



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 05:15 AM GMT

PDB ID : 2PWM  
Title : Crystal Structure of HIV-1 CA146 A92E real cell  
Authors : Kelly, B.N.  
Deposited on : 2007-05-11  
Resolution : 1.90 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 : 1.7 (RC4), CSD as536be (2015)  
Xtriage (Phenix) : 1.9-1692  
EDS : rb-20026688  
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) : trunk26865

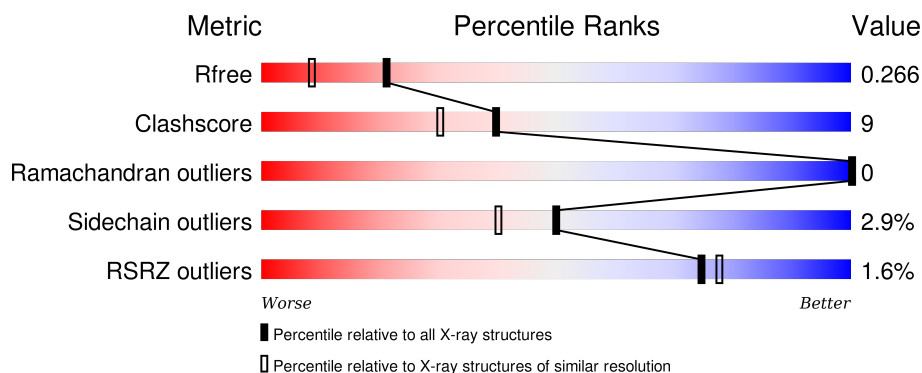
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 1.90 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	4755 (1.90-1.90)
Clashscore	102246	5398 (1.90-1.90)
Ramachandran outliers	100387	5338 (1.90-1.90)
Sidechain outliers	100360	5339 (1.90-1.90)
RSRZ outliers	91569	4766 (1.90-1.90)

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	146	<div> <div>82%</div> <div>17%</div> <div>..</div> </div>
1	B	146	<div> <div>77%</div> <div>16%</div> <div>6%</div> </div>
1	C	146	<div> <div>4%</div> <div>79%</div> <div>18%</div> <div>..</div> </div>
1	D	146	<div> <div>82%</div> <div>14%</div> <div>..</div> </div>
1	E	146	<div> <div>3%</div> <div>88%</div> <div>11%</div> <div>..</div> </div>

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Mol	Chain	Length	Quality of chain
1	F	146	<div><div></div><div>78%</div><div>14%</div><div>• 6%</div></div>
1	G	146	<div><div>3%</div><div></div><div>82%</div><div>15%</div><div>• •</div></div>
1	H	146	<div><div></div><div>82%</div><div>14%</div><div>• •</div></div>

## 2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 9947 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 Gag-Pol polyprotein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	145	Total	C	N	O	S	0	2	0
			1150	727	203	212	8			
1	B	137	Total	C	N	O	S	0	1	0
			1089	689	191	201	8			
1	C	145	Total	C	N	O	S	0	2	0
			1147	726	202	211	8			
1	D	145	Total	C	N	O	S	9	5	0
			1170	741	204	216	9			
1	E	145	Total	C	N	O	S	0	3	0
			1164	734	209	213	8			
1	F	137	Total	C	N	O	S	0	3	0
			1109	700	197	204	8			
1	G	145	Total	C	N	O	S	0	2	0
			1147	725	201	213	8			
1	H	145	Total	C	N	O	S	0	5	0
			1166	737	204	217	8			

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	92	GLU	ALA	ENGINEERED	UNP P12497
B	92	GLU	ALA	ENGINEERED	UNP P12497
C	92	GLU	ALA	ENGINEERED	UNP P12497
D	92	GLU	ALA	ENGINEERED	UNP P12497
E	92	GLU	ALA	ENGINEERED	UNP P12497
F	92	GLU	ALA	ENGINEERED	UNP P12497
G	92	GLU	ALA	ENGINEERED	UNP P12497
H	92	GLU	ALA	ENGINEERED	UNP P12497

- Molecule 2 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	G	1	Total Cl 1 1	0	0
2	D	1	Total Cl 1 1	0	0
2	E	1	Total Cl 1 1	0	0
2	H	1	Total Cl 1 1	0	0
2	B	1	Total Cl 1 1	0	0
2	C	1	Total Cl 1 1	0	0
2	A	1	Total Cl 1 1	0	0
2	F	1	Total Cl 1 1	0	0

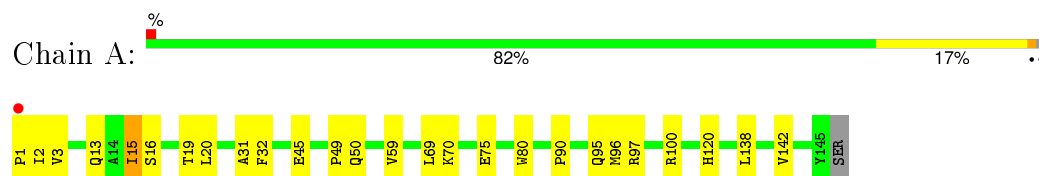
- Molecule 3 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	107	Total O 107 107	0	0
3	B	102	Total O 102 102	0	0
3	C	89	Total O 89 89	0	0
3	D	98	Total O 98 98	0	0
3	E	113	Total O 113 113	0	0
3	F	102	Total O 102 102	0	0
3	G	84	Total O 84 84	0	0
3	H	102	Total O 102 102	0	0

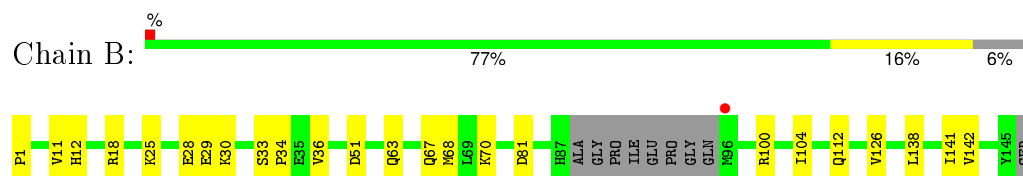
### 3 Residue-property plots [i](#)

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 ( $RSRZ > 2$ ). 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.

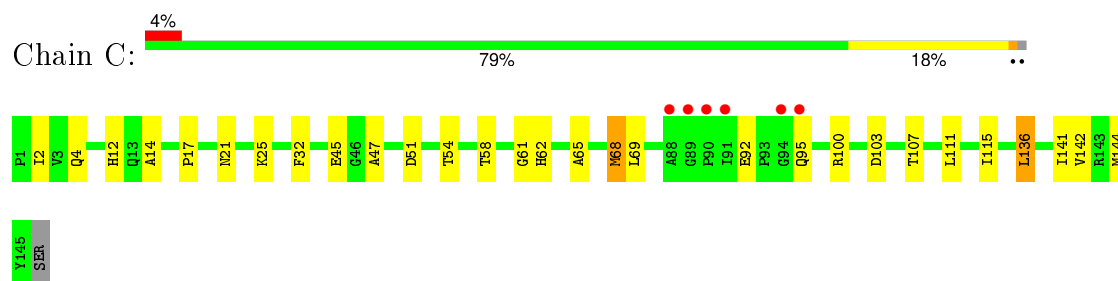
- Molecule 1: Gag-Pol polypeptide



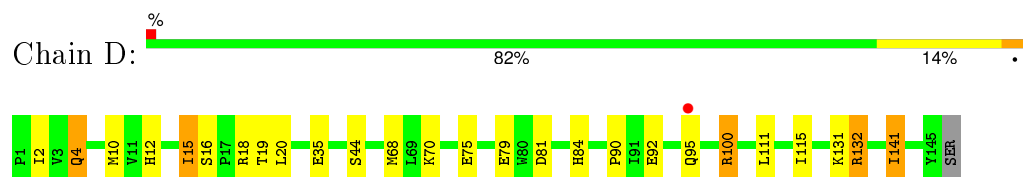
- Molecule 1: Gag-Pol polypeptide



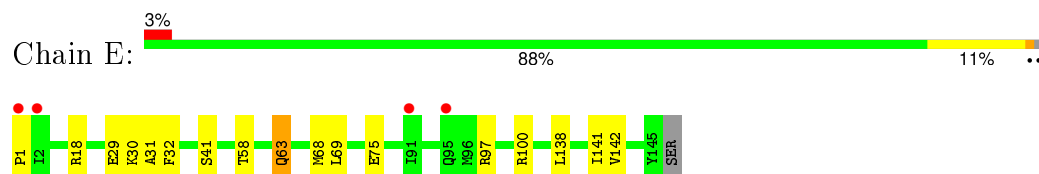
- Molecule 1: Gag-Pol polypeptide



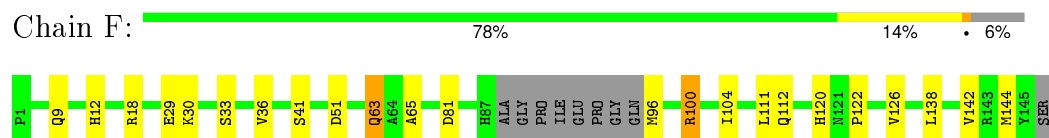
- Molecule 1: Gag-Pol polypeptide



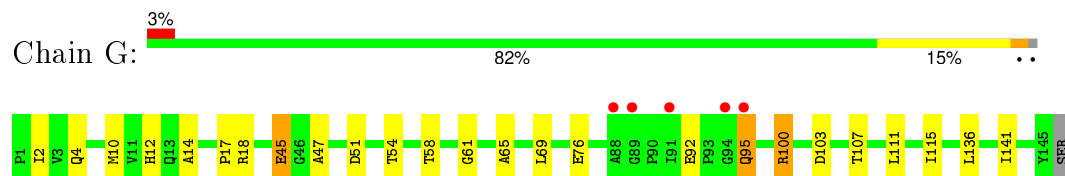
- Molecule 1: Gag-Pol polypeptide



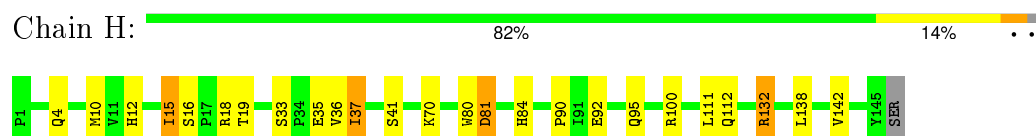
## ● Molecule 1: Gag-Pol polyprotein



## ● Molecule 1: Gag-Pol polyprotein



## ● Molecule 1: Gag-Pol polyprotein



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	48.21Å 58.93Å 92.33Å 71.51° 88.12° 83.01°	Depositor
Resolution (Å)	32.21 – 1.90 32.20 – 1.90	Depositor EDS
% Data completeness (in resolution range)	96.3 (32.21-1.90) 86.6 (32.20-1.90)	Depositor EDS
$R_{merge}$	0.06	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	6.24 (at 1.91Å)	Xtriage
Refinement program	REFMAC 5.3.0008	Depositor
R, $R_{free}$	0.204 , 0.270 0.206 , 0.266	Depositor DCC
$R_{free}$ test set	3669 reflections (5.34%)	DCC
Wilson B-factor (Å <sup>2</sup> )	16.7	Xtriage
Anisotropy	0.049	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.37 , 43.1	EDS
Estimated twinning fraction	0.000 for -h,-k,-k+l	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.45$ , $\langle L^2 \rangle = 0.28$	Xtriage
Outliers	0 of 72334 reflections	Xtriage
$F_o, F_c$ correlation	0.97	EDS
Total number of atoms	9947	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	18.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 97.38 % of the origin peak, indicating pseudo translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo translational symmetry is equal to 1.7599e-10. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

<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

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: CL

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	0.95	2/1181 (0.2%)	0.88	1/1606 (0.1%)
1	B	0.92	1/1114 (0.1%)	0.90	3/1513 (0.2%)
1	C	0.89	0/1178	0.89	3/1602 (0.2%)
1	D	0.90	0/1204	0.89	3/1637 (0.2%)
1	E	0.92	0/1192	0.89	1/1620 (0.1%)
1	F	0.89	0/1134	0.91	3/1539 (0.2%)
1	G	0.93	0/1178	0.90	2/1603 (0.1%)
1	H	0.90	1/1203 (0.1%)	0.86	1/1636 (0.1%)
All	All	0.91	4/9384 (0.0%)	0.89	17/12756 (0.1%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	80	TRP	CB-CG	5.52	1.60	1.50
1	B	11	VAL	CB-CG2	5.38	1.64	1.52
1	A	59	VAL	CB-CG1	5.33	1.64	1.52
1	H	80	TRP	CE3-CZ3	5.13	1.47	1.38

All (17) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	81	ASP	CB-CG-OD2	8.22	125.69	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	132	ARG	NE-CZ-NH2	-7.41	116.59	120.30
1	C	103	ASP	CB-CG-OD2	7.30	124.87	118.30
1	F	81	ASP	CB-CG-OD2	6.91	124.52	118.30
1	G	103	ASP	CB-CG-OD2	6.77	124.39	118.30
1	F	100	ARG	NE-CZ-NH2	-6.65	116.98	120.30
1	F	100	ARG	NE-CZ-NH1	5.95	123.28	120.30
1	A	2	ILE	N-CA-C	5.61	126.14	111.00
1	D	81	ASP	CB-CG-OD2	5.56	123.30	118.30
1	B	100	ARG	NE-CZ-NH2	-5.51	117.54	120.30
1	C	136	LEU	CA-CB-CG	5.50	127.95	115.30
1	C	136	LEU	CB-CG-CD2	-5.34	101.92	111.00
1	H	81	ASP	CB-CG-OD2	5.32	123.09	118.30
1	G	136	LEU	CB-CG-CD1	-5.32	101.96	111.00
1	B	1	PRO	N-CD-CG	-5.18	95.43	103.20
1	D	100	ARG	NE-CZ-NH2	-5.09	117.76	120.30
1	E	58	THR	OG1-CB-CG2	-5.04	98.41	110.00

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	1	PRO	Peptide

## 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	1150	0	1149	23	0
1	B	1089	0	1085	18	0
1	C	1147	0	1149	26	0
1	D	1170	0	1170	38	0
1	E	1164	0	1162	14	0
1	F	1109	0	1104	15	0
1	G	1147	0	1142	24	1
1	H	1166	0	1164	32	1
2	A	1	0	0	0	0
2	B	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	C	1	0	0	0	0
2	D	1	0	0	0	0
2	E	1	0	0	0	0
2	F	1	0	0	0	0
2	G	1	0	0	0	0
2	H	1	0	0	0	0
3	A	107	0	0	2	0
3	B	102	0	0	8	0
3	C	89	0	0	3	0
3	D	98	0	0	4	0
3	E	113	0	0	5	1
3	F	102	0	0	3	0
3	G	84	0	0	3	0
3	H	102	0	0	3	1
All	All	9947	0	9125	160	2

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 (160) 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:B:28[B]:GLU:CD	3:B:996:HOH:O	1.99	1.01
1:B:28[B]:GLU:OE2	3:B:996:HOH:O	1.77	1.00
1:A:70:LYS:NZ	1:D:75[B]:GLU:OE1	2.00	0.95
1:E:18[A]:ARG:NH1	3:E:1014:HOH:O	2.00	0.94
1:G:92:GLU:HB2	1:G:95:GLN:HG3	1.52	0.92
1:H:132:ARG:HH11	1:H:132:ARG:HG2	1.38	0.89
1:G:4:GLN:HB2	1:H:10:MET:CE	2.04	0.88
1:H:35:GLU:HG3	3:H:985:HOH:O	1.74	0.86
1:B:29:GLU:OE2	1:B:30:LYS:NZ	2.08	0.86
1:G:4:GLN:HB2	1:H:10:MET:HE3	1.59	0.85
1:B:28[B]:GLU:CG	3:B:996:HOH:O	2.24	0.85
1:A:75:GLU:OE1	1:D:70:LYS:NZ	2.15	0.80
1:H:12:HIS:CD2	1:H:111:LEU:HD21	2.16	0.80
1:C:12:HIS:HD2	3:C:916:HOH:O	1.64	0.79
1:G:12:HIS:HD2	3:G:923:HOH:O	1.65	0.77
1:G:4:GLN:CB	1:H:10:MET:HE3	2.14	0.77
1:C:4:GLN:HB2	1:D:10:MET:CE	2.15	0.77
1:E:75:GLU:OE1	1:H:70:LYS:NZ	2.18	0.77
1:F:63[A]:GLN:HG2	3:F:963:HOH:O	1.84	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:4:GLN:CD	1:D:10:MET:HE3	2.07	0.75
1:F:12:HIS:HD2	3:F:934:HOH:O	1.68	0.75
1:D:15:ILE:HD12	1:D:20:LEU:HG	1.67	0.75
1:A:15:ILE:HD11	1:A:19:THR:CG2	2.19	0.72
1:B:112:GLN:HG3	3:B:951:HOH:O	1.90	0.71
1:B:25:LYS:O	1:B:28[B]:GLU:HG2	1.90	0.71
1:D:12:HIS:CD2	1:D:111:LEU:HD21	2.26	0.71
1:D:35:GLU:HG3	3:D:976:HOH:O	1.91	0.70
1:B:12:HIS:HD2	3:B:927:HOH:O	1.74	0.70
1:B:18:ARG:CZ	3:B:947:HOH:O	2.41	0.69
1:C:4:GLN:HB2	1:D:10:MET:HE3	1.73	0.69
1:H:15:ILE:HD11	1:H:19:THR:CG2	2.22	0.69
1:G:45[A]:GLU:OE2	1:H:16:SER:OG	2.11	0.69
1:H:132:ARG:NH1	1:H:132:ARG:HG2	2.03	0.68
1:C:45:GLU:OE1	1:D:18:ARG:NE	2.28	0.67
1:E:18[A]:ARG:CZ	3:E:1014:HOH:O	2.40	0.66
1:C:4:GLN:CB	1:D:10:MET:HE3	2.25	0.66
1:G:61:GLY:O	3:G:988:HOH:O	2.14	0.66
1:H:15:ILE:HD11	1:H:19:THR:HG22	1.77	0.66
1:D:68[B]:MET:CE	1:D:141:ILE:HD12	2.26	0.65
1:A:15:ILE:HD11	1:A:19:THR:HG22	1.79	0.63
1:C:69:LEU:HB2	1:C:141:ILE:HD11	1.81	0.63
1:F:112:GLN:HG3	3:F:960:HOH:O	1.99	0.63
1:E:68:MET:HB2	1:E:141:ILE:HD11	1.81	0.62
1:G:4:GLN:HB2	1:H:10:MET:HE1	1.83	0.61
1:G:2:ILE:HG12	1:G:115:ILE:HD12	1.81	0.61
1:A:45:GLU:OE2	1:B:18:ARG:NH2	2.33	0.60
1:G:14:ALA:HB1	3:G:943:HOH:O	2.00	0.60
1:D:12:HIS:HD2	3:D:941:HOH:O	1.84	0.60
1:C:4:GLN:HB2	1:D:10:MET:HE1	1.83	0.60
1:D:15:ILE:HD11	1:D:19:THR:CG2	2.32	0.59
1:A:15:ILE:CD1	1:A:19:THR:HB	2.31	0.59
1:B:18:ARG:NH1	3:B:947:HOH:O	2.35	0.59
1:B:68:MET:HB3	1:B:141:ILE:HD11	1.85	0.59
1:A:97:ARG:HG3	1:A:97:ARG:HH11	1.67	0.58
1:G:69:LEU:HB2	1:G:141:ILE:HD11	1.86	0.58
1:B:138:LEU:O	1:B:142:VAL:HG23	2.04	0.58
1:G:4:GLN:CD	1:H:10:MET:HE3	2.25	0.57
1:D:15:ILE:C	1:D:15:ILE:HD13	2.25	0.56
1:B:67:GLN:HE22	1:B:70:LYS:HE3	1.70	0.56
1:F:120:HIS:HD2	1:F:122:PRO:O	1.88	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:68[B]:MET:HB3	1:D:141:ILE:HD11	1.88	0.56
1:E:100[B]:ARG:NH2	1:H:81:ASP:OD2	2.38	0.56
1:C:14:ALA:HB1	3:C:936:HOH:O	2.04	0.56
1:G:45[A]:GLU:OE2	1:H:16:SER:CB	2.53	0.56
1:B:28[B]:GLU:HG2	3:B:996:HOH:O	1.97	0.56
1:B:33:SER:O	1:B:36:VAL:HG12	2.05	0.55
1:G:65:ALA:HB1	1:G:141:ILE:HG21	1.88	0.55
1:H:92:GLU:HB2	1:H:95:GLN:HE21	1.71	0.55
1:C:54:THR:O	1:C:58:THR:HG23	2.08	0.54
1:D:68[B]:MET:HE3	1:D:141:ILE:HD12	1.90	0.54
1:B:12:HIS:HE1	1:B:51:ASP:OD1	1.90	0.53
1:D:44:SER:OG	1:D:131:LYS:HE3	2.07	0.53
1:C:2:ILE:HG12	1:C:115:ILE:HD12	1.90	0.53
1:C:4:GLN:CD	1:D:10:MET:CE	2.77	0.53
1:A:90:PRO:HB3	1:A:95:GLN:HG3	1.91	0.52
1:D:68[B]:MET:HE3	1:D:141:ILE:CD1	2.40	0.52
1:D:12:HIS:CD2	3:D:941:HOH:O	2.60	0.52
1:C:65:ALA:HB1	1:C:141:ILE:HG21	1.92	0.52
1:F:65:ALA:HB2	1:F:144:MET:HE3	1.90	0.52
1:F:138:LEU:O	1:F:142:VAL:HG23	2.10	0.52
1:D:75[B]:GLU:OE2	1:D:79:GLU:HG2	2.10	0.51
1:E:97:ARG:HG3	1:E:97:ARG:HH11	1.76	0.51
1:G:54:THR:O	1:G:58:THR:HG23	2.11	0.51
1:D:92:GLU:HB2	1:D:95:GLN:HE21	1.76	0.50
1:G:10:MET:CE	1:H:4[B]:GLN:HG2	2.41	0.50
1:H:15:ILE:HD11	1:H:19:THR:HG21	1.94	0.50
1:F:12:HIS:HE1	1:F:51:ASP:OD1	1.94	0.49
1:H:12:HIS:HD2	3:H:949:HOH:O	1.96	0.49
1:A:97:ARG:HG3	1:A:97:ARG:NH1	2.27	0.49
1:C:21[A]:ASN:HD21	1:C:25:LYS:HE2	1.78	0.49
1:G:111:LEU:O	1:G:115:ILE:HG12	2.13	0.49
1:G:18:ARG:HD2	1:H:41[A]:SER:OG	2.12	0.49
1:A:15:ILE:HD13	1:A:16:SER:N	2.28	0.49
1:E:41:SER:OG	1:F:18[B]:ARG:HD3	2.13	0.48
1:A:70:LYS:HG3	3:A:947:HOH:O	2.13	0.48
1:G:4:GLN:CD	1:H:10:MET:CE	2.81	0.48
1:E:29:GLU:OE2	1:E:30:LYS:NZ	2.47	0.48
1:H:37:ILE:HD11	1:H:138:LEU:HB3	1.96	0.48
1:F:33:SER:O	1:F:36:VAL:HG12	2.12	0.48
1:D:15:ILE:HD11	1:D:19:THR:HG22	1.95	0.48
1:A:15:ILE:HD12	1:A:20:LEU:HG	1.96	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:45[A]:GLU:OE1	1:H:18:ARG:NE	2.46	0.48
1:D:90:PRO:CB	1:D:95:GLN:HB3	2.44	0.48
1:A:96:MET:HE2	1:A:120:HIS:CD2	2.49	0.48
1:C:45:GLU:OE1	1:D:18:ARG:CZ	2.62	0.47
1:H:33:SER:O	1:H:36:VAL:HG12	2.15	0.47
1:D:15:ILE:HD13	1:D:16:SER:N	2.29	0.47
1:C:47:ALA:HB1	1:C:51:ASP:HB2	1.97	0.47
1:C:4:GLN:NE2	1:D:10:MET:HE2	2.30	0.46
1:G:2:ILE:HG12	1:G:115:ILE:CD1	2.46	0.46
1:H:15:ILE:CD1	1:H:19:THR:HG21	2.45	0.46
1:A:15:ILE:HD11	1:A:19:THR:CB	2.46	0.46
1:F:29:GLU:OE2	1:F:30:LYS:NZ	2.41	0.46
1:C:61:GLY:O	3:C:985:HOH:O	2.21	0.45
1:D:90:PRO:HB2	1:D:95:GLN:HB3	1.98	0.45
1:E:97:ARG:HG3	1:E:97:ARG:NH1	2.31	0.45
1:E:138:LEU:O	1:E:142:VAL:HG13	2.16	0.45
1:D:68[A]:MET:HB2	1:D:141:ILE:HD11	1.98	0.45
1:H:12:HIS:CD2	3:H:949:HOH:O	2.68	0.45
1:C:4:GLN:NE2	1:D:4[B]:GLN:OE1	2.47	0.45
1:A:15:ILE:HD13	1:A:19:THR:HB	1.97	0.45
1:H:90:PRO:CB	1:H:95:GLN:HB3	2.47	0.45
1:A:138:LEU:O	1:A:142:VAL:HG13	2.17	0.44
1:D:2:ILE:HG12	1:D:115:ILE:HD12	1.98	0.44
1:C:92:GLU:HB2	1:C:95:GLN:HB2	1.99	0.44
1:D:84:HIS:O	1:D:100:ARG:NH2	2.48	0.44
1:H:70:LYS:HZ3	1:H:70:LYS:HG2	1.52	0.44
1:H:36:VAL:HG13	1:H:37:ILE:HD12	1.98	0.44
1:E:31:ALA:HA	1:E:32:PHE:HA	1.82	0.44
1:C:111:LEU:O	1:C:115:ILE:HG12	2.17	0.44
1:C:32:PHE:O	1:C:142:VAL:HG12	2.18	0.44
1:A:96:MET:CE	1:A:120:HIS:CD2	3.01	0.43
1:C:61:GLY:O	1:C:62:HIS:C	2.56	0.43
1:H:84:HIS:O	1:H:100:ARG:NH2	2.50	0.43
1:A:50:GLN:NE2	3:A:916:HOH:O	2.43	0.43
1:A:100[B]:ARG:HA	1:A:100[B]:ARG:HD2	1.72	0.43
1:A:31:ALA:HA	1:A:32:PHE:HA	1.83	0.43
1:F:65:ALA:HA	1:F:144:MET:HE1	2.02	0.42
1:F:104:ILE:HG12	1:F:126:VAL:HG12	2.00	0.42
1:E:18[A]:ARG:NE	3:E:930:HOH:O	2.53	0.42
1:A:75:GLU:CD	1:D:70:LYS:NZ	2.72	0.42
1:B:104:ILE:HG12	1:B:126:VAL:HG12	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:120:HIS:CD2	1:F:122:PRO:O	2.72	0.41
1:C:68:MET:HE1	1:C:144:MET:SD	2.60	0.41
1:E:1:PRO:HG2	3:E:974:HOH:O	2.20	0.41
1:G:47:ALA:HB1	1:G:51:ASP:HB2	2.03	0.41
1:A:3:VAL:CG1	1:A:13:GLN:HB3	2.51	0.41
1:E:63:GLN:HG2	3:E:971:HOH:O	2.19	0.41
1:D:15:ILE:HD11	1:D:19:THR:HB	2.03	0.41
1:H:138:LEU:O	1:H:142:VAL:HG13	2.21	0.41
1:F:12:HIS:CG	1:F:111:LEU:HD21	2.56	0.41
1:C:100:ARG:NE	1:C:100:ARG:HA	2.36	0.41
1:D:68[A]:MET:HG3	3:D:947:HOH:O	2.20	0.41
1:C:2:ILE:HG12	1:C:115:ILE:CD1	2.51	0.41
1:F:65:ALA:CB	1:F:144:MET:HE3	2.51	0.40
1:D:15:ILE:HD11	1:D:19:THR:CB	2.51	0.40
1:B:34:PRO:HD3	1:B:142:VAL:HG13	2.03	0.40
1:G:4:GLN:OE1	1:H:10:MET:HE2	2.22	0.40
1:A:75:GLU:CD	1:D:70:LYS:HZ2	2.25	0.40
1:G:100:ARG:HA	1:G:100:ARG:NE	2.36	0.40

All (2) 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)
1:G:76:GLU:OE1	1:H:132:ARG:NH2[1_455]	2.11	0.09
3:E:976:HOH:O	3:H:988:HOH:O[1_655]	2.15	0.05

## 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	145/146 (99%)	143 (99%)	2 (1%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	B	134/146 (92%)	133 (99%)	1 (1%)	0	100	100
1	C	145/146 (99%)	142 (98%)	3 (2%)	0	100	100
1	D	148/146 (101%)	145 (98%)	3 (2%)	0	100	100
1	E	146/146 (100%)	144 (99%)	2 (1%)	0	100	100
1	F	136/146 (93%)	135 (99%)	1 (1%)	0	100	100
1	G	145/146 (99%)	143 (99%)	2 (1%)	0	100	100
1	H	148/146 (101%)	146 (99%)	2 (1%)	0	100	100
All	All	1147/1168 (98%)	1131 (99%)	16 (1%)	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	125/124 (101%)	122 (98%)	3 (2%)	57	49
1	B	119/124 (96%)	118 (99%)	1 (1%)	86	86
1	C	125/124 (101%)	121 (97%)	4 (3%)	46	35
1	D	128/124 (103%)	123 (96%)	5 (4%)	39	27
1	E	126/124 (102%)	124 (98%)	2 (2%)	70	66
1	F	121/124 (98%)	115 (95%)	6 (5%)	30	18
1	G	125/124 (101%)	119 (95%)	6 (5%)	31	19
1	H	128/124 (103%)	124 (97%)	4 (3%)	47	37
All	All	997/992 (100%)	966 (97%)	31 (3%)	50	37

All (31) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	15	ILE
1	A	49	PRO

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Mol	Chain	Res	Type
1	A	69	LEU
1	B	63	GLN
1	C	17	PRO
1	C	68	MET
1	C	107	THR
1	C	136	LEU
1	D	4[A]	GLN
1	D	4[B]	GLN
1	D	15	ILE
1	D	132	ARG
1	D	141	ILE
1	E	63	GLN
1	E	69	LEU
1	F	9	GLN
1	F	41	SER
1	F	63[A]	GLN
1	F	63[B]	GLN
1	F	96	MET
1	F	100	ARG
1	G	17	PRO
1	G	45[A]	GLU
1	G	45[B]	GLU
1	G	95	GLN
1	G	100	ARG
1	G	107	THR
1	H	15	ILE
1	H	37	ILE
1	H	112	GLN
1	H	132	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (37) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	4	GLN
1	A	50	GLN
1	A	53	ASN
1	A	57	ASN
1	A	120	HIS
1	B	7	GLN
1	B	9	GLN
1	B	12	HIS
1	B	67	GLN

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Mol	Chain	Res	Type
1	C	4	GLN
1	C	9	GLN
1	C	12	HIS
1	C	53	ASN
1	D	9	GLN
1	D	12	HIS
1	D	53	ASN
1	D	57	ASN
1	D	67	GLN
1	D	95	GLN
1	E	4	GLN
1	E	7	GLN
1	E	53	ASN
1	F	7	GLN
1	F	9	GLN
1	F	12	HIS
1	F	53	ASN
1	F	120	HIS
1	G	12	HIS
1	G	53	ASN
1	G	87	HIS
1	H	9	GLN
1	H	12	HIS
1	H	21	ASN
1	H	53	ASN
1	H	57	ASN
1	H	95	GLN
1	H	121	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 8 ligands modelled in this entry, 8 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	145/146 (99%)	-0.25	1 (0%) 89 90	8, 16, 29, 49	0
1	B	137/146 (93%)	-0.40	1 (0%) 89 90	7, 16, 30, 46	0
1	C	145/146 (99%)	-0.18	6 (4%) 41 45	8, 16, 44, 71	0
1	D	145/146 (99%)	-0.32	1 (0%) 89 90	6, 15, 28, 35	0
1	E	145/146 (99%)	-0.23	4 (2%) 56 60	7, 15, 29, 48	0
1	F	137/146 (93%)	-0.42	0 100 100	7, 16, 26, 36	0
1	G	145/146 (99%)	-0.18	5 (3%) 49 52	8, 17, 46, 70	0
1	H	145/146 (99%)	-0.38	0 100 100	8, 16, 28, 35	0
All	All	1144/1168 (97%)	-0.29	18 (1%) 74 78	6, 16, 31, 71	0

All (18) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	1	PRO	7.2
1	G	89	GLY	6.9
1	C	89	GLY	5.3
1	E	1	PRO	4.9
1	C	88	ALA	4.7
1	G	91	ILE	4.1
1	C	91	ILE	3.9
1	G	88	ALA	3.7
1	C	90	PRO	3.4
1	B	96	MET	3.2
1	G	94	GLY	2.8
1	G	95	GLN	2.6
1	C	95	GLN	2.5
1	C	94	GLY	2.4
1	E	2	ILE	2.4
1	E	91	ILE	2.1

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Mol	Chain	Res	Type	RSRZ
1	D	95	GLN	2.1
1	E	95	GLN	2.1

## 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( $\text{\AA}^2$ )	Q<0.9
2	CL	H	906	1/1	0.99	0.04	-2.43	17,17,17,17	0
2	CL	A	902	1/1	1.00	0.02	-4.24	15,15,15,15	0
2	CL	D	903	1/1	0.99	0.03	-4.26	15,15,15,15	0
2	CL	E	905	1/1	1.00	0.02	-5.97	15,15,15,15	0
2	CL	C	901	1/1	1.00	0.04	-	14,14,14,14	0
2	CL	F	907	1/1	0.99	0.06	-	14,14,14,14	0
2	CL	G	908	1/1	1.00	0.02	-	16,16,16,16	0
2	CL	B	904	1/1	0.99	0.04	-	15,15,15,15	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.