



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 10, 2026 – 12:36 PM UTC

PDB ID : 4JRY / pdb_00004jry
Title : Crystal Structure of SB47 TCR-HLA B*3505-LPEP complex
Authors : Liu, Y.C.; Rossjohn, J.; Gras, S.
Deposited on : 2013-03-22
Resolution : 2.80 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

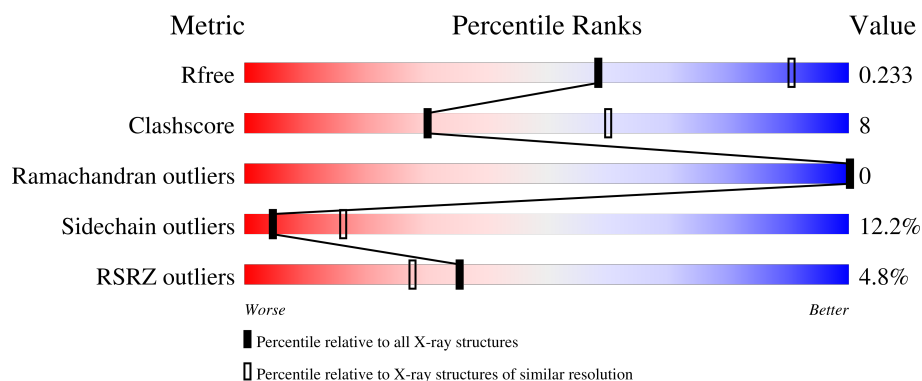
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.80 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	3866 (2.80-2.80)
Clashscore	190562	4276 (2.80-2.80)
Ramachandran outliers	187476	4196 (2.80-2.80)
Sidechain outliers	187428	4198 (2.80-2.80)
RSRZ outliers	180081	3869 (2.80-2.80)

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	5% 71% 23% 6%
2	B	100	4% 73% 25% .
3	C	13	69% 31%
4	D	201	7% 69% 26% . .
5	E	242	4% 79% 19% .

2 Entry composition

There are 8 unique types of molecules in this entry. The entry contains 6830 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	0	0
			2257	1405	414	431	7			

- 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	0	0
			837	533	141	159	4			

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	0	MET	-	expression tag	UNP P61769

- Molecule 3 is a protein called Trans-activator protein BZLF1.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
3	C	13	Total	C	N	O	0	0	0
			101	66	15	20			

- Molecule 4 is a protein called SB47 TCR alpha chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	D	201	Total	C	N	O	S	0	0	0
			1574	991	261	313	9			

- Molecule 5 is a protein called SB47 TCR beta chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	E	242	Total	C	N	O	S	1	0	0
			1934	1216	340	373	5			

- Molecule 6 is SODIUM ION (CCD ID: NA) (formula: Na).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	B	1	Total 1	Na 1	0	0

- Molecule 7 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	B	2	Total 2	Mg 2	0	0

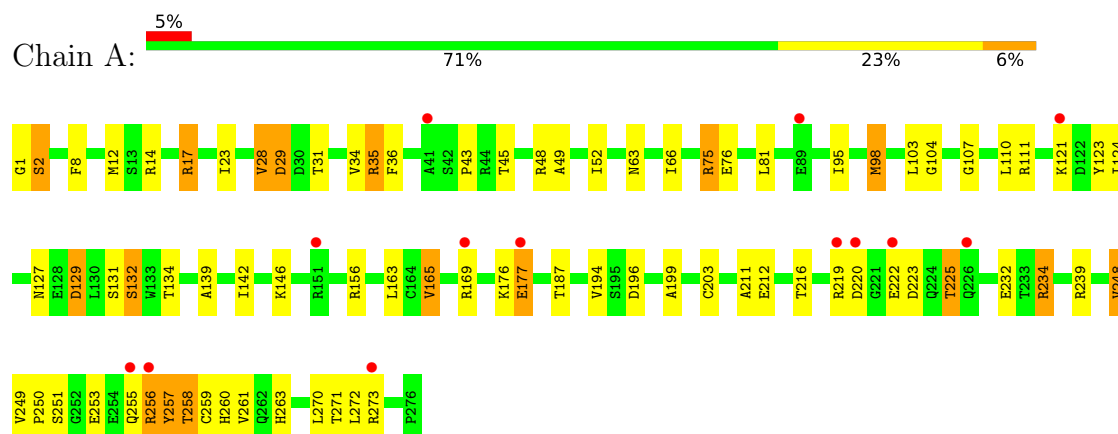
- Molecule 8 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	A	20	Total 20	O 20	0	0
8	B	14	Total 14	O 14	0	0
8	C	2	Total 2	O 2	0	0
8	D	32	Total 32	O 32	0	0
8	E	56	Total 56	O 56	0	0

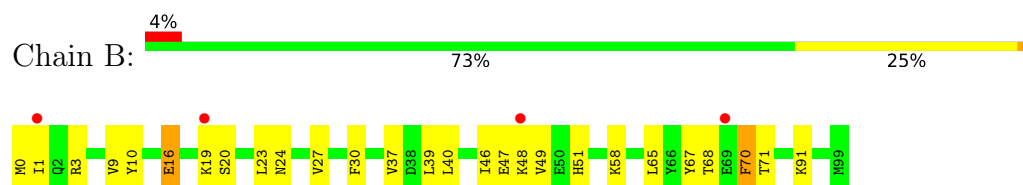
3 Residue-property plots [i](#)

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.

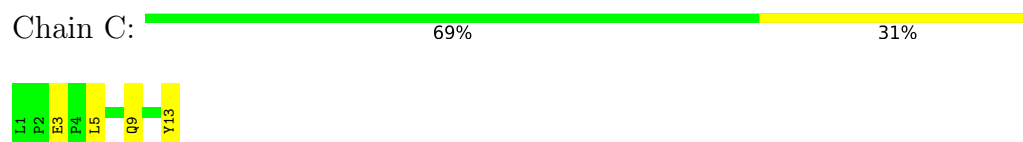
- Molecule 1: MHC class I antigen



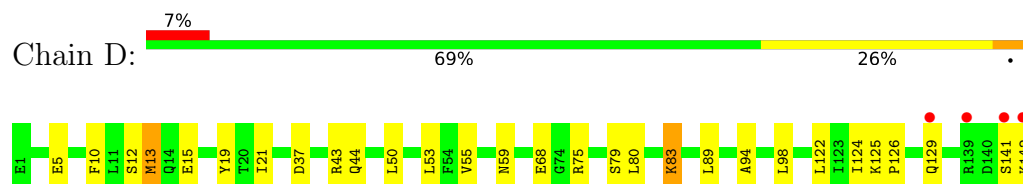
- Molecule 2: Beta-2-microglobulin

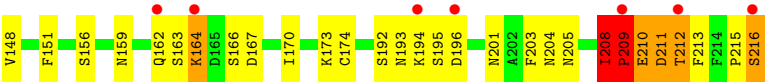


- Molecule 3: Trans-activator protein BZLF1

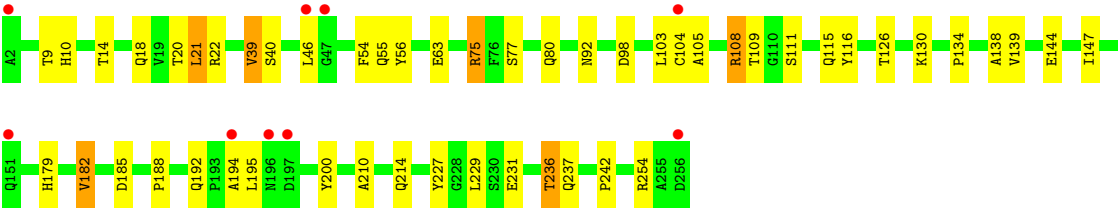
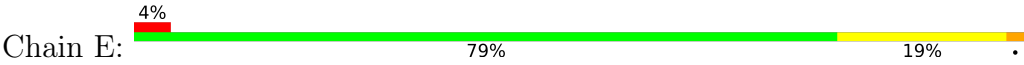


- Molecule 4: SB47 TCR alpha chain





● Molecule 5: SB47 TCR beta chain



4 Data and refinement statistics

Property	Value	Source
Space group	I 4	Depositor
Cell constants a, b, c, α , β , γ	237.60Å 237.60Å 61.20Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	100.00 – 2.80 100.00 – 2.80	Depositor EDS
% Data completeness (in resolution range)	(Not available) (100.00-2.80) 99.9 (100.00-2.80)	Depositor EDS
R_{merge}	0.14	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.11 (at 2.82Å)	Xtriage
Refinement program	BUSTER-TNT, BUSTER	Depositor
R, R_{free}	0.200 , 0.233 0.202 , 0.233	Depositor DCC
R_{free} test set	2147 reflections (5.04%)	wwPDB-VP
Wilson B-factor (Å ²)	48.8	Xtriage
Anisotropy	0.161	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 57.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	0.022 for -k,-h,-l	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	6830	wwPDB-VP
Average B, all atoms (Å ²)	46.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.74% 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, MG

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	0.90	2/2320 (0.1%)	1.33	17/3153 (0.5%)
2	B	0.86	0/860	1.19	3/1162 (0.3%)
3	C	0.76	0/104	1.04	0/142
4	D	0.97	1/1607 (0.1%)	1.28	7/2178 (0.3%)
5	E	0.93	2/1989 (0.1%)	1.20	5/2710 (0.2%)
All	All	0.92	5/6880 (0.1%)	1.26	32/9345 (0.3%)

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	E	103	LEU	CA-C	-5.18	1.46	1.52
1	A	234	ARG	CA-C	-5.17	1.48	1.52
1	A	28	VAL	C-O	-5.11	1.18	1.24
4	D	208	ILE	CA-CB	-5.09	1.49	1.55
5	E	138	ALA	CA-CB	-5.03	1.45	1.53

All (32) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	129	ASP	N-CA-C	-11.57	94.18	110.50
1	A	248	VAL	N-CA-CB	7.58	119.64	111.00
4	D	211	ASP	N-CA-C	-6.71	104.67	112.92
2	B	30	PHE	CA-CB-CG	6.23	120.03	113.80
5	E	236	THR	CB-CA-C	6.18	119.41	109.27
4	D	37	ASP	N-CA-C	-6.08	105.52	113.12
1	A	29	ASP	CB-CA-C	-5.98	109.69	116.63
1	A	95	ILE	N-CA-CB	5.91	118.08	110.99
5	E	144	GLU	CA-C-N	5.85	128.05	120.44
5	E	144	GLU	C-N-CA	5.85	128.05	120.44
4	D	209	PRO	N-CA-C	5.75	121.53	113.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	234	ARG	CA-C-N	5.72	125.48	119.76
1	A	234	ARG	C-N-CA	5.72	125.48	119.76
1	A	257	TYR	N-CA-C	5.71	118.95	109.46
1	A	75	ARG	CA-C-N	5.70	128.24	120.54
1	A	75	ARG	C-N-CA	5.70	128.24	120.54
1	A	28	VAL	N-CA-C	-5.69	99.44	107.75
4	D	192	SER	CA-C-N	5.46	128.05	120.29
4	D	192	SER	C-N-CA	5.46	128.05	120.29
2	B	70	PHE	CA-CB-CG	5.42	119.22	113.80
4	D	55	VAL	N-CA-CB	5.39	119.97	111.99
5	E	185	ASP	CA-CB-CG	5.38	117.98	112.60
5	E	236	THR	N-CA-CB	-5.36	103.91	110.98
1	A	263	HIS	CA-C-N	5.33	127.67	120.38
1	A	263	HIS	C-N-CA	5.33	127.67	120.38
4	D	143	SER	N-CA-C	5.27	115.09	108.45
1	A	196	ASP	CA-CB-CG	5.20	117.80	112.60
2	B	71	THR	CB-CA-C	5.20	117.09	110.34
1	A	75	ARG	N-CA-C	-5.18	105.32	110.97
1	A	256	ARG	N-CA-C	-5.17	106.47	112.89
1	A	212	GLU	CB-CG-CD	5.17	121.38	112.60
1	A	211	ALA	N-CA-C	5.02	117.49	111.71

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	2257	0	2123	37	0
2	B	837	0	803	12	0
3	C	101	0	102	2	0
4	D	1574	0	1522	37	0
5	E	1934	0	1817	23	0
6	B	1	0	0	0	0
7	B	2	0	0	0	0
8	A	20	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
8	B	14	0	0	0	0
8	C	2	0	0	0	0
8	D	32	0	0	1	0
8	E	56	0	0	0	0
All	All	6830	0	6367	106	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 (106) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:146:LYS:N	4:D:147:SER:HA	1.51	1.18
4:D:146:LYS:H	4:D:147:SER:CA	1.59	1.16
5:E:9:THR:HG23	5:E:10:HIS:HD2	1.23	0.97
4:D:13:MET:HG3	4:D:124:ILE:HG13	1.52	0.91
5:E:9:THR:HG23	5:E:10:HIS:CD2	2.07	0.90
4:D:146:LYS:N	4:D:147:SER:CA	2.20	0.86
4:D:146:LYS:H	4:D:147:SER:HA	0.74	0.85
4:D:204:ASN:O	4:D:205:ASN:HB3	1.80	0.82
4:D:209:PRO:O	4:D:210:GLU:CG	2.30	0.80
4:D:209:PRO:O	4:D:210:GLU:CB	2.29	0.77
1:A:17:ARG:HG2	1:A:17:ARG:HH11	1.54	0.72
1:A:129:ASP:OD1	1:A:129:ASP:C	2.32	0.72
4:D:209:PRO:O	4:D:210:GLU:HG3	1.90	0.69
4:D:208:ILE:HG13	4:D:212:THR:HG21	1.75	0.69
4:D:204:ASN:O	4:D:205:ASN:CB	2.41	0.68
5:E:214:GLN:HA	5:E:254:ARG:O	1.95	0.66
1:A:17:ARG:HH11	1:A:17:ARG:CG	2.09	0.66
4:D:205:ASN:O	4:D:205:ASN:ND2	2.30	0.65
1:A:255:GLN:HA	1:A:255:GLN:OE1	1.97	0.65
5:E:9:THR:CG2	5:E:10:HIS:HD2	2.04	0.63
4:D:59:ASN:HD21	4:D:83:LYS:HE2	1.65	0.61
4:D:209:PRO:O	4:D:210:GLU:HB2	1.99	0.61
1:A:103:LEU:HD11	1:A:107:GLY:HA2	1.83	0.60
4:D:210:GLU:H	4:D:212:THR:HG23	1.66	0.60
4:D:94:ALA:HB1	4:D:124:ILE:HG12	1.84	0.60
1:A:28:VAL:O	1:A:29:ASP:HB2	2.04	0.58
4:D:15:GLU:HG2	4:D:126:PRO:HA	1.85	0.58
5:E:192:GLN:C	5:E:194:ALA:H	2.13	0.57
5:E:20:THR:C	5:E:21:LEU:HD23	2.31	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:179:HIS:O	5:E:182:VAL:HG22	2.05	0.56
1:A:121:LYS:HE3	2:B:1:ILE:HD11	1.87	0.56
1:A:260:HIS:CE1	1:A:271:THR:HG23	2.41	0.56
4:D:213:PHE:CE2	4:D:215:PRO:HG3	2.41	0.55
4:D:209:PRO:C	4:D:210:GLU:CG	2.77	0.55
4:D:209:PRO:HB2	4:D:212:THR:HG22	1.88	0.55
4:D:215:PRO:O	4:D:216:SER:HB2	2.07	0.55
4:D:196:ASP:OD1	4:D:196:ASP:C	2.48	0.55
5:E:63:GLU:HA	5:E:80:GLN:HB3	1.89	0.54
1:A:250:PRO:HB2	1:A:253:GLU:HG3	1.91	0.53
4:D:146:LYS:N	4:D:147:SER:CB	2.72	0.53
2:B:1:ILE:HD12	2:B:1:ILE:H	1.72	0.53
1:A:223:ASP:HB3	1:A:225:THR:HG22	1.90	0.53
5:E:18:GLN:HG3	5:E:92:ASN:HB3	1.92	0.52
1:A:203:CYS:CB	1:A:259:CYS:SG	2.98	0.51
5:E:229:LEU:HD12	5:E:242:PRO:HD2	1.92	0.51
5:E:192:GLN:C	5:E:194:ALA:N	2.68	0.51
5:E:10:HIS:CG	5:E:227:TYR:HB3	2.46	0.50
5:E:75:ARG:HH22	5:E:98:ASP:CG	2.20	0.50
2:B:24:ASN:HB3	2:B:65:LEU:HD11	1.94	0.50
1:A:129:ASP:OD2	1:A:132:SER:OG	2.30	0.50
1:A:103:LEU:HD13	1:A:165:VAL:HG22	1.94	0.50
1:A:129:ASP:OD1	1:A:129:ASP:O	2.30	0.49
4:D:210:GLU:H	4:D:212:THR:CG2	2.24	0.49
1:A:129:ASP:OD1	1:A:131:SER:N	2.40	0.49
5:E:105:ALA:HA	5:E:116:TYR:O	2.12	0.49
1:A:127:ASN:O	1:A:129:ASP:O	2.29	0.49
4:D:196:ASP:OD1	4:D:196:ASP:O	2.30	0.49
1:A:81:LEU:HD11	3:C:13:TYR:HB3	1.94	0.49
5:E:39:VAL:HG13	5:E:104:CYS:SG	2.53	0.49
4:D:43:ARG:HB2	4:D:53:LEU:HD11	1.95	0.48
1:A:187:THR:HB	1:A:272:LEU:HD11	1.94	0.48
2:B:16:GLU:HB3	2:B:19:LYS:HG3	1.95	0.48
4:D:163:SER:HB2	4:D:170:ILE:CD1	2.43	0.48
1:A:139:ALA:HA	1:A:142:ILE:HD12	1.95	0.47
4:D:13:MET:HB2	4:D:19:TYR:CE2	2.48	0.47
1:A:35:ARG:HG2	1:A:48:ARG:HD3	1.97	0.47
5:E:108:ARG:HG2	5:E:111:SER:HB2	1.97	0.47
4:D:43:ARG:HD3	8:D:330:HOH:O	2.13	0.47
5:E:134:PRO:HD3	5:E:242:PRO:HB3	1.97	0.47
4:D:151:PHE:HB2	4:D:203:PHE:CE1	2.50	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:261:VAL:HB	1:A:270:LEU:HB2	1.97	0.46
4:D:164:LYS:HE3	4:D:205:ASN:OD1	2.16	0.46
1:A:220:ASP:OD1	1:A:256:ARG:HD2	2.16	0.45
4:D:75:ARG:HD2	4:D:98:LEU:HD11	1.99	0.45
5:E:147:ILE:HG23	5:E:210:ALA:HB1	1.98	0.45
5:E:188:PRO:HB2	5:E:200:TYR:HB3	1.98	0.44
5:E:14:THR:HA	5:E:126:THR:O	2.18	0.44
1:A:123:TYR:HD2	1:A:124:ILE:HG22	1.83	0.44
4:D:167:ASP:HB3	4:D:194:LYS:HE3	1.99	0.43
1:A:66:ILE:HA	3:C:5:LEU:HD21	2.01	0.43
1:A:36:PHE:CE2	1:A:43:PRO:HB2	2.53	0.43
1:A:199:ALA:O	1:A:249:VAL:HG22	2.19	0.43
1:A:104:GLY:CA	1:A:110:LEU:HB2	2.49	0.43
1:A:31:THR:HG23	1:A:239:ARG:HD3	2.00	0.42
4:D:21:ILE:HD11	4:D:89:LEU:HD23	2.01	0.42
1:A:1:GLY:HA3	1:A:2:SER:HA	1.74	0.42
1:A:8:PHE:CE2	1:A:98:MET:HG3	2.54	0.42
1:A:219:ARG:HD3	1:A:257:TYR:OH	2.19	0.42
4:D:125:LYS:HB3	4:D:156:SER:HB3	2.02	0.42
5:E:56:TYR:HB3	5:E:80:GLN:HB2	2.01	0.42
1:A:49:ALA:O	1:A:52:ILE:HG22	2.20	0.41
1:A:234:ARG:HG3	2:B:10:TYR:CE2	2.55	0.41
4:D:13:MET:CB	4:D:19:TYR:CE2	3.03	0.41
5:E:105:ALA:HB1	5:E:115:GLN:HG2	2.02	0.41
2:B:23:LEU:HB2	2:B:70:PHE:CD2	2.55	0.41
2:B:49:VAL:HG22	2:B:68:THR:HB	2.03	0.41
2:B:51:HIS:HA	2:B:65:LEU:O	2.21	0.41
1:A:45:THR:HG21	1:A:63:ASN:HB3	2.02	0.41
2:B:23:LEU:O	2:B:67:TYR:HA	2.21	0.41
2:B:39:LEU:HB3	2:B:46:ILE:HD12	2.02	0.41
5:E:192:GLN:O	5:E:194:ALA:N	2.53	0.41
1:A:177:GLU:OE1	1:A:177:GLU:HA	2.20	0.41
1:A:258:THR:HG22	1:A:260:HIS:NE2	2.36	0.41
4:D:44:GLN:HB2	4:D:50:LEU:HD23	2.03	0.41
1:A:234:ARG:HG3	2:B:10:TYR:CZ	2.57	0.40
2:B:27:VAL:HG21	2:B:37:VAL:HG21	2.03	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	274/276 (99%)	267 (97%)	7 (3%)	0	100	100
2	B	98/100 (98%)	95 (97%)	3 (3%)	0	100	100
3	C	11/13 (85%)	11 (100%)	0	0	100	100
4	D	199/201 (99%)	196 (98%)	3 (2%)	0	100	100
5	E	240/242 (99%)	233 (97%)	7 (3%)	0	100	100
All	All	822/832 (99%)	802 (98%)	20 (2%)	0	100	100

There are no Ramachandran outliers to report.

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	234/234 (100%)	205 (88%)	29 (12%)	4	16
2	B	95/95 (100%)	85 (90%)	10 (10%)	6	22
3	C	11/11 (100%)	9 (82%)	2 (18%)	2	6
4	D	178/178 (100%)	148 (83%)	30 (17%)	2	7
5	E	210/210 (100%)	192 (91%)	18 (9%)	10	31
All	All	728/728 (100%)	639 (88%)	89 (12%)	5	16

All (89) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	2	SER
1	A	12	MET
1	A	14	ARG
1	A	17	ARG
1	A	23	ILE
1	A	34	VAL
1	A	35	ARG
1	A	75	ARG
1	A	76	GLU
1	A	98	MET
1	A	111	ARG
1	A	132	SER
1	A	134	THR
1	A	146	LYS
1	A	156	ARG
1	A	163	LEU
1	A	165	VAL
1	A	169	ARG
1	A	176	LYS
1	A	177	GLU
1	A	194	VAL
1	A	216	THR
1	A	222	GLU
1	A	225	THR
1	A	232	GLU
1	A	248	VAL
1	A	251	SER
1	A	258	THR
1	A	273	ARG
2	B	0	MET
2	B	3	ARG
2	B	9	VAL
2	B	16	GLU
2	B	20	SER
2	B	40	LEU
2	B	47	GLU
2	B	48	LYS
2	B	58	LYS
2	B	91	LYS
3	C	3	GLU
3	C	9	GLN
4	D	5	GLU
4	D	10	PHE

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Mol	Chain	Res	Type
4	D	12	SER
4	D	13	MET
4	D	68	GLU
4	D	79	SER
4	D	80	LEU
4	D	83	LYS
4	D	122	LEU
4	D	129	GLN
4	D	141	SER
4	D	142	LYS
4	D	143	SER
4	D	144	SER
4	D	148	VAL
4	D	159	ASN
4	D	162	GLN
4	D	164	LYS
4	D	166	SER
4	D	173	LYS
4	D	174	CYS
4	D	193	ASN
4	D	195	SER
4	D	201	ASN
4	D	208	ILE
4	D	209	PRO
4	D	210	GLU
4	D	211	ASP
4	D	212	THR
4	D	216	SER
5	E	21	LEU
5	E	22	ARG
5	E	39	VAL
5	E	40	SER
5	E	46	LEU
5	E	54	PHE
5	E	55	GLN
5	E	75	ARG
5	E	77	SER
5	E	108	ARG
5	E	109	THR
5	E	130	LYS
5	E	139	VAL
5	E	182	VAL

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Mol	Chain	Res	Type
5	E	195	LEU
5	E	231	GLU
5	E	236	THR
5	E	237	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (13) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	70	ASN
1	A	80	ASN
1	A	127	ASN
1	A	141	GLN
1	A	224	GLN
4	D	44	GLN
4	D	59	ASN
4	D	96	HIS
4	D	162	GLN
5	E	44	GLN
5	E	55	GLN
5	E	90	ASN
5	E	237	GLN

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 3 ligands modelled in this entry, 3 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%)	0.23	13 (4%) 36 29	31, 49, 68, 87	25 (9%)
2	B	100/100 (100%)	0.16	4 (4%) 42 33	31, 45, 64, 75	6 (6%)
3	C	13/13 (100%)	0.20	0 100 100	34, 51, 72, 73	0
4	D	201/201 (100%)	0.21	14 (6%) 22 16	27, 42, 77, 91	11 (5%)
5	E	242/242 (100%)	-0.23	9 (3%) 45 36	22, 37, 54, 112	14 (5%)
All	All	832/832 (100%)	0.08	40 (4%) 35 28	22, 43, 71, 112	56 (6%)

All (40) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	48	LYS	8.0
4	D	164	LYS	6.7
4	D	139	ARG	5.8
1	A	222	GLU	5.6
4	D	129	GLN	5.0
1	A	273	ARG	4.9
1	A	219	ARG	4.8
4	D	209	PRO	3.8
4	D	194	LYS	3.7
1	A	226	GLN	3.6
1	A	89	GLU	3.6
1	A	151	ARG	3.5
2	B	1	ILE	3.2
4	D	216	SER	3.2
1	A	256	ARG	3.1
5	E	46	LEU	3.1
1	A	121	LYS	3.1
4	D	142	LYS	3.1
1	A	41	ALA	2.9
4	D	145	ASP	2.8

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Mol	Chain	Res	Type	RSRZ
4	D	143	SER	2.8
2	B	19	LYS	2.7
4	D	196	ASP	2.7
5	E	194	ALA	2.7
1	A	177	GLU	2.5
5	E	151	GLN	2.5
5	E	256	ASP	2.5
5	E	47	GLY	2.4
1	A	169	ARG	2.4
1	A	220	ASP	2.4
4	D	144	SER	2.4
5	E	197	ASP	2.4
1	A	255	GLN	2.4
2	B	69	GLU	2.3
4	D	162	GLN	2.2
5	E	104	CYS	2.1
5	E	196	ASN	2.1
4	D	212	THR	2.0
4	D	141	SER	2.0
5	E	2	ALA	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
7	MG	B	102	1/1	0.88	0.18	60,60,60,60	0
6	NA	B	101	1/1	0.94	0.12	44,44,44,44	0
7	MG	B	103	1/1	0.95	0.23	53,53,53,53	0

6.5 Other polymers [i](#)

There are no such residues in this entry.