



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 19, 2016 – 09:19 PM GMT

PDB ID : 4ZXS  
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](mailto:validation@mail.wwpdb.org)  
A user guide is available at  
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>  
with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467  
Mogul : unknown  
Xtriage (Phenix) : 1.9-1692  
EDS : rb-20026982  
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)  
Refmac : 5.8.0135  
CCP4 : 6.5.0  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : rb-20026982

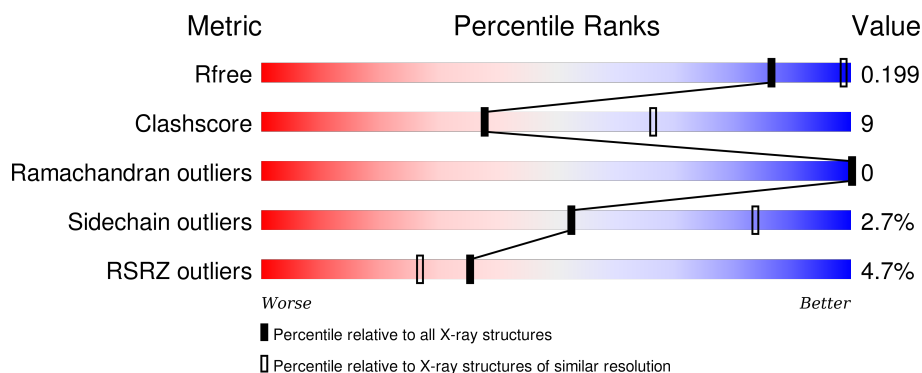
# 1 Overall quality at a glance

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))
$R_{free}$	91344	3004 (2.80-2.76)
Clashscore	102246	3480 (2.80-2.76)
Ramachandran outliers	100387	3423 (2.80-2.76)
Sidechain outliers	100360	3425 (2.80-2.76)
RSRZ outliers	91569	3016 (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 on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria. 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	<div> <div>5%</div> <div>66% 21% 13%</div> </div>
1	C	183	<div> <div>5%</div> <div>64% 21% 12%</div> </div>
2	B	260	<div> <div>3%</div> <div>75% 18% 7%</div> </div>
2	D	260	<div> <div>4%</div> <div>75% 18% 7%</div> </div>

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	X
5	ZN	B	401	-	-	-	X
6	NA	B	402	-	-	-	X
6	NA	D	402	-	-	-	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 (three-letter code: 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 (three-letter code: 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 (three-letter code: 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 (three-letter code: NA) (formula: Na).

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

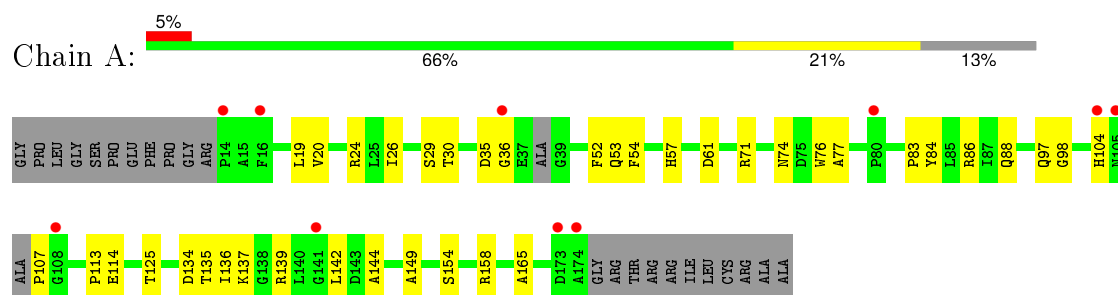
- Molecule 7 is water.

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

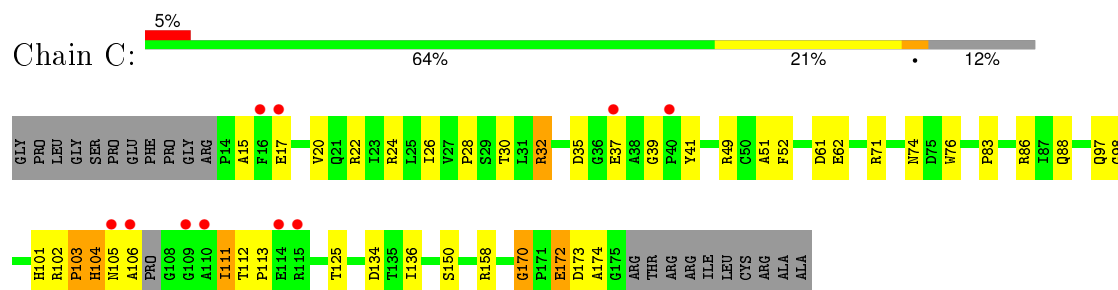
### 3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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 ( $\text{RSRZ} > 2$ ). 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.

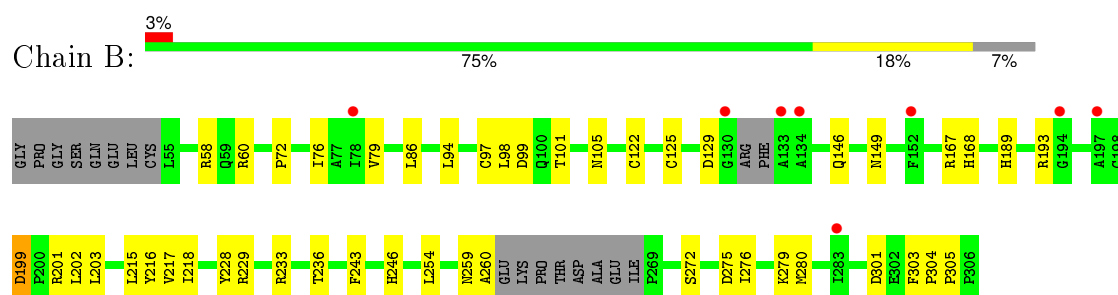
- Molecule 1: Virion egress protein UL34



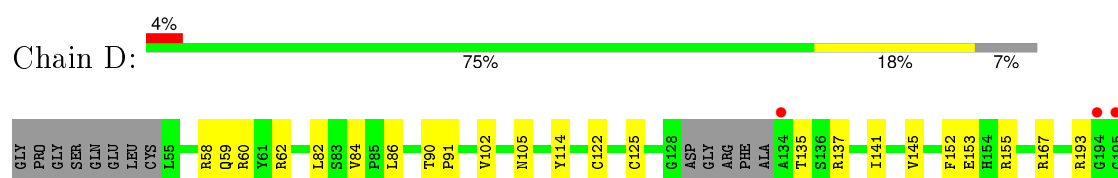
- Molecule 1: Virion egress protein UL34

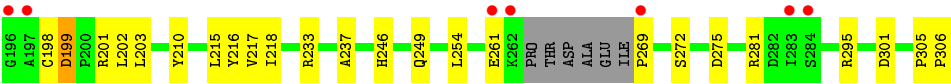


- Molecule 2: Virion egress protein UL31



- Molecule 2: Virion egress protein UL31





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 6	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	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) 99.8 (47.86-2.77)	Depositor EDS
$R_{merge}$	0.08	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	3.08 (at 2.77Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.9_1692)	Depositor
R, $R_{free}$	0.217 , 0.265 0.179 , 0.199	Depositor DCC
$R_{free}$ test set	1368 reflections (5.00%)	DCC
Wilson B-factor (Å <sup>2</sup> )	56.3	Xtriage
Anisotropy	0.332	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.33 , 36.9	EDS
Estimated twinning fraction	0.294 for h,-h-k,-l	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.41$ , $\langle L^2 \rangle = 0.23$	Xtriage
Outliers	0 of 27365 reflections	Xtriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	6319	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	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.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical values of  $\langle |L| \rangle$ ,  $\langle L^2 \rangle$  for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 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: 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	0.34	0/1266	0.47	0/1713
1	C	0.47	0/1273	0.56	1/1724 (0.1%)
2	B	0.48	0/1928	0.48	0/2622
2	D	0.37	0/1929	0.49	0/2622
All	All	0.42	0/6396	0.50	1/8681 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	170	GLY	C-N-CD	5.14	139.20	128.40

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	1234	0	1204	25	0
1	C	1241	0	1210	34	0
2	B	1880	0	1861	28	0
2	D	1881	0	1868	36	1
3	A	1	0	0	0	0
3	C	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
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	114	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 9.

All (114) 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
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
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
2:D:210:TYR:HD1	2:D:261:GLU:HG3	1.64	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:32:ARG:NH1	7:C:302:HOH:O	2.32	0.62
2:D:193:ARG:CG	2:D:193:ARG:HH11	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
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
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:C:39:GLY:O	1:C:41:TYR:HD2	1.90	0.54
1:A:88:GLN:HG3	1:A:125:THR:HG22	1.89	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
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
2:D:58:ARG:CZ	2:D:62:ARG:HH11	2.25	0.50
1:A:144:ALA:O	2:B:60:ARG:NH1	2.45	0.50
1:C:15:ALA:HB1	1:C:76:TRP:CZ2	2.45	0.49
1:C:24:ARG:NH2	1:C:28:PRO:O	2.46	0.49
2:B:202:LEU:HD22	2:B:215:LEU:HD11	1.94	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:CG	2:D:193:ARG:NH1	2.73	0.49
2:D:59:GLN:HG3	2:D:60:ARG:HG3	1.94	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:102:ARG:HA	1:C:103:PRO:HD2	1.76	0.47
2:D:137:ARG:NH1	2:D:237:ALA:O	2.46	0.47
1:A:20:VAL:HG21	1:A:35:ASP:HA	1.97	0.47
1:C:111:ILE:HG12	1:C:112:THR:N	2.30	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: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
2:B:275:ASP:OD1	2:D:281:ARG:NH2	2.46	0.46
2:B:94:LEU:HB3	2:B:246:HIS:HD2	1.81	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
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:D:305:PRO:HA	2:D:306:PRO:HD3	1.84	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
1:C:172:GLU:OE1	1:C:174:ALA:N	2.40	0.43
1:A:137:LYS:HE3	1:A:149:ALA:HB3	1.99	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:105:ASN:CG	1:C:106:ALA:H	2.12	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:58:ARG:HH22	2:D:62:ARG:NH1	2.17	0.41
1:C:51:ALA:N	1:C:98:GLY:O	2.39	0.41
1:A:142:LEU:HD22	2:B:86:LEU:HD13	2.03	0.41
2:D:145:VAL:HG11	2:D:269:PRO:HB3	2.02	0.40
2:B:72:PRO:O	2:B:76:ILE:HG13	2.21	0.40
1:A:86:ARG:HH11	1:A:97:GLN:HE21	1.69	0.40
1:C:30:THR:HG21	1:C:62:GLU:OE2	2.21	0.40
2:D:193:ARG:NH1	2:D:199:ASP:CG	2.72	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 [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	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%)	60	88
1	C	133/150 (89%)	127 (96%)	6 (4%)	34	67
2	B	199/214 (93%)	195 (98%)	4 (2%)	63	89
2	D	200/214 (94%)	195 (98%)	5 (2%)	55	85
All	All	666/728 (92%)	648 (97%)	18 (3%)	52	84

All (18) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	29	SER
1	A	30	THR
1	A	104	HIS
2	B	105	ASN
2	B	129	ASP
2	B	199	ASP
2	B	279	LYS
1	C	32	ARG
1	C	35	ASP
1	C	103	PRO
1	C	104	HIS
1	C	111	ILE
1	C	172	GLU
2	D	114	TYR
2	D	198	CYS
2	D	199	ASP
2	D	246	HIS
2	D	249	GLN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	117	ASN

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Mol	Chain	Res	Type
2	B	168	HIS
2	B	246	HIS
2	D	149	ASN

### 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 carbohydrates in this entry.

### 5.6 Ligand geometry ⓘ

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 ⓘ

There are no such residues in this entry.

### 5.8 Polymer linkage issues ⓘ

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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	159/183 (86%)	0.41	10 (6%) 23 16	24, 61, 115, 169	0
1	C	161/183 (87%)	0.54	10 (6%) 24 17	37, 68, 124, 168	0
2	B	242/260 (93%)	0.27	8 (3%) 50 42	32, 56, 100, 154	0
2	D	241/260 (92%)	0.34	10 (4%) 41 33	41, 60, 110, 155	0
All	All	803/886 (90%)	0.37	38 (4%) 35 27	24, 61, 118, 169	0

All (38) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	174	ALA	6.5
2	B	133	ALA	5.6
2	D	195	GLY	5.1
2	D	262	LYS	5.0
2	D	194	GLY	4.8
1	A	173	ASP	4.4
1	A	105	ASN	4.4
1	C	37	GLU	4.3
1	C	16	PHE	4.2
1	A	14	PRO	4.0
1	C	109	GLY	3.9
2	B	197	ALA	3.9
2	D	197	ALA	3.8
1	C	114	GLU	3.8
2	B	130	GLY	3.4
1	C	106	ALA	3.3
1	C	110	ALA	3.3
2	D	269	PRO	3.3
2	B	78	ILE	3.2
1	C	40	PRO	3.2
1	A	104	HIS	3.2

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Mol	Chain	Res	Type	RSRZ
2	B	194	GLY	2.9
2	B	283	ILE	2.9
2	D	261	GLU	2.8
2	D	134	ALA	2.6
2	B	152	PHE	2.6
2	B	134	ALA	2.6
1	C	17	GLU	2.6
1	C	105	ASN	2.6
1	A	36	GLY	2.6
2	D	284	SER	2.5
1	A	16	PHE	2.5
2	D	283	ILE	2.3
1	A	141	GLY	2.1
2	D	196	GLY	2.1
1	A	108	GLY	2.0
1	C	115	ARG	2.0
1	A	80	PRO	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 carbohydrates 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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95<sup>th</sup> 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	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
4	CL	A	203	1/1	0.89	0.28	8.92	101,101,101,101	0
5	ZN	B	401	1/1	0.97	0.28	7.49	66,66,66,66	0
6	NA	D	402	1/1	0.89	0.40	6.70	47,47,47,47	0
6	NA	B	402	1/1	0.80	0.29	5.89	49,49,49,49	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
5	ZN	D	401	1/1	0.98	0.24	1.35	61,61,61,61	0
3	NI	C	201	1/1	0.93	0.21	-	74,74,74,74	0
3	NI	A	201	1/1	0.41	0.52	-	153,153,153,153	0
4	CL	C	202	1/1	0.72	0.18	-	99,99,99,99	0
4	CL	A	202	1/1	0.74	0.24	-	92,92,92,92	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.