



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 10, 2026 – 12:17 AM UTC

PDB ID : 4ZXS / pdb_00004zxs
Title : HSV-1 nuclear egress complex
Authors : Bigalke, J.M.; Heldwein, E.E.
Deposited on : 2015-05-20
Resolution : 2.77 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

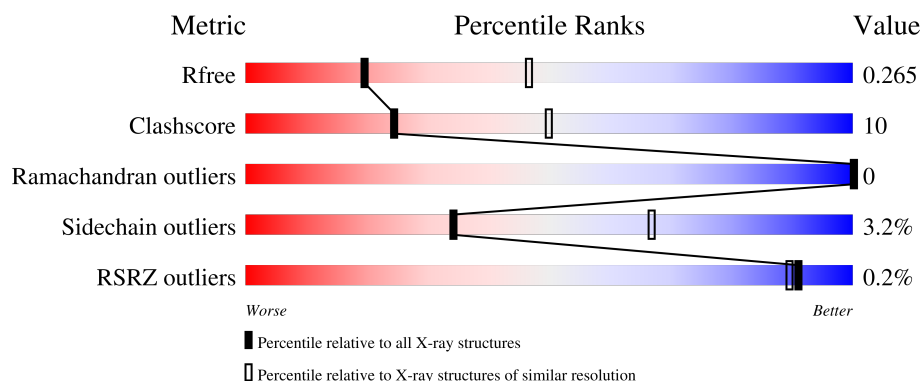
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

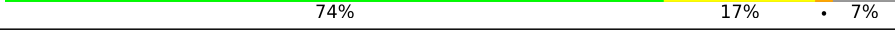
The reported resolution of this entry is 2.77 Å.

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	5248 (2.80-2.76)
Clashscore	190562	5693 (2.80-2.76)
Ramachandran outliers	187476	5590 (2.80-2.76)
Sidechain outliers	187428	5592 (2.80-2.76)
RSRZ outliers	180081	5251 (2.80-2.76)

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	183	
1	C	183	
2	B	260	
2	D	260	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard

residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
4	CL	A	203	-	-	X	-

2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 6319 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 Virion egress protein UL34.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	159	Total	C	N	O	S	0	0	0
			1234	782	219	224	9			
1	C	161	Total	C	N	O	S	0	0	0
			1241	785	221	226	9			

There are 24 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	3	GLY	-	expression tag	UNP P10218
A	4	PRO	-	expression tag	UNP P10218
A	5	LEU	-	expression tag	UNP P10218
A	6	GLY	-	expression tag	UNP P10218
A	7	SER	-	expression tag	UNP P10218
A	8	PRO	-	expression tag	UNP P10218
A	9	GLU	-	expression tag	UNP P10218
A	10	PHE	-	expression tag	UNP P10218
A	11	PRO	-	expression tag	UNP P10218
A	12	GLY	-	expression tag	UNP P10218
A	13	ARG	-	expression tag	UNP P10218
A	14	PRO	-	expression tag	UNP P10218
C	3	GLY	-	expression tag	UNP P10218
C	4	PRO	-	expression tag	UNP P10218
C	5	LEU	-	expression tag	UNP P10218
C	6	GLY	-	expression tag	UNP P10218
C	7	SER	-	expression tag	UNP P10218
C	8	PRO	-	expression tag	UNP P10218
C	9	GLU	-	expression tag	UNP P10218
C	10	PHE	-	expression tag	UNP P10218
C	11	PRO	-	expression tag	UNP P10218
C	12	GLY	-	expression tag	UNP P10218
C	13	ARG	-	expression tag	UNP P10218
C	14	PRO	-	expression tag	UNP P10218

- Molecule 2 is a protein called Virion egress protein UL31.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	242	Total	C	N	O	S	0	0	0
			1880	1211	323	333	13			
2	D	241	Total	C	N	O	S	0	0	0
			1881	1213	323	332	13			

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	47	GLY	-	expression tag	UNP P10215
B	48	PRO	-	expression tag	UNP P10215
B	49	GLY	-	expression tag	UNP P10215
B	50	SER	-	expression tag	UNP P10215
D	47	GLY	-	expression tag	UNP P10215
D	48	PRO	-	expression tag	UNP P10215
D	49	GLY	-	expression tag	UNP P10215
D	50	SER	-	expression tag	UNP P10215

- Molecule 3 is NICKEL (II) ION (CCD ID: NI) (formula: Ni).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	1	Total	Ni	0	0
			1	1		
3	C	1	Total	Ni	0	0
			1	1		

- Molecule 4 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	2	Total	Cl	0	0
			2	2		
4	C	1	Total	Cl	0	0
			1	1		

- Molecule 5 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	B	1	Total	Zn	0	0
			1	1		
5	D	1	Total	Zn	0	0
			1	1		

- 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
6	D	1	Total 1	Na 1	0	0

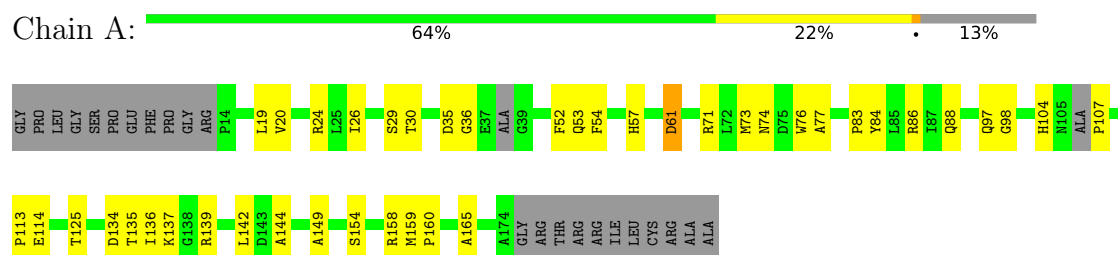
- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	12	Total 12	O 12	0	0
7	B	30	Total 30	O 30	0	0
7	C	13	Total 13	O 13	0	0
7	D	19	Total 19	O 19	0	0

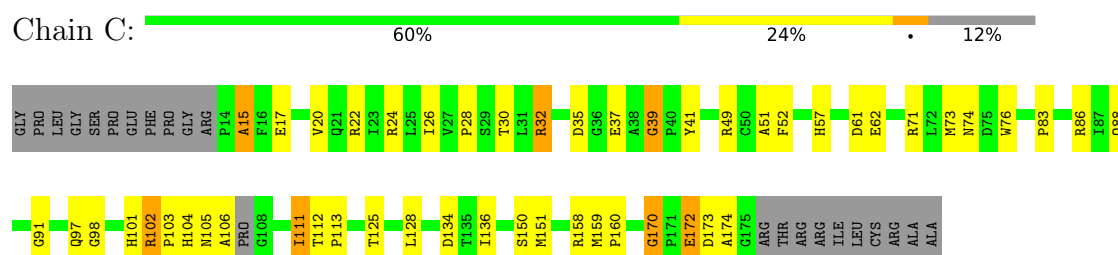
3 Residue-property plots

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

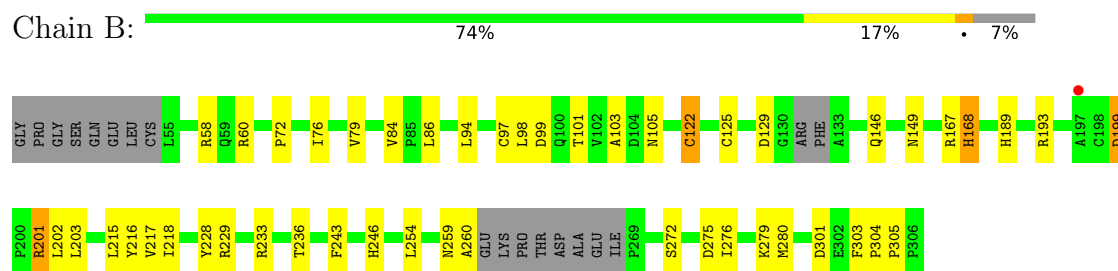
• Molecule 1: Virion egress protein UL34



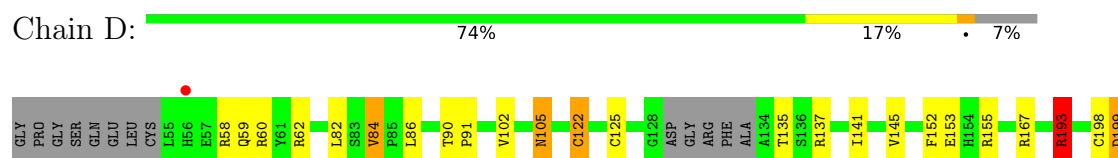
• Molecule 1: Virion egress protein UL34



• Molecule 2: Virion egress protein UL31



• Molecule 2: Virion egress protein UL31



P200	R201	L202	L203	Y210	L215	Y216	V217	I218	R233	A237	H246	Q249	L254	E261	K262	PRO	THR	ASP	ALA	GLU	ILE	P269	S272	D275	R281	F285	M290	R295	D301	P305	P306
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4 Data and refinement statistics

Property	Value	Source
Space group	P 6	Depositor
Cell constants a, b, c, α , β , γ	110.53Å 110.53Å 155.85Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	47.86 – 2.77 47.86 – 2.77	Depositor EDS
% Data completeness (in resolution range)	99.8 (47.86-2.77) 99.9 (47.86-2.77)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.08 (at 2.77Å)	Xtriage
Refinement program	PHENIX 1.9_1692	Depositor
R, R_{free}	0.217 , 0.265 0.225 , 0.265	Depositor DCC
R_{free} test set	1369 reflections (4.99%)	wwPDB-VP
Wilson B-factor (Å ²)	56.3	Xtriage
Anisotropy	0.332	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 42.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.41$, $\langle L^2 \rangle = 0.23$	Xtriage
Estimated twinning fraction	0.294 for h,-h-k,-l	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	6319	wwPDB-VP
Average B, all atoms (Å ²)	66.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.68% 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: NI, ZN, 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	0.47	1/1266 (0.1%)	0.83	0/1713
1	C	0.62	0/1273	0.93	6/1724 (0.3%)
2	B	0.63	1/1928 (0.1%)	0.82	1/2622 (0.0%)
2	D	0.50	2/1929 (0.1%)	0.82	6/2622 (0.2%)
All	All	0.56	4/6396 (0.1%)	0.84	13/8681 (0.1%)

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	84	VAL	C-N	5.68	1.40	1.33
2	D	122	CYS	C-N	5.41	1.41	1.34
2	B	122	CYS	C-N	5.19	1.41	1.34
1	A	61	ASP	C-O	-5.07	1.18	1.24

All (13) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	84	VAL	CA-C-O	7.97	124.37	119.19
2	D	84	VAL	N-CA-C	7.05	116.36	108.05
1	C	15	ALA	N-CA-C	6.92	118.47	111.07
1	C	170	GLY	CA-C-N	-6.63	113.85	120.21
1	C	170	GLY	C-N-CA	-6.63	113.85	120.21
1	C	57	HIS	N-CA-C	5.37	117.76	110.35
2	D	84	VAL	CA-C-N	-5.17	114.29	120.13
2	D	84	VAL	C-N-CA	-5.17	114.29	120.13
2	B	103	ALA	N-CA-C	5.08	121.61	110.80
2	D	122	CYS	O-C-N	5.03	125.86	121.18
2	D	193	ARG	N-CA-C	-5.02	105.94	111.71
1	C	39	GLY	CA-C-N	-5.01	114.62	119.78
1	C	39	GLY	C-N-CA	-5.01	114.62	119.78

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	1234	0	1204	27	0
1	C	1241	0	1210	38	0
2	B	1880	0	1861	29	0
2	D	1881	0	1868	37	1
3	A	1	0	0	0	0
3	C	1	0	0	0	0
4	A	2	0	0	5	0
4	C	1	0	0	0	0
5	B	1	0	0	0	0
5	D	1	0	0	0	0
6	B	1	0	0	0	0
6	D	1	0	0	0	0
7	A	12	0	0	3	0
7	B	30	0	0	0	0
7	C	13	0	0	1	0
7	D	19	0	0	0	0
All	All	6319	0	6143	122	1

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 10.

All (122) 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:158:ARG:NE	4:A:203:CL:CL	2.05	1.24
1:C:172:GLU:HG2	2:D:84:VAL:HG11	1.47	0.94
2:D:193:ARG:NH1	2:D:199:ASP:OD1	2.04	0.90
2:D:135:THR:O	2:D:233:ARG:NH1	2.05	0.88
1:C:105:ASN:OD1	1:C:106:ALA:N	2.08	0.86
1:A:57:HIS:CE1	7:A:308:HOH:O	2.34	0.81
1:C:172:GLU:CG	2:D:84:VAL:HG11	2.12	0.80

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:58:ARG:NH1	2:D:62:ARG:HH11	1.86	0.74
2:D:167:ARG:NH2	2:D:301:ASP:OD2	2.21	0.74
1:C:101:HIS:O	1:C:103:PRO:HD3	1.90	0.71
2:D:122:CYS:HB3	2:D:125:CYS:HB2	1.72	0.71
2:B:201:ARG:HB2	2:B:218:ILE:HB	1.71	0.71
4:A:202:CL:CL	7:A:311:HOH:O	2.46	0.70
1:A:159:MET:HE3	1:A:160:PRO:HA	1.74	0.69
2:D:58:ARG:HH12	2:D:62:ARG:HH11	1.38	0.69
2:D:272:SER:OG	2:D:275:ASP:OD2	2.09	0.67
1:A:57:HIS:HE1	7:A:308:HOH:O	1.73	0.67
2:D:193:ARG:HH11	2:D:193:ARG:HG3	1.59	0.66
2:B:122:CYS:HB3	2:B:125:CYS:HB2	1.78	0.65
1:C:113:PRO:HG3	1:C:136:ILE:HG23	1.78	0.65
1:C:61:ASP:OD1	1:C:158:ARG:NH2	2.29	0.64
2:B:203:LEU:HB2	2:B:216:TYR:HB2	1.80	0.63
2:B:146:GLN:OE1	2:B:149:ASN:ND2	2.32	0.62
1:C:32:ARG:NH1	7:C:302:HOH:O	2.32	0.62
2:D:210:TYR:HD1	2:D:261:GLU:HG3	1.64	0.62
2:D:193:ARG:HH11	2:D:193:ARG:CG	2.11	0.61
1:C:88:GLN:HG3	1:C:125:THR:HG22	1.82	0.61
1:C:15:ALA:HB1	1:C:76:TRP:HZ2	1.66	0.60
1:C:159:MET:HE3	1:C:160:PRO:HA	1.83	0.60
2:B:199:ASP:HB3	2:B:201:ARG:HH21	1.67	0.60
1:A:71:ARG:NH2	1:A:134:ASP:OD1	2.33	0.59
2:B:98:LEU:O	2:B:101:THR:OG1	2.18	0.59
1:C:113:PRO:HD3	1:C:136:ILE:HG12	1.84	0.59
2:B:272:SER:OG	2:B:275:ASP:OD2	2.11	0.59
1:C:37:GLU:OE1	1:C:49:ARG:HD2	2.03	0.58
1:A:74:ASN:HB2	1:A:83:PRO:HG2	1.85	0.58
2:B:259:ASN:OD1	2:B:260:ALA:N	2.37	0.57
2:D:285:PHE:HB2	2:D:290:MET:HE2	1.86	0.57
1:C:105:ASN:CG	1:C:106:ALA:H	2.12	0.56
1:C:173:ASP:O	1:C:174:ALA:HB3	2.05	0.56
1:C:101:HIS:O	1:C:103:PRO:CD	2.54	0.55
1:A:36:GLY:HA2	1:A:53:GLN:HB2	1.88	0.54
1:A:88:GLN:HG3	1:A:125:THR:HG22	1.89	0.54
1:C:39:GLY:O	1:C:41:TYR:HD2	1.90	0.54
1:A:158:ARG:CZ	4:A:203:CL:CL	2.88	0.54
2:B:233:ARG:NH2	2:B:236:THR:OG1	2.41	0.54
1:A:77:ALA:O	2:B:58:ARG:NH2	2.41	0.54
1:C:105:ASN:O	1:C:106:ALA:HB2	2.08	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:217:VAL:HB	2:D:254:LEU:HB3	1.91	0.53
1:C:74:ASN:HB2	1:C:83:PRO:HG2	1.91	0.53
1:A:114:GLU:N	1:A:114:GLU:OE1	2.43	0.52
1:A:113:PRO:HG3	1:A:136:ILE:HG23	1.91	0.52
2:D:203:LEU:HB2	2:D:216:TYR:HB2	1.92	0.52
1:C:150:SER:HB3	2:D:82:LEU:HD13	1.92	0.52
1:C:172:GLU:CG	2:D:84:VAL:CG1	2.85	0.51
1:A:158:ARG:CD	4:A:203:CL:CL	2.94	0.51
1:A:26:ILE:HD12	2:B:79:VAL:HG21	1.91	0.51
2:B:243:PHE:CD1	2:B:243:PHE:N	2.78	0.51
2:D:137:ARG:O	2:D:141:ILE:HG13	2.12	0.50
1:A:144:ALA:O	2:B:60:ARG:NH1	2.45	0.50
2:D:58:ARG:CZ	2:D:62:ARG:HH11	2.25	0.50
1:C:15:ALA:HB1	1:C:76:TRP:CZ2	2.45	0.49
2:B:202:LEU:HD22	2:B:215:LEU:HD11	1.94	0.49
1:C:24:ARG:NH2	1:C:28:PRO:O	2.46	0.49
1:A:154:SER:HB2	1:A:165:ALA:HB3	1.94	0.49
2:D:201:ARG:HB2	2:D:218:ILE:HB	1.94	0.49
2:D:193:ARG:NH1	2:D:193:ARG:CG	2.73	0.49
2:D:59:GLN:HG3	2:D:60:ARG:HG3	1.94	0.48
1:C:102:ARG:HA	1:C:103:PRO:HD2	1.76	0.47
1:A:20:VAL:HG21	1:A:35:ASP:HA	1.97	0.47
2:D:137:ARG:NH1	2:D:237:ALA:O	2.46	0.47
1:A:52:PHE:CE2	1:A:98:GLY:HA3	2.50	0.47
2:B:217:VAL:HB	2:B:254:LEU:HB3	1.96	0.47
1:C:71:ARG:NH2	1:C:134:ASP:OD1	2.41	0.47
1:C:111:ILE:HG12	1:C:112:THR:N	2.30	0.47
1:C:170:GLY:HA3	2:D:86:LEU:HD21	1.96	0.47
1:C:104:HIS:O	1:C:104:HIS:ND1	2.47	0.46
2:D:210:TYR:CD1	2:D:261:GLU:HG3	2.48	0.46
2:B:276:ILE:O	2:B:280:MET:HG3	2.15	0.46
1:A:84:TYR:OH	1:A:107:PRO:HB2	2.15	0.46
2:D:152:PHE:O	2:D:155:ARG:HG3	2.16	0.46
2:B:216:TYR:OH	2:B:305:PRO:HG3	2.15	0.46
2:B:168:HIS:CD2	2:B:168:HIS:N	2.83	0.46
1:A:73:MET:HE3	1:A:83:PRO:HB3	1.99	0.46
2:B:94:LEU:HB3	2:B:246:HIS:HD2	1.81	0.46
2:B:275:ASP:OD1	2:D:281:ARG:NH2	2.46	0.46
2:B:167:ARG:NH2	2:B:301:ASP:OD2	2.37	0.45
1:A:24:ARG:HD2	1:A:54:PHE:HE1	1.82	0.45
1:C:128:LEU:HD23	1:C:151:MET:HE1	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:193:ARG:NH1	2:D:199:ASP:CG	2.72	0.45
2:B:199:ASP:HB3	2:B:201:ARG:NH2	2.30	0.45
2:D:90:THR:HA	2:D:91:PRO:HD3	1.88	0.44
1:C:86:ARG:HH11	1:C:97:GLN:HE21	1.65	0.44
2:D:102:VAL:HG22	2:D:105:ASN:OD1	2.17	0.44
1:C:22:ARG:O	1:C:26:ILE:HG12	2.18	0.44
2:B:280:MET:HB3	2:B:280:MET:HE2	1.75	0.44
1:C:104:HIS:O	1:C:104:HIS:CG	2.70	0.44
2:D:202:LEU:HD22	2:D:215:LEU:HD11	2.00	0.44
2:D:305:PRO:HA	2:D:306:PRO:HD3	1.84	0.44
1:A:137:LYS:HE3	1:A:149:ALA:HB3	1.99	0.43
1:C:172:GLU:OE1	1:C:174:ALA:N	2.40	0.43
1:A:135:THR:O	1:A:139:ARG:HG2	2.19	0.43
1:C:52:PHE:CE2	1:C:98:GLY:HA3	2.52	0.43
1:A:61:ASP:OD1	4:A:203:CL:CL	2.74	0.43
2:B:303:PHE:HA	2:B:304:PRO:HD3	1.92	0.42
2:D:216:TYR:OH	2:D:305:PRO:HG3	2.18	0.42
1:C:91:GLY:C	1:C:159:MET:HE2	2.44	0.42
1:C:17:GLU:O	1:C:20:VAL:HG12	2.19	0.42
2:B:97:CYS:SG	2:B:99:ASP:OD1	2.78	0.42
2:B:228:TYR:OH	2:B:229:ARG:NH1	2.52	0.42
2:B:189:HIS:CE1	2:B:193:ARG:HD2	2.54	0.42
1:A:19:LEU:HD22	1:A:76:TRP:CG	2.55	0.41
2:D:135:THR:OG1	2:D:233:ARG:HD3	2.20	0.41
2:D:58:ARG:HH22	2:D:62:ARG:NH1	2.17	0.41
1:A:142:LEU:HD22	2:B:86:LEU:HD13	2.03	0.41
1:C:51:ALA:N	1:C:98:GLY:O	2.39	0.41
2:D:145:VAL:HG11	2:D:269:PRO:HB3	2.02	0.40
1:A:86:ARG:HH11	1:A:97:GLN:HE21	1.69	0.40
2:B:72:PRO:O	2:B:76:ILE:HG13	2.21	0.40
1:C:73:MET:HE3	1:C:83:PRO:HB3	2.02	0.40
1:C:30:THR:HG21	1:C:62:GLU:OE2	2.21	0.40
2:D:58:ARG:NH2	2:D:62:ARG:HH11	2.20	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:153:GLU:OE2	2:D:295:ARG:NH1[3_655]	2.08	0.12

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	153/183 (84%)	152 (99%)	1 (1%)	0	100	100
1	C	157/183 (86%)	151 (96%)	6 (4%)	0	100	100
2	B	236/260 (91%)	229 (97%)	7 (3%)	0	100	100
2	D	235/260 (90%)	226 (96%)	9 (4%)	0	100	100
All	All	781/886 (88%)	758 (97%)	23 (3%)	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	134/150 (89%)	131 (98%)	3 (2%)	45	75
1	C	133/150 (89%)	128 (96%)	5 (4%)	29	61
2	B	199/214 (93%)	192 (96%)	7 (4%)	32	64
2	D	200/214 (94%)	194 (97%)	6 (3%)	36	69
All	All	666/728 (92%)	645 (97%)	21 (3%)	34	67

All (21) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	29	SER
1	A	30	THR

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Mol	Chain	Res	Type
1	A	104	HIS
2	B	84	VAL
2	B	105	ASN
2	B	129	ASP
2	B	168	HIS
2	B	199	ASP
2	B	201	ARG
2	B	279	LYS
1	C	32	ARG
1	C	35	ASP
1	C	102	ARG
1	C	111	ILE
1	C	172	GLU
2	D	105	ASN
2	D	193	ARG
2	D	198	CYS
2	D	199	ASP
2	D	246	HIS
2	D	249	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (7) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	117	ASN
2	B	147	GLN
2	B	168	HIS
2	B	213	HIS
2	B	246	HIS
2	D	149	ASN
2	D	249	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 [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 9 ligands modelled in this entry, 9 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 [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	159/183 (86%)	-0.69	0	100 100	24, 61, 115, 169	0
1	C	161/183 (87%)	-0.51	0	100 100	37, 68, 124, 168	0
2	B	242/260 (93%)	-0.74	1 (0%)	88 85	32, 56, 100, 154	0
2	D	241/260 (92%)	-0.72	1 (0%)	88 85	41, 60, 110, 155	0
All	All	803/886 (90%)	-0.68	2 (0%)	91 89	24, 61, 118, 169	0

All (2) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	197	ALA	2.7
2	D	56	HIS	2.0

6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
4	CL	C	202	1/1	0.96	0.07	99,99,99,99	0
4	CL	A	202	1/1	0.98	0.06	92,92,92,92	0
6	NA	D	402	1/1	0.98	0.07	47,47,47,47	0
6	NA	B	402	1/1	0.99	0.07	49,49,49,49	0
4	CL	A	203	1/1	0.99	0.05	101,101,101,101	0
5	ZN	B	401	1/1	1.00	0.02	66,66,66,66	0
5	ZN	D	401	1/1	1.00	0.01	61,61,61,61	0
3	NI	C	201	1/1	1.00	0.02	74,74,74,74	0
3	NI	A	201	1/1	1.00	0.05	153,153,153,153	0

6.5 Other polymers [i](#)

There are no such residues in this entry.