



# Full wwPDB X-ray Structure Validation Report ⓘ

Oct 11, 2021 – 07:39 AM EDT

PDB ID : 2PWO  
Title : Crystal Structure of HIV-1 CA146 A92E Psuedo Cell  
Authors : Kelly, B.N.  
Deposited on : 2007-05-11  
Resolution : 1.45 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

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

---

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

MolProbity : 4.02b-467  
Xtriage (Phenix) : 1.13  
EDS : 2.23.2  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
Refmac : 5.8.0158  
CCP4 : 7.0.044 (Gargrove)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.23.2

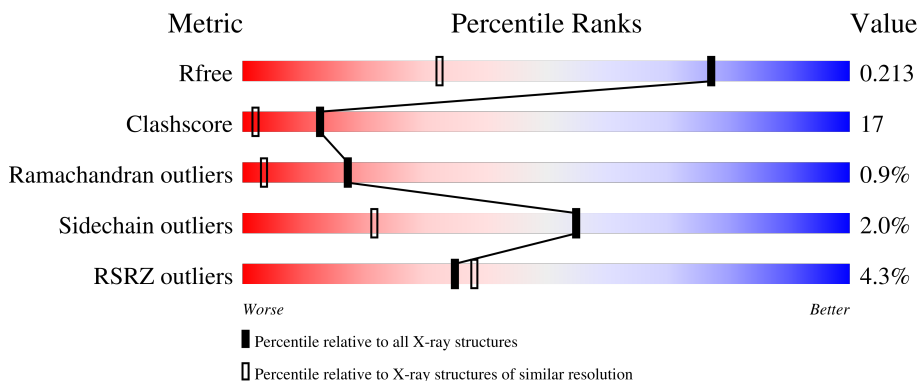
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*


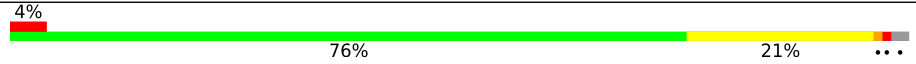
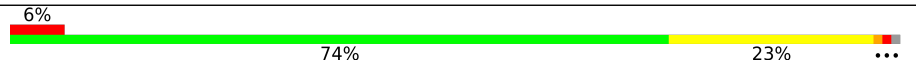

The reported resolution of this entry is 1.45 Å.

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))
$R_{free}$	130704	1156 (1.46-1.46)
Clashscore	141614	1202 (1.46-1.46)
Ramachandran outliers	138981	1178 (1.46-1.46)
Sidechain outliers	138945	1178 (1.46-1.46)
RSRZ outliers	127900	1139 (1.46-1.46)

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  $\geq 3$ , 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	146	 4% 84% 14% ..
1	B	146	 4% 76% 21% ...
1	C	146	 6% 74% 23% ...
1	D	146	 3% 82% 16% ..

## 2 Entry composition [i](#)

There are 3 unique types of molecules in this entry. The entry contains 5361 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 (Pr160Gag-Pol).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	144	1211	766	213	223	9	0	12	0
1	B	143	1181	751	202	219	9	0	10	0
1	C	145	1219	768	215	227	9	0	11	0
1	D	145	1213	772	209	223	9	0	13	0

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	92	GLU	ALA	engineered mutation	UNP P12497
B	92	GLU	ALA	engineered mutation	UNP P12497
C	92	GLU	ALA	engineered mutation	UNP P12497
D	92	GLU	ALA	engineered mutation	UNP P12497

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

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

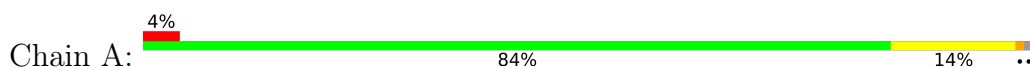
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	138	Total 138	O 138	0	0
3	B	123	Total 123	O 123	0	0
3	C	126	Total 126	O 126	0	0
3	D	146	Total 146	O 146	0	0

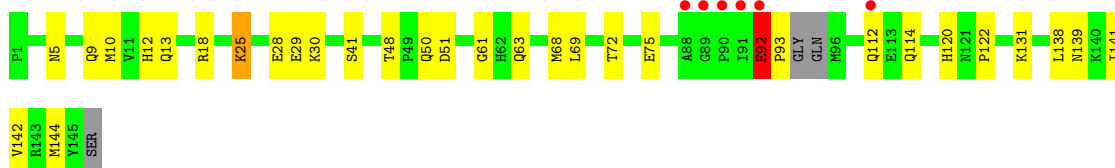
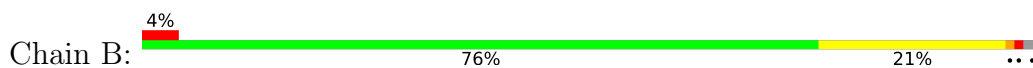
### 3 Residue-property plots [i](#)

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.

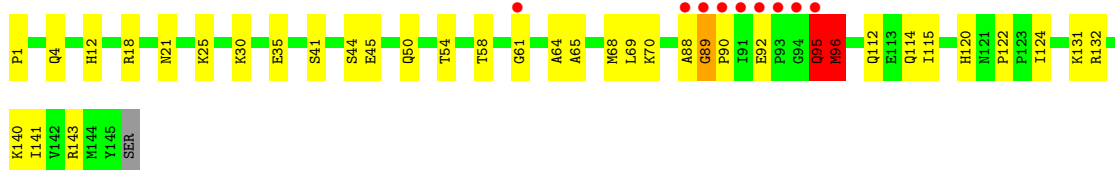
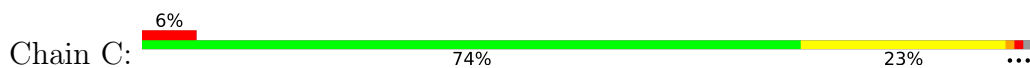
- Molecule 1: Gag-Pol polyprotein (Pr160Gag-Pol)



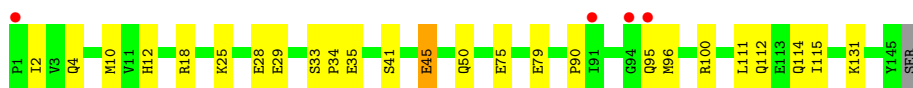
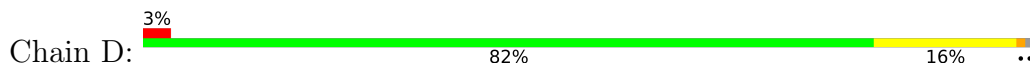
- Molecule 1: Gag-Pol polyprotein (Pr160Gag-Pol)



- Molecule 1: Gag-Pol polyprotein (Pr160Gag-Pol)



- Molecule 1: Gag-Pol polyprotein (Pr160Gag-Pol)



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	46.23Å 48.21Å 58.93Å 83.01° 71.28° 87.43°	Depositor
Resolution (Å)	30.03 – 1.45 30.03 – 1.45	Depositor EDS
% Data completeness (in resolution range)	90.7 (30.03-1.45) 90.7 (30.03-1.45)	Depositor EDS
$R_{merge}$	0.06	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.92 (at 1.45Å)	Xtrriage
Refinement program	REFMAC	Depositor
R, $R_{free}$	0.170 , 0.216 0.168 , 0.213	Depositor DCC
$R_{free}$ test set	3881 reflections (5.03%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	16.0	Xtrriage
Anisotropy	0.077	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.36 , 44.1	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.33$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
$F_o, F_c$ correlation	0.97	EDS
Total number of atoms	5361	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	20.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 75.14 % 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 1.3372e-06. 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, 0.333 respectively for untwinned datasets, and 0.375, 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: 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	0.82	0/1259	0.85	0/1708
1	B	0.74	0/1235	0.80	0/1675
1	C	0.73	0/1259	0.86	3/1709 (0.2%)
1	D	0.78	0/1271	0.79	0/1726
All	All	0.77	0/5024	0.83	3/6818 (0.0%)

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	96	MET	N-CA-C	-7.09	91.85	111.00
1	C	1	PRO	N-CD-CG	-6.58	93.33	103.20
1	C	132	ARG	NE-CZ-NH2	-6.48	117.06	120.30

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	1211	0	1220	35	0
1	B	1181	0	1196	38	0
1	C	1219	0	1216	55	0
1	D	1213	0	1237	59	0

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	A	1	0	0	0	0
2	B	1	0	0	0	0
2	C	1	0	0	0	0
2	D	1	0	0	0	0
3	A	138	0	0	7	2
3	B	123	0	0	15	0
3	C	126	0	0	17	0
3	D	146	0	0	24	2
All	All	5361	0	4869	161	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 17.

All (161) 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:C:45[B]:GLU:OE2	1:C:131[B]:LYS:NZ	1.67	1.27
1:D:75[B]:GLU:CD	3:D:1025:HOH:O	1.72	1.25
1:C:18[A]:ARG:HD3	1:D:41[A]:SER:OG	1.32	1.23
1:B:92:GLU:HB3	1:B:93:PRO:HA	1.23	1.19
1:C:18[A]:ARG:CD	1:D:41[A]:SER:OG	1.98	1.11
1:B:92:GLU:HB3	1:B:93:PRO:CA	1.83	1.09
1:B:61:GLY:O	3:B:980:HOH:O	1.74	1.05
1:A:2:ILE:HD11	1:A:10:MET:HB3	1.33	1.04
1:B:18[B]:ARG:CZ	3:B:951:HOH:O	2.04	1.02
1:C:143[A]:ARG:HG3	3:C:977:HOH:O	1.58	1.02
1:B:92:GLU:CB	1:B:93:PRO:HA	1.90	1.01
1:C:143[B]:ARG:CD	3:C:977:HOH:O	2.07	0.99
1:D:75[B]:GLU:OE2	3:D:1025:HOH:O	1.71	0.99
1:C:143[B]:ARG:HD3	3:C:977:HOH:O	1.58	0.98
1:A:100[B]:ARG:NH2	3:A:906:HOH:O	1.95	0.98
1:C:45[B]:GLU:OE2	1:D:18[B]:ARG:CZ	2.16	0.93
1:A:2:ILE:CD1	1:A:10:MET:HB3	1.99	0.92
1:C:18[A]:ARG:HD3	1:D:41[A]:SER:HG	1.13	0.92
1:A:70:LYS:NZ	1:D:75[B]:GLU:OE1	2.03	0.92
1:C:45[B]:GLU:OE1	1:D:18[B]:ARG:NE	2.05	0.90
1:B:139:ASN:O	1:B:142:VAL:HG22	1.71	0.90
1:B:18[B]:ARG:NH1	3:B:951:HOH:O	2.07	0.87
1:A:2:ILE:HD11	1:A:10:MET:CB	2.06	0.85
1:C:30:LYS:HE3	1:C:35[A]:GLU:HG2	1.57	0.85
1:C:4:GLN:HE21	1:D:4[A]:GLN:HE21	1.25	0.84

*Continued on next page...*



*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:45[A]:GLU:HG2	3:C:1022:HOH:O	1.78	0.84
1:C:18[A]:ARG:NE	1:D:41[A]:SER:OG	2.12	0.83
1:D:112[A]:GLN:HG3	3:D:1038:HOH:O	1.78	0.82
1:C:61:GLY:O	3:C:1000:HOH:O	1.95	0.82
1:C:70:LYS:HE2	3:C:1002:HOH:O	1.79	0.82
1:D:112[A]:GLN:NE2	3:D:1038:HOH:O	2.14	0.80
1:C:18[B]:ARG:CZ	1:D:45[B]:GLU:OE2	2.17	0.80
1:C:12:HIS:HD2	3:C:916:HOH:O	1.65	0.79
1:C:45[B]:GLU:CD	1:D:18[B]:ARG:NE	2.38	0.77
1:D:112[C]:GLN:NE2	3:D:986:HOH:O	1.69	0.77
1:C:18[B]:ARG:NH1	1:D:45[B]:GLU:OE2	2.18	0.76
1:B:18[B]:ARG:HG3	3:B:931:HOH:O	1.87	0.74
1:B:72:THR:O	1:B:75[B]:GLU:HG3	1.86	0.74
1:D:112[C]:GLN:HG2	3:D:1038:HOH:O	1.87	0.73
1:B:18[B]:ARG:NE	3:B:951:HOH:O	2.19	0.72
1:D:112[A]:GLN:CG	3:D:1038:HOH:O	2.37	0.71
1:B:25[A]:LYS:NZ	1:B:28[A]:GLU:OE1	2.23	0.71
1:B:18[B]:ARG:CD	3:B:951:HOH:O	2.40	0.69
1:C:44:SER:OG	1:C:131[B]:LYS:HE3	1.93	0.69
1:B:18[A]:ARG:NH1	3:B:1007:HOH:O	2.22	0.68
1:C:120:HIS:CD2	3:C:1018:HOH:O	2.47	0.67
1:B:112:GLN:HG3	3:B:957:HOH:O	1.93	0.67
1:D:75[A]:GLU:HG3	3:D:1025:HOH:O	1.94	0.67
1:C:112[B]:GLN:HG3	3:C:952:HOH:O	1.94	0.67
1:C:21[A]:ASN:OD1	3:C:978:HOH:O	2.12	0.67
1:C:18[B]:ARG:HG3	3:C:981:HOH:O	1.95	0.66
1:C:45[B]:GLU:OE2	1:D:18[B]:ARG:NE	2.28	0.66
1:D:112[A]:GLN:OE1	3:D:1044:HOH:O	2.13	0.66
1:B:50:GLN:H	1:B:114:GLN:HE22	1.45	0.65
1:D:45[B]:GLU:OE2	1:D:131[B]:LYS:NZ	2.29	0.64
1:D:75[A]:GLU:OE1	3:D:1005:HOH:O	2.15	0.64
1:B:18[B]:ARG:HD2	3:B:951:HOH:O	1.98	0.63
1:A:91:ILE:HD12	1:A:91:ILE:O	1.99	0.62
1:B:12:HIS:HD2	3:B:929:HOH:O	1.82	0.62
1:C:4:GLN:NE2	1:D:4[A]:GLN:HE21	1.94	0.62
1:D:12:HIS:CD2	1:D:111:LEU:HD21	2.35	0.61
1:C:18[A]:ARG:CZ	1:D:41[A]:SER:OG	2.48	0.61
1:D:75[B]:GLU:OE2	1:D:79:GLU:HG2	1.99	0.61
1:C:21[A]:ASN:HD21	1:C:25:LYS:HE3	1.65	0.61
1:C:92:GLU:HB2	1:C:95:GLN:HG2	1.82	0.61
1:C:12:HIS:HB2	1:C:115:ILE:HD11	1.82	0.60

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:3:VAL:HG22	3:A:1026:HOH:O	2.02	0.60
1:C:30:LYS:HE3	1:C:35[A]:GLU:CG	2.30	0.60
1:B:92:GLU:HB3	1:B:93:PRO:C	2.21	0.60
1:C:18[A]:ARG:CD	1:D:41[A]:SER:HG	1.94	0.60
1:D:12:HIS:HD2	3:D:946:HOH:O	1.85	0.59
1:C:21[A]:ASN:HD21	1:C:25:LYS:CE	2.16	0.59
1:C:95:GLN:HA	3:C:1024:HOH:O	2.02	0.58
1:D:28[A]:GLU:HG3	3:D:930:HOH:O	2.04	0.57
1:D:96:MET:HG3	3:D:998:HOH:O	2.03	0.57
1:B:131:LYS:NZ	3:B:1017:HOH:O	2.11	0.56
1:D:50[B]:GLN:H	1:D:114:GLN:HE22	1.53	0.56
1:D:50[A]:GLN:H	1:D:114:GLN:HE22	1.53	0.56
1:B:5:ASN:HD21	1:B:9[A]:GLN:HE21	1.54	0.55
1:C:45[B]:GLU:CD	1:D:18[B]:ARG:CZ	2.73	0.55
1:C:54:THR:O	1:C:58:THR:HG23	2.06	0.55
1:D:35:GLU:HG3	3:D:990:HOH:O	2.06	0.55
1:A:5:ASN:HD21	1:A:9[B]:GLN:HE21	1.53	0.55
1:A:3:VAL:HG23	1:A:13[B]:GLN:CD	2.28	0.55
1:C:50:GLN:H	1:C:114:GLN:HE22	1.54	0.54
1:A:50:GLN:HG2	3:A:919:HOH:O	2.07	0.54
1:C:143[A]:ARG:CG	3:C:977:HOH:O	2.32	0.54
1:A:30[B]:LYS:HD3	1:A:35[B]:GLU:HB3	1.89	0.53
1:C:120:HIS:HD2	1:C:122:PRO:O	1.92	0.53
1:D:75[B]:GLU:CG	3:D:1025:HOH:O	2.37	0.53
1:A:3:VAL:HG21	1:A:13[B]:GLN:OE1	2.09	0.53
1:B:25[A]:LYS:HD3	3:B:945:HOH:O	2.07	0.53
1:A:2:ILE:CD1	1:B:10:MET:HE1	2.39	0.53
1:B:120:HIS:HD2	1:B:122:PRO:O	1.91	0.53
1:A:18[B]:ARG:CZ	3:A:962:HOH:O	2.57	0.52
1:C:65:ALA:HB1	1:C:141:ILE:HG21	1.90	0.52
1:D:18[A]:ARG:NE	3:D:943:HOH:O	2.42	0.52
1:B:25[A]:LYS:HA	1:B:28[A]:GLU:HG2	1.91	0.52
1:B:25[A]:LYS:CE	1:B:28[A]:GLU:OE1	2.58	0.52
1:B:138:LEU:O	1:B:142:VAL:HG13	2.10	0.51
1:A:5:ASN:ND2	1:A:9[B]:GLN:HG2	2.26	0.51
1:D:112[A]:GLN:CD	3:D:1038:HOH:O	2.49	0.50
1:A:138:LEU:O	1:A:142:VAL:HG13	2.11	0.50
1:C:18[B]:ARG:CD	1:D:45[B]:GLU:OE2	2.52	0.50
1:B:13:GLN:HG3	3:B:1019:HOH:O	2.10	0.50
1:D:25:LYS:HA	1:D:28[A]:GLU:HG2	1.93	0.50
1:A:100[B]:ARG:NH2	1:D:100:ARG:HB3	2.26	0.50

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:18[A]:ARG:HD2	3:D:943:HOH:O	2.12	0.50
1:A:50:GLN:HG3	1:A:114:GLN:HE22	1.77	0.49
1:D:90:PRO:HB2	1:D:95:GLN:HB3	1.94	0.49
1:A:5:ASN:HD21	1:A:9[B]:GLN:NE2	2.10	0.49
1:A:91:ILE:HD12	1:A:91:ILE:C	2.34	0.49
1:D:112[A]:GLN:CD	1:D:112[A]:GLN:H	2.16	0.48
1:D:12:HIS:CD2	3:D:946:HOH:O	2.64	0.48
1:A:2:ILE:CD1	1:B:10:MET:CE	2.91	0.47
1:B:12:HIS:HE1	1:B:51:ASP:OD1	1.97	0.47
1:D:4[B]:GLN:HG3	3:D:991:HOH:O	2.12	0.47
1:A:3:VAL:CG2	1:A:13[B]:GLN:CD	2.83	0.47
1:A:18[B]:ARG:NE	3:A:962:HOH:O	2.48	0.47
1:C:45[B]:GLU:OE1	1:D:18[B]:ARG:CZ	2.62	0.46
1:C:143[B]:ARG:CG	3:C:977:HOH:O	2.57	0.46
1:C:18[B]:ARG:HD2	1:D:45[B]:GLU:OE2	2.14	0.46
1:A:131:LYS:NZ	3:B:951:HOH:O	2.27	0.46
1:A:132:ARG:HG3	1:A:132:ARG:NH1	2.32	0.45
1:C:64:ALA:O	1:C:68[B]:MET:HG3	2.16	0.45
1:A:50:GLN:H	1:A:114:GLN:HE22	1.64	0.45
1:C:4:GLN:HE21	1:D:4[A]:GLN:NE2	2.01	0.45
1:A:100[B]:ARG:NH2	1:D:100:ARG:CB	2.79	0.45
1:C:69:LEU:HB2	1:C:141:ILE:HD11	1.99	0.45
1:A:70:LYS:HG3	3:A:946:HOH:O	2.17	0.45
1:D:29:GLU:OE2	3:D:953:HOH:O	2.21	0.45
1:B:18[A]:ARG:NH2	3:B:987:HOH:O	2.49	0.44
1:B:48:THR:HB	1:B:114:GLN:HE21	1.83	0.44
1:B:29[B]:GLU:OE1	1:B:30:LYS:NZ	2.50	0.44
1:A:132:ARG:HG3	1:A:132:ARG:HH11	1.83	0.44
1:C:140:LYS:O	1:C:143[A]:ARG:HG2	2.18	0.44
1:B:68[B]:MET:SD	1:B:144:MET:SD	3.15	0.43
1:D:90:PRO:CB	1:D:95:GLN:HB3	2.47	0.43
1:A:2:ILE:CG1	1:A:10:MET:HB3	2.48	0.43
1:A:5:ASN:HD21	1:A:9[B]:GLN:HG2	1.83	0.43
1:C:25:LYS:HG3	3:C:978:HOH:O	2.18	0.43
1:C:30:LYS:HD3	1:C:35[A]:GLU:HG3	2.01	0.43
1:D:4[B]:GLN:CG	3:D:991:HOH:O	2.66	0.43
1:C:131[B]:LYS:HE2	3:C:933:HOH:O	2.19	0.42
1:D:2:ILE:HG12	1:D:115:ILE:HD12	2.01	0.42
1:D:25:LYS:HG3	3:D:996:HOH:O	2.19	0.42
1:D:33:SER:HB2	1:D:34:PRO:HD2	2.02	0.42
1:A:35[A]:GLU:CG	3:A:959:HOH:O	2.68	0.42

*Continued on next page...*

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:124:ILE:HD11	3:C:1018:HOH:O	2.20	0.42
1:B:50:GLN:H	1:B:114:GLN:NE2	2.12	0.42
1:B:92:GLU:CB	1:B:93:PRO:CA	2.62	0.41
1:C:41[B]:SER:OG	1:D:18[B]:ARG:HD2	2.19	0.41
1:A:13[A]:GLN:NE2	1:A:14:ALA:H	2.19	0.41
1:C:88:ALA:O	1:C:89:GLY:O	2.37	0.41
1:A:63:GLN:H	1:A:63:GLN:HG2	1.67	0.41
1:B:69:LEU:HB2	1:B:141:ILE:HD11	2.03	0.41
1:C:90:PRO:HB2	1:C:95:GLN:HG3	2.03	0.41
1:A:18[B]:ARG:HD3	1:B:41[B]:SER:OG	2.20	0.41
1:D:18[A]:ARG:CD	3:D:943:HOH:O	2.68	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)
3:A:960:HOH:O	3:D:1023:HOH:O[1_545]	1.84	0.36
3:A:972:HOH:O	3:D:999:HOH:O[1_545]	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	154/146 (106%)	152 (99%)	1 (1%)	1 (1%)	25	7
1	B	149/146 (102%)	146 (98%)	2 (1%)	1 (1%)	22	5
1	C	154/146 (106%)	150 (97%)	1 (1%)	3 (2%)	8	1
1	D	156/146 (107%)	155 (99%)	1 (1%)	0	100	100
All	All	613/584 (105%)	603 (98%)	5 (1%)	5 (1%)	17	4

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	92	GLU
1	C	89	GLY
1	C	95	GLN
1	C	96	MET
1	A	93	PRO

### 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	134/124 (108%)	130 (97%)	4 (3%)	41 9
1	B	132/124 (106%)	128 (97%)	4 (3%)	41 9
1	C	134/124 (108%)	132 (98%)	2 (2%)	65 35
1	D	136/124 (110%)	133 (98%)	3 (2%)	52 18
All	All	536/496 (108%)	523 (98%)	13 (2%)	55 16

All (13) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	13[A]	GLN
1	A	13[B]	GLN
1	A	69	LEU
1	A	91	ILE
1	B	25[A]	LYS
1	B	25[B]	LYS
1	B	63	GLN
1	B	92	GLU
1	C	95	GLN
1	C	96	MET
1	D	10	MET
1	D	45[A]	GLU
1	D	45[B]	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (23) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	4	GLN
1	A	7	GLN
1	A	21	ASN
1	A	53	ASN
1	A	57	ASN
1	A	114	GLN
1	B	7	GLN
1	B	12	HIS
1	B	53	ASN
1	B	114	GLN
1	B	120	HIS
1	C	9	GLN
1	C	12	HIS
1	C	53	ASN
1	C	87	HIS
1	C	114	GLN
1	C	120	HIS
1	D	7	GLN
1	D	9	GLN
1	D	12	HIS
1	D	53	ASN
1	D	57	ASN
1	D	114	GLN

### 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 monosaccharides in this entry.

### 5.6 Ligand geometry [i](#)

Of 4 ligands modelled in this entry, 4 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	144/146 (98%)	0.14	6 (4%) 36 39	10, 16, 28, 38	0
1	B	143/146 (97%)	0.04	6 (4%) 36 39	11, 18, 32, 62	0
1	C	145/146 (99%)	0.16	9 (6%) 20 22	10, 18, 38, 56	0
1	D	145/146 (99%)	0.03	4 (2%) 53 55	10, 17, 28, 32	0
All	All	577/584 (98%)	0.09	25 (4%) 35 38	10, 18, 29, 62	0

All (25) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	2	ILE	7.8
1	C	89	GLY	7.1
1	C	88	ALA	6.5
1	B	88	ALA	5.6
1	C	91	ILE	5.0
1	C	95	GLN	5.0
1	A	91	ILE	4.5
1	B	90	PRO	4.4
1	B	89	GLY	4.1
1	A	93	PRO	3.7
1	B	92	GLU	3.7
1	C	94	GLY	3.4
1	B	91	ILE	3.2
1	A	6	LEU	3.1
1	C	93	PRO	3.0
1	D	95	GLN	2.9
1	C	90	PRO	2.8
1	D	1	PRO	2.8
1	D	94	GLY	2.8
1	C	92	GLU	2.6
1	A	95	GLN	2.3

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
1	D	91	ILE	2.3
1	A	94	GLY	2.2
1	C	61	GLY	2.1
1	B	112	GLN	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 monosaccharides 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, 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	B-factors(Å <sup>2</sup> )	Q<0.9
2	CL	A	902	1/1	1.00	0.04	17,17,17,17	0
2	CL	B	904	1/1	1.00	0.04	15,15,15,15	0
2	CL	C	901	1/1	1.00	0.04	15,15,15,15	0
2	CL	D	903	1/1	1.00	0.04	17,17,17,17	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.