



wwPDB X-ray Structure Validation Summary Report ⓘ

Jun 29, 2026 – 04:15 pm BST

PDB ID : 28ZB / pdb_000028zb
Title : Crystal Structure of HLA class II major histocompatibility complex bound to HCMV-IE1 peptide
Authors : Krey, T.; Nagarathinam, K.; Ssebyatika, G.
Deposited on : 2026-03-02
Resolution : 2.43 Å(reported)

This is a wwPDB X-ray Structure Validation Summary 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 : 1.8.4, CSD as541be (2020)
Xtriage (Phenix) : 2.0
EDS : 3.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.015 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.50

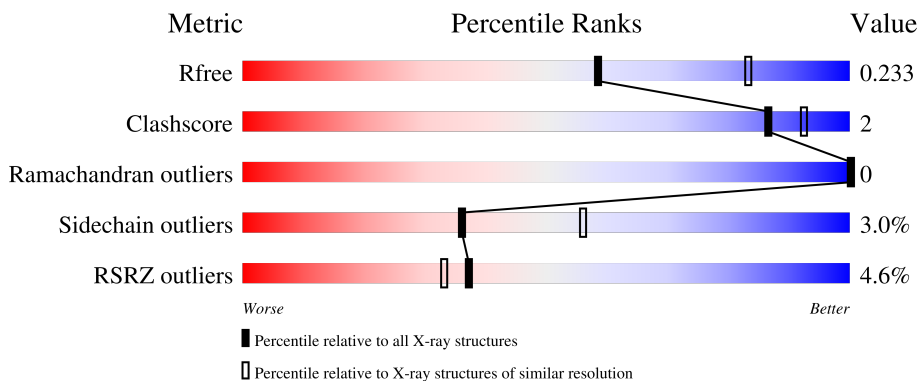
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.43 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.



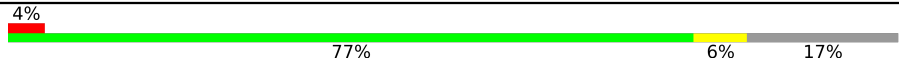

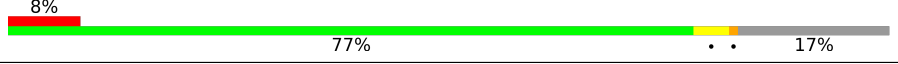
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	6062 (2.44-2.40)
Clashscore	190562	6562 (2.44-2.40)
Ramachandran outliers	187476	6481 (2.44-2.40)
Sidechain outliers	187428	6482 (2.44-2.40)
RSRZ outliers	180081	6066 (2.44-2.40)

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	202	 3% 84% 6% 11%
1	D	202	 0% 84% 6% 10%
1	G	202	 3% 83% 6% 11%
1	J	202	 4% 84% 6% 10%
2	B	239	 4% 74% 8% 17%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
2	E	239	 4% 77% 6% 17%
2	H	239	 3% 74% 8% 16%
2	K	239	 8% 77% 8% 17%

2 Entry composition i

There are 5 unique types of molecules in this entry. The entry contains 12754 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 II histocompatibility antigen, DR alpha chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	179	1474	956	240	273	5	0	0	0
1	D	181	1487	963	242	277	5	0	0	0
1	G	179	1474	956	240	273	5	0	0	0
1	J	181	1487	963	242	277	5	0	0	0

There are 44 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	217	ASP	-	expression tag	UNP P01903
A	218	ASP	-	expression tag	UNP P01903
A	219	ASP	-	expression tag	UNP P01903
A	220	ASP	-	expression tag	UNP P01903
A	221	LYS	-	expression tag	UNP P01903
A	222	GLU	-	expression tag	UNP P01903
A	223	ASN	-	expression tag	UNP P01903
A	224	LEU	-	expression tag	UNP P01903
A	225	TYR	-	expression tag	UNP P01903
A	226	PHE	-	expression tag	UNP P01903
A	227	GLN	-	expression tag	UNP P01903
D	217	ASP	-	expression tag	UNP P01903
D	218	ASP	-	expression tag	UNP P01903
D	219	ASP	-	expression tag	UNP P01903
D	220	ASP	-	expression tag	UNP P01903
D	221	LYS	-	expression tag	UNP P01903
D	222	GLU	-	expression tag	UNP P01903
D	223	ASN	-	expression tag	UNP P01903
D	224	LEU	-	expression tag	UNP P01903
D	225	TYR	-	expression tag	UNP P01903
D	226	PHE	-	expression tag	UNP P01903

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
D	227	GLN	-	expression tag	UNP P01903
G	217	ASP	-	expression tag	UNP P01903
G	218	ASP	-	expression tag	UNP P01903
G	219	ASP	-	expression tag	UNP P01903
G	220	ASP	-	expression tag	UNP P01903
G	221	LYS	-	expression tag	UNP P01903
G	222	GLU	-	expression tag	UNP P01903
G	223	ASN	-	expression tag	UNP P01903
G	224	LEU	-	expression tag	UNP P01903
G	225	TYR	-	expression tag	UNP P01903
G	226	PHE	-	expression tag	UNP P01903
G	227	GLN	-	expression tag	UNP P01903
J	217	ASP	-	expression tag	UNP P01903
J	218	ASP	-	expression tag	UNP P01903
J	219	ASP	-	expression tag	UNP P01903
J	220	ASP	-	expression tag	UNP P01903
J	221	LYS	-	expression tag	UNP P01903
J	222	GLU	-	expression tag	UNP P01903
J	223	ASN	-	expression tag	UNP P01903
J	224	LEU	-	expression tag	UNP P01903
J	225	TYR	-	expression tag	UNP P01903
J	226	PHE	-	expression tag	UNP P01903
J	227	GLN	-	expression tag	UNP P01903

- Molecule 2 is a protein called Regulatory protein IE1,HLA class II histocompatibility antigen DR beta chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	B	199	1653	1039	305	303	6	0	0	0
2	E	199	1653	1039	305	303	6	0	0	0
2	H	200	1660	1043	306	305	6	0	0	0
2	K	198	1642	1030	301	305	6	0	0	0

There are 136 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	15	GLY	-	linker	PDB ?
B	16	GLY	-	linker	PDB ?

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
B	17	GLY	-	linker	PDB ?
B	18	GLY	-	linker	PDB ?
B	19	SER	-	linker	PDB ?
B	20	GLY	-	linker	PDB ?
B	21	GLY	-	linker	PDB ?
B	22	GLY	-	linker	PDB ?
B	23	GLY	-	linker	PDB ?
B	24	SER	-	linker	PDB ?
B	25	GLY	-	linker	PDB ?
B	26	GLY	-	linker	PDB ?
B	27	GLY	-	linker	PDB ?
B	28	GLY	-	linker	PDB ?
B	29	SER	-	linker	PDB ?
B	220	LEU	-	expression tag	UNP Q5Y7D1
B	221	GLU	-	expression tag	UNP Q5Y7D1
B	222	THR	-	expression tag	UNP Q5Y7D1
B	223	VAL	-	expression tag	UNP Q5Y7D1
B	224	PRO	-	expression tag	UNP Q5Y7D1
B	225	ARG	-	expression tag	UNP Q5Y7D1
B	226	SER	-	expression tag	UNP Q5Y7D1
B	227	GLY	-	expression tag	UNP Q5Y7D1
B	228	GLU	-	expression tag	UNP Q5Y7D1
B	229	VAL	-	expression tag	UNP Q5Y7D1
B	230	TYR	-	expression tag	UNP Q5Y7D1
B	231	THR	-	expression tag	UNP Q5Y7D1
B	232	CYS	-	expression tag	UNP Q5Y7D1
B	233	GLN	-	expression tag	UNP Q5Y7D1
B	234	VAL	-	expression tag	UNP Q5Y7D1
B	235	GLU	-	expression tag	UNP Q5Y7D1
B	236	HIS	-	expression tag	UNP Q5Y7D1
B	237	PRO	-	expression tag	UNP Q5Y7D1
B	238	SER	-	expression tag	UNP Q5Y7D1
E	15	GLY	-	linker	PDB ?
E	16	GLY	-	linker	PDB ?
E	17	GLY	-	linker	PDB ?
E	18	GLY	-	linker	PDB ?
E	19	SER	-	linker	PDB ?
E	20	GLY	-	linker	PDB ?
E	21	GLY	-	linker	PDB ?
E	22	GLY	-	linker	PDB ?
E	23	GLY	-	linker	PDB ?
E	24	SER	-	linker	PDB ?

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
E	25	GLY	-	linker	PDB ?
E	26	GLY	-	linker	PDB ?
E	27	GLY	-	linker	PDB ?
E	28	GLY	-	linker	PDB ?
E	29	SER	-	linker	PDB ?
E	220	LEU	-	expression tag	UNP Q5Y7D1
E	221	GLU	-	expression tag	UNP Q5Y7D1
E	222	THR	-	expression tag	UNP Q5Y7D1
E	223	VAL	-	expression tag	UNP Q5Y7D1
E	224	PRO	-	expression tag	UNP Q5Y7D1
E	225	ARG	-	expression tag	UNP Q5Y7D1
E	226	SER	-	expression tag	UNP Q5Y7D1
E	227	GLY	-	expression tag	UNP Q5Y7D1
E	228	GLU	-	expression tag	UNP Q5Y7D1
E	229	VAL	-	expression tag	UNP Q5Y7D1
E	230	TYR	-	expression tag	UNP Q5Y7D1
E	231	THR	-	expression tag	UNP Q5Y7D1
E	232	CYS	-	expression tag	UNP Q5Y7D1
E	233	GLN	-	expression tag	UNP Q5Y7D1
E	234	VAL	-	expression tag	UNP Q5Y7D1
E	235	GLU	-	expression tag	UNP Q5Y7D1
E	236	HIS	-	expression tag	UNP Q5Y7D1
E	237	PRO	-	expression tag	UNP Q5Y7D1
E	238	SER	-	expression tag	UNP Q5Y7D1
H	15	GLY	-	linker	PDB ?
H	16	GLY	-	linker	PDB ?
H	17	GLY	-	linker	PDB ?
H	18	GLY	-	linker	PDB ?
H	19	SER	-	linker	PDB ?
H	20	GLY	-	linker	PDB ?
H	21	GLY	-	linker	PDB ?
H	22	GLY	-	linker	PDB ?
H	23	GLY	-	linker	PDB ?
H	24	SER	-	linker	PDB ?
H	25	GLY	-	linker	PDB ?
H	26	GLY	-	linker	PDB ?
H	27	GLY	-	linker	PDB ?
H	28	GLY	-	linker	PDB ?
H	29	SER	-	linker	PDB ?
H	220	LEU	-	expression tag	UNP Q5Y7D1
H	221	GLU	-	expression tag	UNP Q5Y7D1
H	222	THR	-	expression tag	UNP Q5Y7D1

Continued on next page...

Continued from previous page...

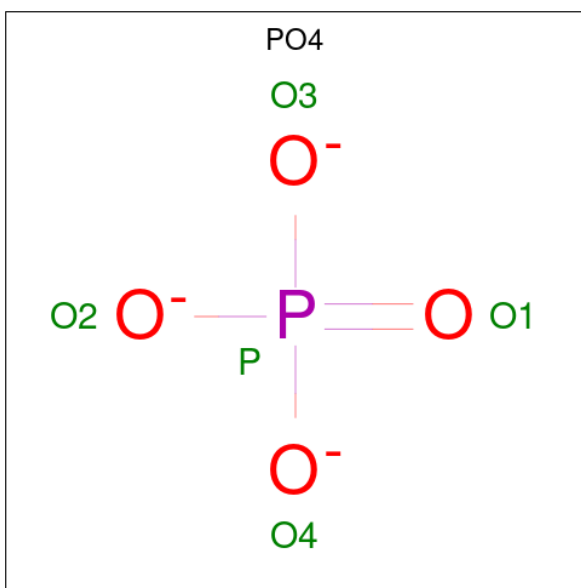
Chain	Residue	Modelled	Actual	Comment	Reference
H	223	VAL	-	expression tag	UNP Q5Y7D1
H	224	PRO	-	expression tag	UNP Q5Y7D1
H	225	ARG	-	expression tag	UNP Q5Y7D1
H	226	SER	-	expression tag	UNP Q5Y7D1
H	227	GLY	-	expression tag	UNP Q5Y7D1
H	228	GLU	-	expression tag	UNP Q5Y7D1
H	229	VAL	-	expression tag	UNP Q5Y7D1
H	230	TYR	-	expression tag	UNP Q5Y7D1
H	231	THR	-	expression tag	UNP Q5Y7D1
H	232	CYS	-	expression tag	UNP Q5Y7D1
H	233	GLN	-	expression tag	UNP Q5Y7D1
H	234	VAL	-	expression tag	UNP Q5Y7D1
H	235	GLU	-	expression tag	UNP Q5Y7D1
H	236	HIS	-	expression tag	UNP Q5Y7D1
H	237	PRO	-	expression tag	UNP Q5Y7D1
H	238	SER	-	expression tag	UNP Q5Y7D1
K	15	GLY	-	linker	PDB ?
K	16	GLY	-	linker	PDB ?
K	17	GLY	-	linker	PDB ?
K	18	GLY	-	linker	PDB ?
K	19	SER	-	linker	PDB ?
K	20	GLY	-	linker	PDB ?
K	21	GLY	-	linker	PDB ?
K	22	GLY	-	linker	PDB ?
K	23	GLY	-	linker	PDB ?
K	24	SER	-	linker	PDB ?
K	25	GLY	-	linker	PDB ?
K	26	GLY	-	linker	PDB ?
K	27	GLY	-	linker	PDB ?
K	28	GLY	-	linker	PDB ?
K	29	SER	-	linker	PDB ?
K	220	LEU	-	expression tag	UNP Q5Y7D1
K	221	GLU	-	expression tag	UNP Q5Y7D1
K	222	THR	-	expression tag	UNP Q5Y7D1
K	223	VAL	-	expression tag	UNP Q5Y7D1
K	224	PRO	-	expression tag	UNP Q5Y7D1
K	225	ARG	-	expression tag	UNP Q5Y7D1
K	226	SER	-	expression tag	UNP Q5Y7D1
K	227	GLY	-	expression tag	UNP Q5Y7D1
K	228	GLU	-	expression tag	UNP Q5Y7D1
K	229	VAL	-	expression tag	UNP Q5Y7D1
K	230	TYR	-	expression tag	UNP Q5Y7D1

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
K	231	THR	-	expression tag	UNP Q5Y7D1
K	232	CYS	-	expression tag	UNP Q5Y7D1
K	233	GLN	-	expression tag	UNP Q5Y7D1
K	234	VAL	-	expression tag	UNP Q5Y7D1
K	235	GLU	-	expression tag	UNP Q5Y7D1
K	236	HIS	-	expression tag	UNP Q5Y7D1
K	237	PRO	-	expression tag	UNP Q5Y7D1
K	238	SER	-	expression tag	UNP Q5Y7D1

- Molecule 3 is PHOSPHATE ION (CCD ID: PO4) (formula: O₄P).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total O P 5 4 1	0	0
3	B	1	Total O P 5 4 1	0	0
3	E	1	Total O P 5 4 1	0	0
3	E	1	Total O P 5 4 1	0	0
3	H	1	Total O P 5 4 1	0	0

- Molecule 4 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula: C₈H₁₅NO₆).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	N	O		
4	D	1	14	8	1	5	0	0
4	E	1	14	8	1	5	0	0
4	G	1	14	8	1	5	0	0
4	K	1	14	8	1	5	0	0

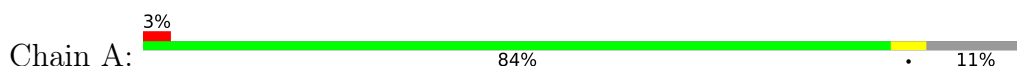
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
5	A	15	15	15	0	0
5	B	23	23	23	0	0
5	D	30	30	30	0	0
5	E	27	27	27	0	0
5	G	11	11	11	0	0
5	H	16	16	16	0	0
5	J	13	13	13	0	0
5	K	8	8	8	0	0

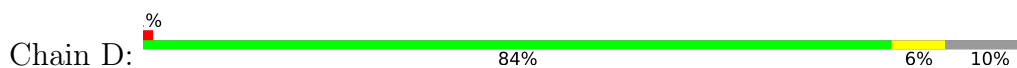
3 Residue-property plots [i](#)

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.

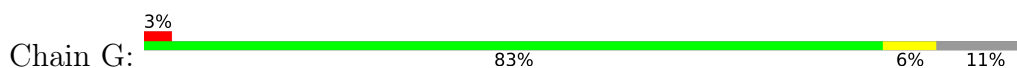
- Molecule 1: HLA class II histocompatibility antigen, DR alpha chain



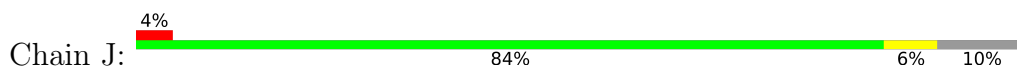
- Molecule 1: HLA class II histocompatibility antigen, DR alpha chain



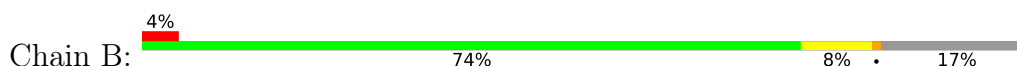
- Molecule 1: HLA class II histocompatibility antigen, DR alpha chain

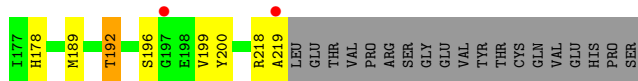


- Molecule 1: HLA class II histocompatibility antigen, DR alpha chain

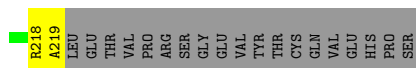
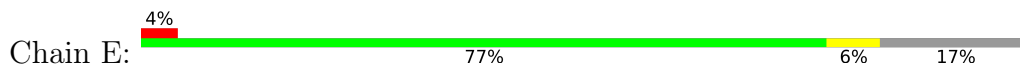


- Molecule 2: Regulatory protein IE1, HLA class II histocompatibility antigen DR beta chain

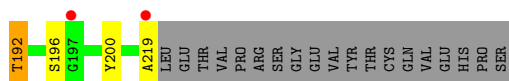
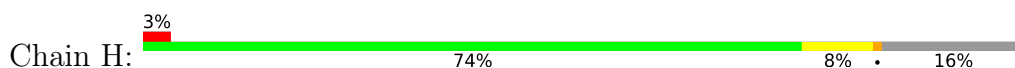




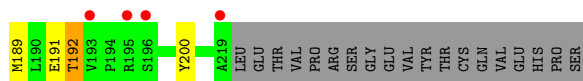
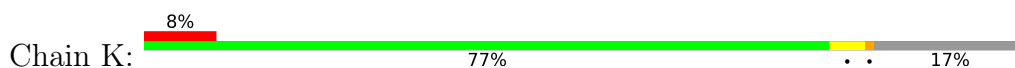
- Molecule 2: Regulatory protein IE1,HLA class II histocompatibility antigen DR beta chain



- Molecule 2: Regulatory protein IE1,HLA class II histocompatibility antigen DR beta chain



- Molecule 2: Regulatory protein IE1,HLA class II histocompatibility antigen DR beta chain



4 Data and refinement statistics i

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	71.27Å 96.18Å 160.09Å 90.00° 92.66° 90.00°	Depositor
Resolution (Å)	35.30 – 2.43 35.30 – 2.43	Depositor EDS
% Data completeness (in resolution range)	99.8 (35.30-2.43) 99.8 (35.30-2.43)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.82 (at 2.42Å)	Xtrriage
Refinement program	BUSTER 2.10.4	Depositor
R, R_{free}	0.225 , 0.244 0.212 , 0.233	Depositor DCC
R_{free} test set	4090 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	52.9	Xtrriage
Anisotropy	0.414	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.39 , 41.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtrriage
Estimated twinning fraction	0.010 for h,-k,-l	Xtrriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	12754	wwPDB-VP
Average B, all atoms (Å ²)	62.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.44% 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: NAG, PO4

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	0.61	0/1519	0.95	1/2070 (0.0%)
1	D	0.67	0/1532	0.95	0/2088
1	G	0.60	0/1519	0.95	1/2070 (0.0%)
1	J	0.61	0/1532	0.94	1/2088 (0.0%)
2	B	0.63	0/1696	0.95	0/2299
2	E	0.65	0/1696	0.96	0/2299
2	H	0.65	0/1703	0.96	1/2309 (0.0%)
2	K	0.59	0/1682	0.95	0/2277
All	All	0.63	0/12879	0.95	4/17500 (0.0%)

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	56	ILE	N-CA-C	-5.62	106.22	111.45
1	J	56	ILE	N-CA-C	-5.47	106.36	111.45
1	G	56	ILE	N-CA-C	-5.38	106.44	111.45
2	H	-26	LYS	N-CA-C	5.08	118.09	109.76

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	1474	0	1416	3	0
1	D	1487	0	1424	4	0
1	G	1474	0	1415	6	0
1	J	1487	0	1425	4	0
2	B	1653	0	1585	16	0
2	E	1653	0	1584	7	0
2	H	1660	0	1592	11	0
2	K	1642	0	1562	9	0
3	A	5	0	0	0	0
3	B	5	0	0	1	0
3	E	10	0	0	0	0
3	H	5	0	0	0	0
4	D	14	0	13	0	0
4	E	14	0	13	0	0
4	G	14	0	13	0	0
4	K	14	0	13	0	0
5	A	15	0	0	0	0
5	B	23	0	0	0	0
5	D	30	0	0	0	0
5	E	27	0	0	0	0
5	G	11	0	0	0	0
5	H	16	0	0	0	0
5	J	13	0	0	0	0
5	K	8	0	0	0	0
All	All	12754	0	12055	51	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 2.

The worst 5 of 51 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:K:-17:ARG:NH1	2:K:38:GLU:OE2	2.21	0.74
2:H:-17:ARG:NH1	2:H:38:GLU:OE2	2.21	0.72
2:K:157:GLU:OE2	2:K:159:ARG:NH1	2.24	0.71
2:K:-27:ILE:HG23	2:K:114:VAL:HB	1.74	0.69
2:H:-17:ARG:NH2	2:H:66:ASN:OD1	2.26	0.68

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	177/202 (88%)	176 (99%)	1 (1%)	0	100	100
1	D	179/202 (89%)	178 (99%)	1 (1%)	0	100	100
1	G	177/202 (88%)	176 (99%)	1 (1%)	0	100	100
1	J	179/202 (89%)	177 (99%)	2 (1%)	0	100	100
2	B	195/239 (82%)	188 (96%)	7 (4%)	0	100	100
2	E	195/239 (82%)	190 (97%)	5 (3%)	0	100	100
2	H	196/239 (82%)	191 (97%)	5 (3%)	0	100	100
2	K	190/239 (80%)	185 (97%)	5 (3%)	0	100	100
All	All	1488/1764 (84%)	1461 (98%)	27 (2%)	0	100	100

There are no Ramachandran outliers to report.

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	164/186 (88%)	160 (98%)	4 (2%)	43	63
1	D	165/186 (89%)	161 (98%)	4 (2%)	43	63
1	G	164/186 (88%)	161 (98%)	3 (2%)	51	71
1	J	165/186 (89%)	161 (98%)	4 (2%)	43	63
2	B	184/210 (88%)	177 (96%)	7 (4%)	29	47
2	E	184/210 (88%)	176 (96%)	8 (4%)	26	42

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	H	185/210 (88%)	177 (96%)	8 (4%)	26	42
2	K	183/210 (87%)	179 (98%)	4 (2%)	45	66
All	All	1394/1584 (88%)	1352 (97%)	42 (3%)	36	56

5 of 42 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	H	52	ARG
1	J	142	VAL
2	H	97	LEU
2	H	192	THR
1	J	168	HIS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 17 such sidechains are listed below:

Mol	Chain	Res	Type
2	K	93	GLN
2	K	139	GLN
2	E	165	GLN
1	G	174	HIS
2	H	48	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 oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

9 ligands are 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
4	NAG	E	301	2	14,14,15	0.32	0	17,19,21	0.62	0
3	PO4	E	303	-	4,4,4	0.16	0	6,6,6	0.29	0
3	PO4	B	301	-	4,4,4	0.15	0	6,6,6	0.28	0
3	PO4	E	302	-	4,4,4	0.26	0	6,6,6	0.21	0
4	NAG	D	301	1	14,14,15	0.31	0	17,19,21	0.78	1 (5%)
4	NAG	K	301	2	14,14,15	0.31	0	17,19,21	0.55	0
3	PO4	H	301	-	4,4,4	0.25	0	6,6,6	0.29	0
4	NAG	G	301	1	14,14,15	0.32	0	17,19,21	0.51	0
3	PO4	A	301	-	4,4,4	0.40	0	6,6,6	0.24	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	NAG	D	301	1	-	0/6/23/26	0/1/1/1
4	NAG	K	301	2	-	0/6/23/26	0/1/1/1
4	NAG	G	301	1	-	0/6/23/26	0/1/1/1
4	NAG	E	301	2	-	0/6/23/26	0/1/1/1

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	D	301	NAG	C1-O5-C5	2.29	115.30	112.19

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	301	PO4	1	0

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 [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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	179/202 (88%)	0.22	6 (3%) 48 44	44, 57, 76, 87	0
1	D	181/202 (89%)	0.02	2 (1%) 78 75	37, 52, 67, 77	0
1	G	179/202 (88%)	0.39	7 (3%) 43 39	47, 64, 87, 101	0
1	J	181/202 (89%)	0.36	9 (4%) 34 30	50, 66, 85, 89	0
2	B	199/239 (83%)	0.30	10 (5%) 34 30	43, 59, 79, 86	0
2	E	199/239 (83%)	0.19	9 (4%) 38 34	36, 53, 73, 93	0
2	H	200/239 (83%)	0.42	8 (4%) 42 38	47, 63, 88, 98	0
2	K	198/239 (82%)	0.69	18 (9%) 15 12	52, 73, 104, 110	0
All	All	1516/1764 (85%)	0.33	69 (4%) 37 33	36, 61, 87, 110	0

The worst 5 of 69 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	H	219	ALA	3.9
2	B	-16	ILE	3.7
1	G	205	PHE	3.6
1	A	124	LEU	3.6
2	K	135	THR	3.5

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
4	NAG	K	301	14/15	0.54	0.18	93,95,96,96	0
4	NAG	E	301	14/15	0.65	0.17	79,81,82,83	0
3	PO4	H	301	5/5	0.74	0.15	111,111,111,111	0
4	NAG	G	301	14/15	0.81	0.14	83,84,85,85	0
4	NAG	D	301	14/15	0.81	0.13	71,73,74,74	0
3	PO4	E	303	5/5	0.84	0.12	93,93,93,93	0
3	PO4	E	302	5/5	0.85	0.14	107,107,107,107	0
3	PO4	A	301	5/5	0.89	0.13	108,109,109,109	0
3	PO4	B	301	5/5	0.92	0.15	76,76,77,77	0

6.5 Other polymers [i](#)

There are no such residues in this entry.