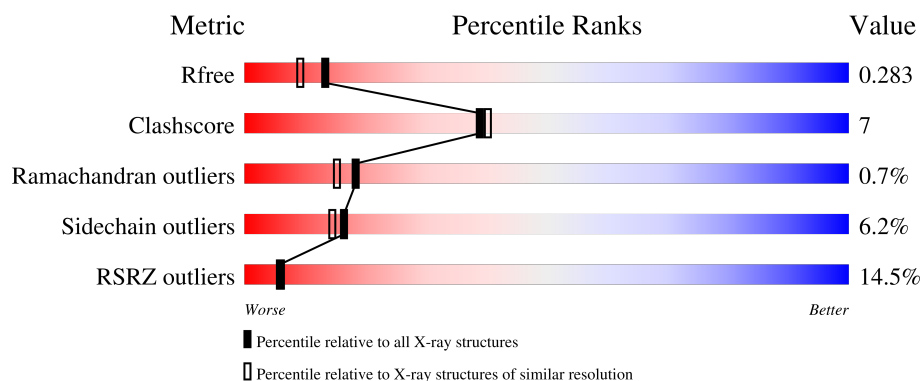
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.10 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	6658 (2.10-2.10)
Clashscore	190562	7164 (2.10-2.10)
Ramachandran outliers	187476	7099 (2.10-2.10)
Sidechain outliers	187428	7100 (2.10-2.10)
RSRZ outliers	180081	6662 (2.10-2.10)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	276	17% 84% 14% .
2	B	100	36% 74% 24% .
3	C	11	55% 45%
4	D	200	6% 76% 18% .

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
5	E	242	10% 85% 14%

2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 7064 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called HLA class I histocompatibility antigen, B-35 alpha chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	276	Total	C	N	O	S	0	7	0
			2320	1442	428	442	8			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	100	Total	C	N	O	S	0	2	0
			852	544	143	161	4			

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	0	MET	-	initiating methionine	UNP P61769

- Molecule 3 is a protein called HPVG peptide from 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			

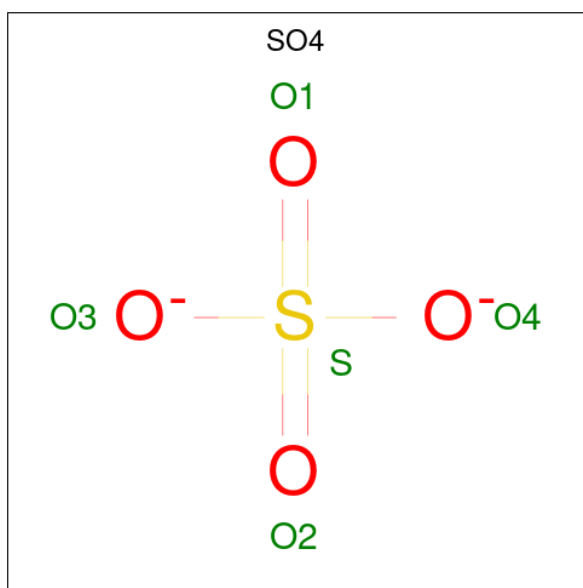
- Molecule 4 is a protein called alpha chain of the TK3 TCR.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	D	200	Total	C	N	O	S	0	11	0
			1648	1024	274	343	7			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	E	242	Total	C	N	O	S	0	2	0
			1943	1221	338	378	6			

- Molecule 6 is SULFATE ION (CCD ID: SO4) (formula: O₄S).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	E	1	Total	O	S	0	0
			5	4	1		

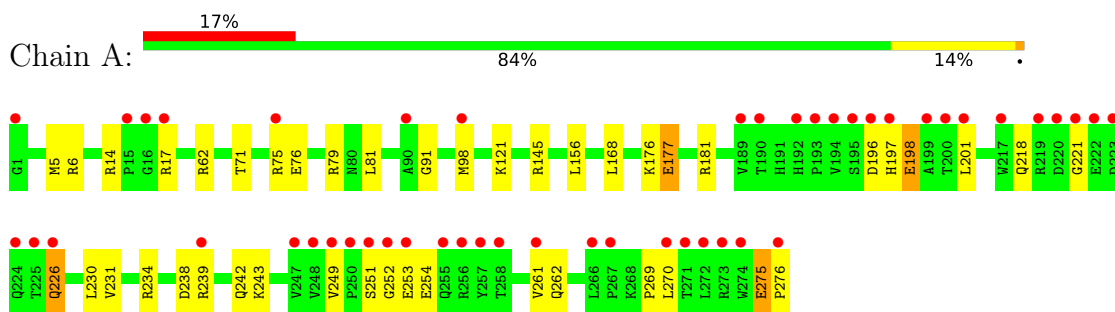
- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	69	Total	O	0	0
			69	69		
7	B	14	Total	O	0	0
			14	14		
7	C	5	Total	O	0	0
			5	5		
7	D	66	Total	O	0	0
			66	66		
7	E	47	Total	O	0	0
			47	47		

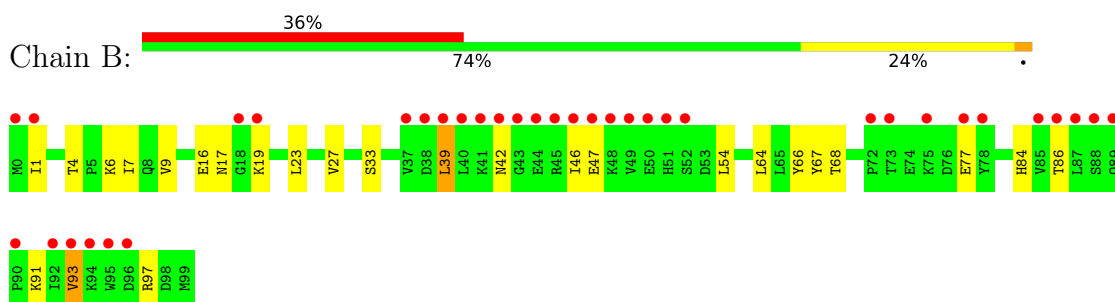
3 Residue-property plots [i](#)

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

- Molecule 1: HLA class I histocompatibility antigen, B-35 alpha chain



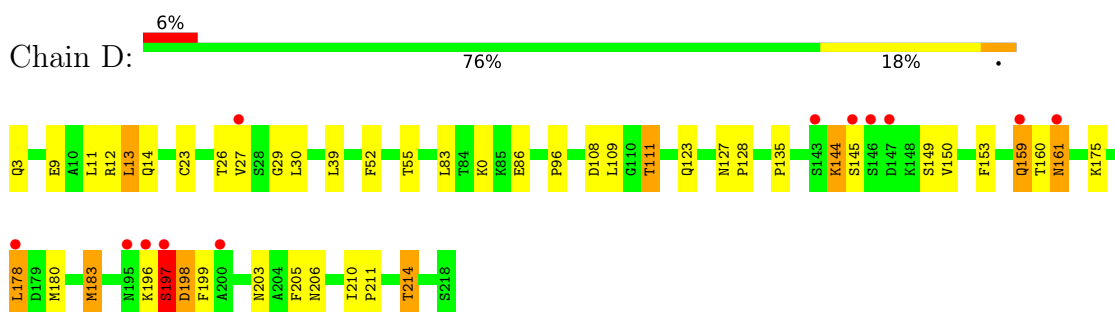
- Molecule 2: Beta-2-microglobulin



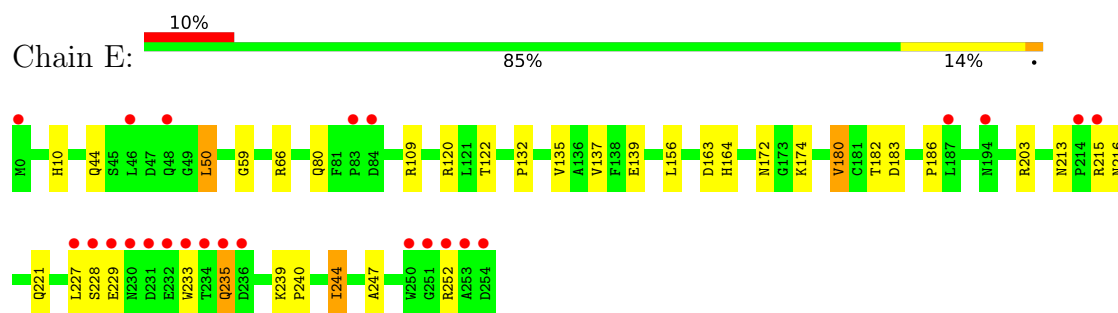
- Molecule 3: HPVG peptide from Epstein-Barr nuclear antigen 1



- Molecule 4: alpha chain of the TK3 TCR



● Molecule 5: beta chain of the TK3 TCR



4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	44.76Å 63.61Å 88.14Å 101.12° 97.60° 112.00°	Depositor
Resolution (Å)	84.22 – 2.10 84.22 – 2.10	Depositor EDS
% Data completeness (in resolution range)	98.2 (84.22-2.10) 98.2 (84.22-2.10)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.69 (at 2.10Å)	Xtriage
Refinement program	REFMAC 5.5.0088	Depositor
R, R_{free}	0.229 , 0.276 0.243 , 0.283	Depositor DCC
R_{free} test set	2513 reflections (5.08%)	wwPDB-VP
Wilson B-factor (Å ²)	23.9	Xtriage
Anisotropy	0.624	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 30.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	7064	wwPDB-VP
Average B, all atoms (Å ²)	30.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.52% 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: SO4

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	0.43	0/2383	0.75	0/3237
2	B	0.42	0/875	0.74	0/1183
3	C	0.54	0/99	0.61	0/133
4	D	0.42	0/1680	0.76	1/2272 (0.0%)
5	E	0.41	0/1993	0.70	0/2708
All	All	0.42	0/7030	0.74	1/9533 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	D	144	LYS	N-CA-C	6.36	117.90	110.97

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	2320	0	2180	26	0
2	B	852	0	821	13	0
3	C	95	0	76	5	0
4	D	1648	0	1567	27	0
5	E	1943	0	1839	23	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	E	5	0	0	0	0
7	A	69	0	0	1	0
7	B	14	0	0	0	0
7	C	5	0	0	0	0
7	D	66	0	0	3	0
7	E	47	0	0	0	0
All	All	7064	0	6483	91	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 7.

All (91) 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:62:ARG:HE	3:C:1:HIS:HE1	1.18	0.87
5:E:10:HIS:ND1	5:E:164:HIS:HD2	1.79	0.80
1:A:6:ARG:HE	1:A:98[A]:MET:HE3	1.49	0.78
4:D:14:GLN:NE2	4:D:127:ASN:HD22	1.81	0.77
4:D:108:ASP:HB3	4:D:111:THR:HG23	1.69	0.74
4:D:12[A]:ARG:HH22	4:D:123:GLN:HE22	1.35	0.74
2:B:4:THR:HA	2:B:86:THR:HG21	1.71	0.72
4:D:14:GLN:HE22	4:D:127:ASN:HD22	1.35	0.72
4:D:144:LYS:HB3	4:D:145:SER:HA	1.72	0.72
4:D:135:PRO:HB2	4:D:214[A]:THR:HG22	1.74	0.70
4:D:52:PHE:HZ	4:D:55[B]:THR:HG23	1.57	0.69
1:A:62:ARG:HE	3:C:1:HIS:CE1	2.07	0.69
4:D:12[B]:ARG:HH22	4:D:123:GLN:HE22	1.39	0.68
4:D:52:PHE:CZ	4:D:55[B]:THR:HG23	2.28	0.67
1:A:176:LYS:O	1:A:177:GLU:HB3	1.94	0.66
4:D:161:ASN:HB3	7:D:227:HOH:O	1.95	0.66
2:B:7:ILE:HG21	2:B:93[A]:VAL:HG21	1.79	0.65
5:E:122:THR:OG1	5:E:164:HIS:HE1	1.80	0.65
5:E:227:LEU:HD22	5:E:240:PRO:HD2	1.80	0.64
5:E:59:GLY:H	5:E:80:GLN:NE2	1.98	0.61
5:E:10:HIS:ND1	5:E:164:HIS:CD2	2.67	0.60
1:A:239:ARG:HH11	1:A:239:ARG:HA	1.66	0.59
2:B:7:ILE:CG2	2:B:93[A]:VAL:HG21	2.33	0.59
4:D:160:THR:HG21	4:D:211:PRO:HG3	1.85	0.57
4:D:27[A]:VAL:HG13	4:D:108:ASP:CG	2.30	0.57
4:D:203:ASN:O	4:D:206:ASN:HB2	2.05	0.56
2:B:33:SER:HB2	2:B:54:LEU:HD21	1.87	0.56

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:163:ASP:OD1	5:E:186:PRO:HG2	2.07	0.55
5:E:183:ASP:OD2	5:E:203:ARG:NH1	2.35	0.55
4:D:14:GLN:HE22	4:D:127:ASN:ND2	2.05	0.54
1:A:230:LEU:HD12	1:A:243:LYS:HE3	1.91	0.52
2:B:42:ASN:ND2	2:B:77:GLU:H	2.07	0.52
1:A:91:GLY:HA2	7:A:288:HOH:O	2.10	0.51
1:A:198:GLU:HG2	1:A:251:SER:HB3	1.91	0.51
3:C:1:HIS:HD2	3:C:2:PRO:O	1.94	0.51
2:B:27:VAL:HG22	2:B:64:LEU:HD12	1.93	0.50
1:A:5:MET:HB2	1:A:168:LEU:HD13	1.93	0.50
4:D:12[A]:ARG:NH2	4:D:123:GLN:HE22	2.08	0.50
4:D:27[A]:VAL:HG12	4:D:29:GLY:N	2.27	0.50
2:B:84:HIS:ND1	2:B:86:THR:HG22	2.27	0.50
2:B:39:LEU:HD23	2:B:68:THR:HG22	1.93	0.49
4:D:197:SER:O	4:D:199:PHE:N	2.45	0.49
4:D:96:PRO:HG3	4:D:128:PRO:HB3	1.94	0.48
1:A:238:ASP:O	1:A:239:ARG:HB2	2.13	0.48
1:A:262:GLN:HE21	1:A:269:PRO:HG3	1.78	0.48
1:A:6:ARG:NE	1:A:98[A]:MET:HE3	2.23	0.47
3:C:8:TYR:CD2	5:E:109:ARG:HA	2.49	0.47
5:E:44:GLN:HB2	5:E:50:LEU:CD1	2.45	0.47
4:D:23:CYS:O	4:D:86[A]:GLU:HB2	2.15	0.47
5:E:44:GLN:HB2	5:E:50:LEU:HD12	1.97	0.47
5:E:172:ASN:HD21	5:E:216:ASN:HD22	1.63	0.47
1:A:181:ARG:O	1:A:181:ARG:HG3	2.15	0.46
4:D:11:LEU:HD22	4:D:13:LEU:HD13	1.96	0.46
2:B:16:GLU:HB3	2:B:19:LYS:HB3	1.98	0.46
5:E:213:ASN:HD21	5:E:215:ARG:NH1	2.13	0.46
1:A:251:SER:O	1:A:253:GLU:N	2.48	0.46
4:D:144:LYS:N	4:D:145:SER:HB2	2.31	0.46
4:D:180:MET:HE2	4:D:183:MET:HE3	1.98	0.46
2:B:23:LEU:O	2:B:67:TYR:HA	2.16	0.46
2:B:17:ASN:ND2	2:B:97:ARG:HH12	2.15	0.45
2:B:64:LEU:HD13	2:B:66:TYR:CE2	2.51	0.45
1:A:251:SER:C	1:A:253:GLU:H	2.24	0.45
4:D:210:ILE:HB	7:D:258:HOH:O	2.15	0.45
5:E:137:VAL:HG23	5:E:247:ALA:HB3	2.00	0.43
5:E:221:GLN:HG3	5:E:244:ILE:HD13	2.00	0.43
1:A:239:ARG:HA	1:A:239:ARG:NH1	2.33	0.43
1:A:198:GLU:CG	1:A:251:SER:HB3	2.48	0.43
1:A:76:GLU:HG3	1:A:79:ARG:NH2	2.34	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:46[B]:ILE:C	2:B:46[B]:ILE:HD13	2.43	0.43
1:A:201:LEU:HD12	1:A:249:VAL:HG11	2.01	0.42
4:D:3:GLN:HG3	4:D:26:THR:O	2.19	0.42
5:E:120:ARG:HH22	5:E:163:ASP:HB3	1.84	0.42
5:E:132:PRO:HD3	5:E:240:PRO:HB3	2.02	0.42
5:E:233:TRP:CE2	5:E:235:GLN:HB2	2.54	0.42
1:A:261:VAL:CG1	1:A:270:LEU:HB2	2.50	0.42
4:D:159:GLN:HE21	4:D:159:GLN:HA	1.84	0.42
5:E:59:GLY:H	5:E:80:GLN:HE21	1.67	0.42
1:A:71:THR:O	1:A:75[A]:ARG:HG3	2.20	0.42
1:A:196:ASP:O	1:A:197:HIS:HB2	2.19	0.42
4:D:178:LEU:HB2	7:D:248:HOH:O	2.20	0.42
1:A:218:GLN:HE21	1:A:221:GLY:HA2	1.85	0.41
1:A:234:ARG:HE	1:A:242:GLN:HE21	1.68	0.41
1:A:226:GLN:H	1:A:226:GLN:HG2	1.67	0.41
5:E:239:LYS:HA	5:E:240:PRO:HD3	1.86	0.41
4:D:153:PHE:HB2	4:D:205:PHE:CE1	2.55	0.41
5:E:180:VAL:HA	5:E:203:ARG:O	2.21	0.40
1:A:275:GLU:HA	1:A:276:PRO:HD3	1.90	0.40
3:C:6:ALA:HB3	3:C:9:PHE:CE1	2.56	0.40
5:E:139:GLU:OE1	5:E:252:ARG:NH1	2.54	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	281/276 (102%)	264 (94%)	15 (5%)	2 (1%)	18	15
2	B	100/100 (100%)	97 (97%)	2 (2%)	1 (1%)	12	9
3	C	9/11 (82%)	9 (100%)	0	0	100	100
4	D	209/200 (104%)	201 (96%)	6 (3%)	2 (1%)	12	9

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
5	E	242/242 (100%)	232 (96%)	8 (3%)	2 (1%)	16	12
All	All	841/829 (101%)	803 (96%)	31 (4%)	7 (1%)	18	12

All (7) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
4	D	198	ASP
2	B	47	GLU
1	A	198	GLU
1	A	252	GLY
4	D	197	SER
5	E	229[A]	GLU
5	E	229[B]	GLU

5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	241/234 (103%)	230 (95%)	11 (5%)	24	25
2	B	97/95 (102%)	90 (93%)	7 (7%)	13	11
3	C	9/9 (100%)	9 (100%)	0	100	100
4	D	189/178 (106%)	168 (89%)	21 (11%)	6	3
5	E	212/210 (101%)	203 (96%)	9 (4%)	26	28
All	All	748/726 (103%)	700 (94%)	48 (6%)	16	14

All (48) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	14	ARG
1	A	17	ARG
1	A	81	LEU
1	A	121	LYS
1	A	145	ARG

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	156	LEU
1	A	177	GLU
1	A	226	GLN
1	A	231	VAL
1	A	254	GLU
1	A	275	GLU
2	B	1	ILE
2	B	6	LYS
2	B	9	VAL
2	B	39	LEU
2	B	91	LYS
2	B	93[A]	VAL
2	B	93[B]	VAL
4	D	9[A]	GLU
4	D	9[B]	GLU
4	D	13	LEU
4	D	30	LEU
4	D	39	LEU
4	D	83	LEU
4	D	0	LYS
4	D	109	LEU
4	D	111	THR
4	D	149	SER
4	D	150	VAL
4	D	159	GLN
4	D	161	ASN
4	D	175	LYS
4	D	178	LEU
4	D	183	MET
4	D	196	LYS
4	D	197	SER
4	D	198	ASP
4	D	214[A]	THR
4	D	214[B]	THR
5	E	50	LEU
5	E	66	ARG
5	E	135	VAL
5	E	156	LEU
5	E	174	LYS
5	E	180	VAL
5	E	182	THR
5	E	235	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
5	E	244	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (30) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	32	GLN
1	A	115	GLN
1	A	127	ASN
1	A	191	HIS
1	A	218	GLN
1	A	242	GLN
1	A	262	GLN
2	B	2	GLN
2	B	17	ASN
2	B	24	ASN
2	B	42	ASN
2	B	83	ASN
3	C	1	HIS
4	D	14	GLN
4	D	44	GLN
4	D	123	GLN
4	D	129	ASN
4	D	132	ASN
4	D	159	GLN
4	D	161	ASN
4	D	188	ASN
4	D	207	ASN
5	E	51	GLN
5	E	80	GLN
5	E	164	HIS
5	E	212	GLN
5	E	213	ASN
5	E	216	ASN
5	E	230	ASN
5	E	243	GLN

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](#)

1 ligand is modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. 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 $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
6	SO4	E	255	-	4,4,4	0.24	0	6,6,6	0.09	0

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%)	0.79	48 (17%)	4 4	8, 26, 74, 91	14 (5%)
2	B	100/100 (100%)	1.71	36 (36%)	1 1	18, 43, 78, 87	2 (2%)
3	C	11/11 (100%)	-0.46	0	100 100	13, 15, 18, 19	0
4	D	200/200 (100%)	0.48	12 (6%)	27 29	8, 23, 50, 59	12 (6%)
5	E	242/242 (100%)	0.67	24 (9%)	13 13	14, 26, 50, 87	13 (5%)
All	All	829/829 (100%)	0.77	120 (14%)	6 6	8, 26, 68, 91	41 (4%)

All (120) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	46[A]	ILE	7.0
2	B	37	VAL	5.6
2	B	49	VAL	5.4
2	B	38	ASP	4.7
2	B	43	GLY	4.7
2	B	40	LEU	4.6
5	E	0	MET	4.4
2	B	0	MET	4.4
2	B	39	LEU	4.4
2	B	92	ILE	4.4
1	A	15	PRO	4.3
1	A	251	SER	4.3
2	B	1	ILE	4.2
1	A	276	PRO	4.1
2	B	51	HIS	4.0
4	D	195	ASN	4.0
5	E	254	ASP	3.9
1	A	194	VAL	3.9
2	B	18	GLY	3.9
4	D	146	SER	3.7

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
2	B	42	ASN	3.6
4	D	196	LYS	3.6
5	E	229[A]	GLU	3.6
4	D	197	SER	3.6
5	E	228	SER	3.6
1	A	253	GLU	3.5
1	A	250	PRO	3.5
1	A	272	LEU	3.4
2	B	41	LYS	3.4
2	B	48	LYS	3.4
2	B	52	SER	3.4
1	A	249	VAL	3.4
1	A	199	ALA	3.4
1	A	274	TRP	3.3
1	A	196	ASP	3.3
1	A	197	HIS	3.3
1	A	270	LEU	3.3
1	A	252	GLY	3.2
5	E	46	LEU	3.2
5	E	215	ARG	3.2
2	B	50	GLU	3.2
1	A	239	ARG	3.2
2	B	86	THR	3.2
1	A	248	VAL	3.2
5	E	252	ARG	3.2
1	A	257	TYR	3.1
2	B	85	VAL	3.1
2	B	90	PRO	3.1
2	B	94	LYS	3.1
2	B	44	GLU	3.0
4	D	147	ASP	3.0
1	A	98[A]	MET	3.0
1	A	193	PRO	3.0
1	A	267	PRO	3.0
1	A	271	THR	3.0
5	E	231	ASP	2.9
1	A	195	SER	2.9
1	A	189	VAL	2.9
1	A	220	ASP	2.9
1	A	256	ARG	2.9
2	B	88	SER	2.9
5	E	230	ASN	2.9

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
2	B	73	THR	2.8
4	D	145	SER	2.7
5	E	253	ALA	2.7
1	A	201	LEU	2.7
2	B	89	GLN	2.7
1	A	90	ALA	2.7
1	A	219	ARG	2.7
2	B	78	TYR	2.7
1	A	17	ARG	2.7
2	B	45	ARG	2.7
2	B	77	GLU	2.7
1	A	16	GLY	2.6
4	D	27[A]	VAL	2.6
5	E	234	THR	2.6
5	E	232	GLU	2.6
2	B	75	LYS	2.6
1	A	255	GLN	2.5
5	E	214	PRO	2.5
5	E	250	TRP	2.5
1	A	190	THR	2.5
4	D	178	LEU	2.5
5	E	227	LEU	2.5
5	E	233	TRP	2.5
2	B	95	TRP	2.5
2	B	47	GLU	2.4
5	E	84	ASP	2.4
5	E	235	GLN	2.4
1	A	261	VAL	2.4
1	A	225	THR	2.4
5	E	251	GLY	2.3
1	A	217	TRP	2.3
1	A	192	HIS	2.3
2	B	93[A]	VAL	2.3
1	A	226	GLN	2.3
4	D	143	SER	2.3
1	A	258	THR	2.3
1	A	266	LEU	2.3
5	E	48	GLN	2.2
1	A	200	THR	2.2
5	E	83	PRO	2.2
1	A	1	GLY	2.2
1	A	221	GLY	2.2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	273	ARG	2.2
5	E	236	ASP	2.2
1	A	222	GLU	2.2
4	D	161	ASN	2.2
1	A	224	GLN	2.2
5	E	187	LEU	2.2
5	E	194	ASN	2.2
2	B	96	ASP	2.2
4	D	200	ALA	2.1
1	A	75[A]	ARG	2.1
2	B	19	LYS	2.1
2	B	87	LEU	2.1
2	B	72	PRO	2.1
1	A	223	ASP	2.0
1	A	247	VAL	2.0
4	D	159	GLN	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(Å ²)	Q<0.9
6	SO4	E	255	5/5	0.88	0.09	59,59,60,60	0

6.5 Other polymers [i](#)

There are no such residues in this entry.