



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 1, 2026 – 01:20 PM UTC

PDB ID : 3P05 / pdb_00003p05
Title : X-ray structure of pentameric HIV-1 CA
Authors : Pornillos, O.
Deposited on : 2010-09-27
Resolution : 2.50 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

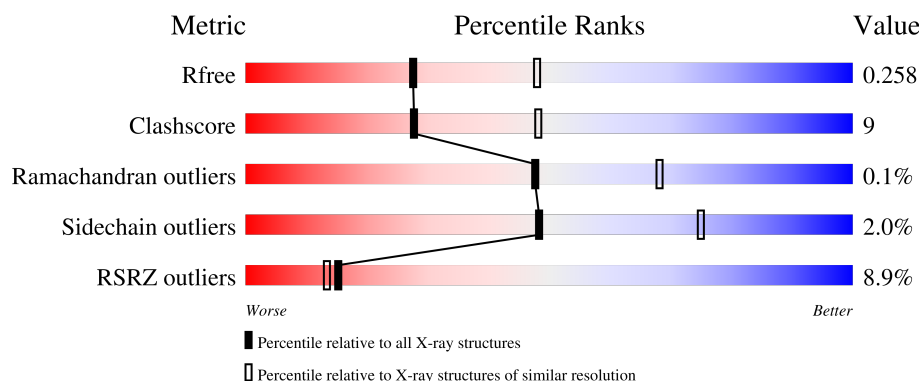
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.50 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	5829 (2.50-2.50)
Clashscore	190562	6492 (2.50-2.50)
Ramachandran outliers	187476	6378 (2.50-2.50)
Sidechain outliers	187428	6380 (2.50-2.50)
RSRZ outliers	180081	5833 (2.50-2.50)

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	231	10% 74% 16% • 9%
1	B	231	12% 65% 23% • 10%
1	C	231	6% 76% 13% • 10%
1	D	231	8% 71% 19% 11%
1	E	231	4% 69% 16% • 14%

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
2	IOD	D	233	-	-	X	-
2	IOD	E	233	-	-	X	-

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 7918 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 HIV-1 CA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	210	Total	C	N	O	S	0	0	0
			1606	1013	278	302	13			
1	B	209	Total	C	N	O	S	0	0	0
			1594	1001	275	304	14			
1	C	209	Total	C	N	O	S	0	0	0
			1592	1003	273	302	14			
1	D	206	Total	C	N	O	S	0	0	0
			1582	997	271	300	14			
1	E	199	Total	C	N	O	S	0	0	0
			1534	968	263	291	12			

There are 20 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	21	CYS	ASN	engineered mutation	UNP Q72497
A	22	CYS	ALA	engineered mutation	UNP Q72497
A	184	ALA	TRP	engineered mutation	UNP Q72497
A	185	ALA	MET	engineered mutation	UNP Q72497
B	21	CYS	ASN	engineered mutation	UNP Q72497
B	22	CYS	ALA	engineered mutation	UNP Q72497
B	184	ALA	TRP	engineered mutation	UNP Q72497
B	185	ALA	MET	engineered mutation	UNP Q72497
C	21	CYS	ASN	engineered mutation	UNP Q72497
C	22	CYS	ALA	engineered mutation	UNP Q72497
C	184	ALA	TRP	engineered mutation	UNP Q72497
C	185	ALA	MET	engineered mutation	UNP Q72497
D	21	CYS	ASN	engineered mutation	UNP Q72497
D	22	CYS	ALA	engineered mutation	UNP Q72497
D	184	ALA	TRP	engineered mutation	UNP Q72497
D	185	ALA	MET	engineered mutation	UNP Q72497
E	21	CYS	ASN	engineered mutation	UNP Q72497
E	22	CYS	ALA	engineered mutation	UNP Q72497
E	184	ALA	TRP	engineered mutation	UNP Q72497

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Chain	Residue	Modelled	Actual	Comment	Reference
E	185	ALA	MET	engineered mutation	UNP Q72497

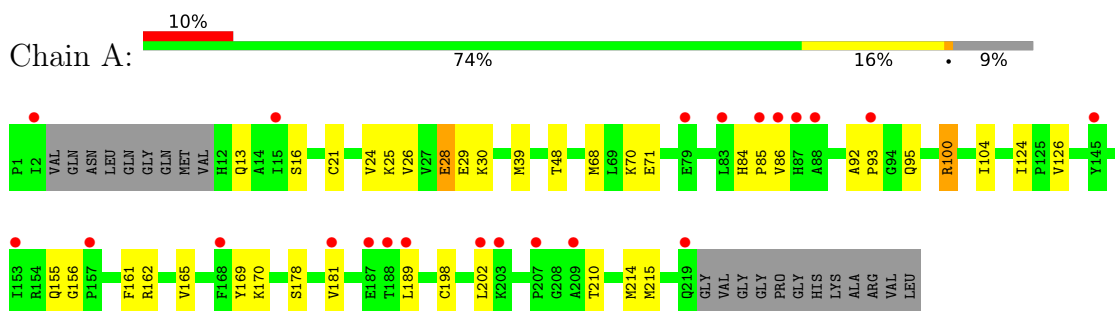
- Molecule 2 is IODIDE ION (CCD ID: IOD) (formula: I).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	4	Total I 4 4	0	0
2	B	1	Total I 1 1	0	0
2	C	1	Total I 1 1	0	0
2	D	2	Total I 2 2	0	0
2	E	2	Total I 2 2	0	0

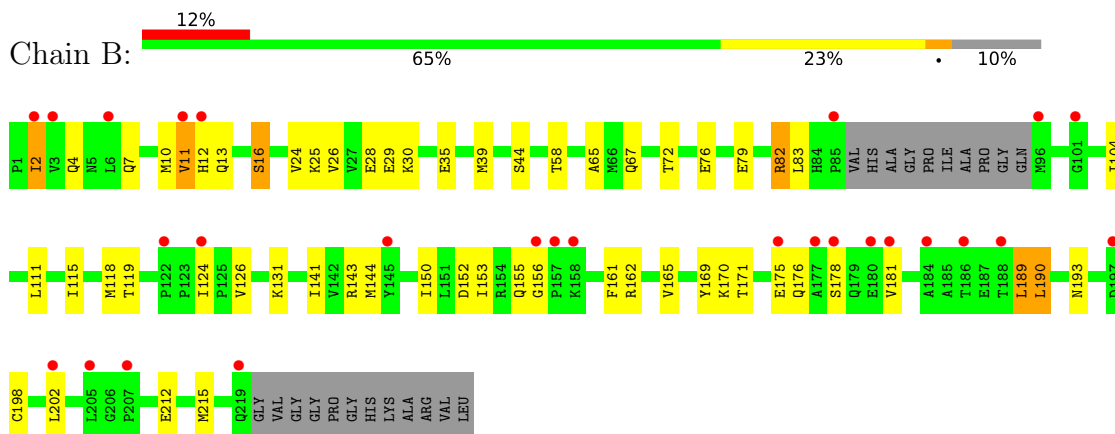
3 Residue-property plots [i](#)

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.

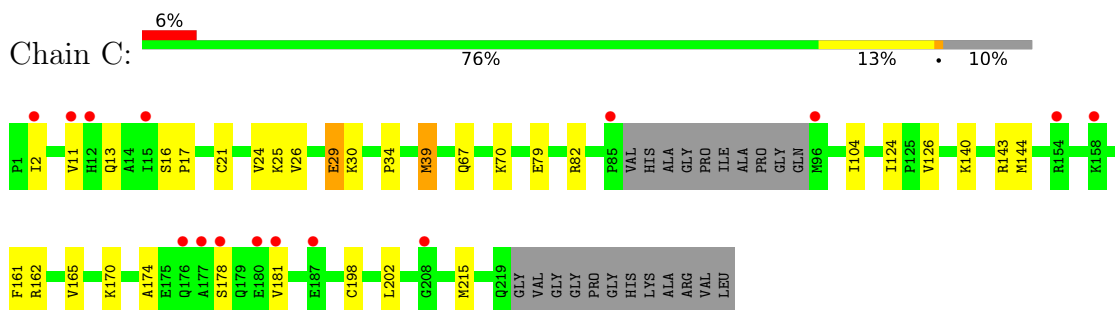
• Molecule 1: HIV-1 CA



• Molecule 1: HIV-1 CA

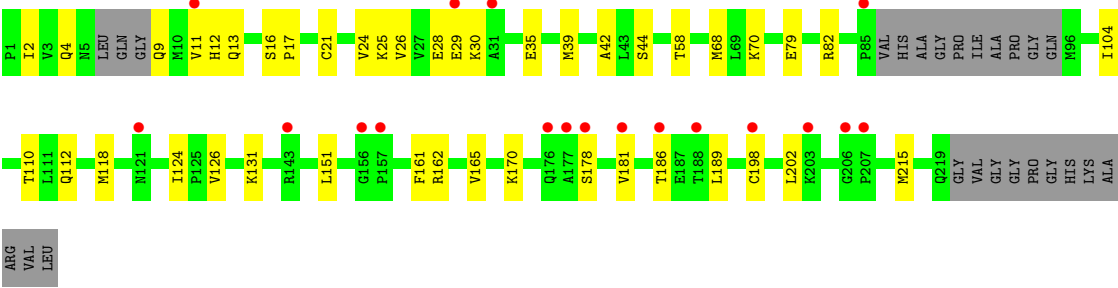


• Molecule 1: HIV-1 CA

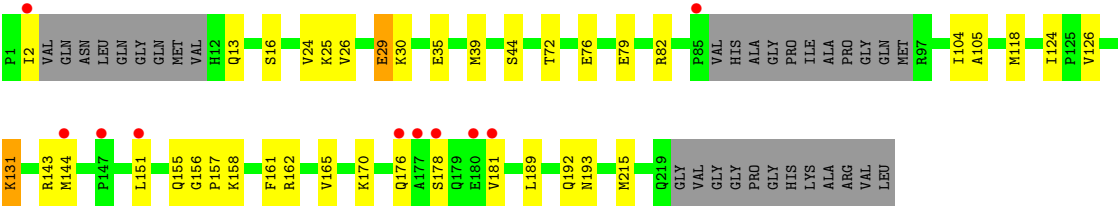


• Molecule 1: HIV-1 CA





• Molecule 1: HIV-1 CA



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	58.72Å 130.31Å 81.83Å 90.00° 97.37° 90.00°	Depositor
Resolution (Å)	32.58 – 2.50 32.58 – 2.50	Depositor EDS
% Data completeness (in resolution range)	97.4 (32.58-2.50) 97.4 (32.58-2.50)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.52 (at 2.51Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.6.1_357)	Depositor
R, R_{free}	0.230 , 0.266 0.222 , 0.258	Depositor DCC
R_{free} test set	2083 reflections (4.93%)	wwPDB-VP
Wilson B-factor (Å ²)	54.0	Xtriage
Anisotropy	0.124	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 40.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	7918	wwPDB-VP
Average B, all atoms (Å ²)	64.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.91% 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: IOD

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	0.88	1/1642 (0.1%)	1.03	2/2236 (0.1%)
1	B	0.94	3/1627 (0.2%)	1.17	8/2214 (0.4%)
1	C	0.88	0/1625	1.02	2/2212 (0.1%)
1	D	0.85	1/1614 (0.1%)	1.01	2/2195 (0.1%)
1	E	0.87	0/1566	0.99	2/2129 (0.1%)
All	All	0.89	5/8074 (0.1%)	1.05	16/10986 (0.1%)

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	189	LEU	CA-C	-6.87	1.44	1.52
1	B	2	ILE	CA-CB	-5.95	1.47	1.54
1	A	48	THR	CA-CB	5.59	1.60	1.53
1	B	190	LEU	N-CA	-5.01	1.40	1.46
1	D	42	ALA	CA-CB	-5.01	1.45	1.53

All (16) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	82	ARG	NE-CZ-NH2	12.03	130.02	119.20
1	B	82	ARG	NE-CZ-NH1	-11.37	110.13	121.50
1	B	82	ARG	CD-NE-CZ	9.22	137.31	124.40
1	B	189	LEU	CA-C-N	-7.40	110.50	120.79
1	B	189	LEU	C-N-CA	-7.40	110.50	120.79
1	E	105	ALA	N-CA-C	-7.08	104.53	113.02
1	E	29	GLU	N-CA-C	5.86	118.14	111.11
1	A	189	LEU	N-CA-C	5.53	118.23	111.82
1	D	189	LEU	N-CA-C	5.32	117.99	111.82
1	B	152	ASP	N-CA-C	5.22	115.90	108.54
1	C	29	GLU	N-CA-C	5.18	116.61	111.07

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	100	ARG	NE-CZ-NH1	-5.16	116.34	121.50
1	C	39	MET	N-CA-C	5.14	116.57	111.07
1	D	186	THR	N-CA-C	-5.10	105.37	111.03
1	B	16	SER	CA-C-N	5.02	125.04	119.32
1	B	16	SER	C-N-CA	5.02	125.04	119.32

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	1606	0	1584	30	0
1	B	1594	0	1552	52	0
1	C	1592	0	1558	25	0
1	D	1582	0	1556	27	0
1	E	1534	0	1515	25	0
2	A	4	0	0	3	0
2	B	1	0	0	1	0
2	C	1	0	0	1	0
2	D	2	0	0	3	0
2	E	2	0	0	3	0
All	All	7918	0	7765	141	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 9.

All (141) 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:D:39:MET:HE1	1:E:24:VAL:HG21	1.26	1.14
1:A:39:MET:HE1	1:B:24:VAL:HG21	1.21	1.10
1:B:39:MET:HE1	1:C:24:VAL:HG21	1.38	1.06
1:A:84:HIS:O	1:A:100:ARG:NH1	1.94	0.98
1:E:158:LYS:HB2	2:E:233:IOD:I	2.45	0.86

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:85:PRO:HA	1:A:100:ARG:NH2	1.94	0.83
1:A:24:VAL:HG21	1:E:39:MET:HE1	1.60	0.82
1:A:28:GLU:HA	1:A:28:GLU:OE1	1.79	0.82
1:B:143:ARG:NH1	1:B:176:GLN:OE1	2.12	0.82
1:B:212:GLU:OE2	1:C:143:ARG:NH2	2.13	0.81
1:B:143:ARG:CZ	1:B:176:GLN:OE1	2.31	0.79
1:B:10:MET:HB3	1:B:119:THR:HG22	1.65	0.76
1:A:85:PRO:HA	1:A:100:ARG:HH22	1.52	0.74
1:B:11:VAL:HG12	1:B:12:HIS:H	1.52	0.74
1:B:11:VAL:HG12	1:B:12:HIS:N	2.02	0.74
1:C:39:MET:HE1	1:D:24:VAL:HG21	1.71	0.72
1:B:189:LEU:O	1:B:190:LEU:C	2.26	0.71
1:B:2:ILE:HD12	1:B:118:MET:HE2	1.73	0.71
1:A:178:SER:OG	1:A:181:VAL:HG23	1.92	0.70
1:B:143:ARG:NH2	1:B:176:GLN:OE1	2.25	0.69
1:E:189:LEU:HD22	1:E:193:ASN:HD21	1.58	0.67
1:C:2:ILE:HA	1:C:11:VAL:O	1.95	0.67
1:B:150:ILE:N	1:B:175:GLU:OE2	2.27	0.67
1:B:189:LEU:HD22	1:B:193:ASN:ND2	2.11	0.66
1:A:39:MET:HE1	1:B:24:VAL:CG2	2.13	0.66
1:B:178:SER:OG	1:B:181:VAL:HG23	1.97	0.64
1:B:39:MET:CE	1:C:24:VAL:HG21	2.23	0.63
1:B:153:ILE:HD11	1:B:171:THR:HG21	1.80	0.63
1:D:13:GLN:HA	1:D:13:GLN:OE1	1.98	0.63
1:D:151:LEU:HD21	2:D:232:IOD:I	2.69	0.63
1:A:39:MET:CE	1:B:24:VAL:HG21	2.13	0.62
1:E:189:LEU:HD22	1:E:193:ASN:ND2	2.15	0.62
1:E:178:SER:OG	1:E:181:VAL:HG23	2.00	0.60
1:A:71:GLU:HB2	2:A:235:IOD:I	2.71	0.60
1:B:44:SER:OG	1:B:131:LYS:HE3	2.01	0.60
1:C:178:SER:OG	1:C:181:VAL:HG23	2.01	0.59
1:B:79:GLU:OE1	1:B:82:ARG:NH1	2.35	0.59
1:A:104:ILE:HG12	1:A:126:VAL:HG12	1.85	0.58
1:C:25:LYS:HD2	1:C:29:GLU:OE2	2.04	0.58
1:D:79:GLU:OE1	1:D:82:ARG:NH1	2.37	0.58
1:D:161:PHE:O	1:D:165:VAL:HG23	2.04	0.58
1:D:178:SER:OG	1:D:181:VAL:HG23	2.05	0.57
1:B:13:GLN:HA	1:B:13:GLN:OE1	2.04	0.57
1:D:170:LYS:HD2	2:D:233:IOD:I	2.75	0.56
2:A:233:IOD:I	1:B:144:MET:CE	3.24	0.56
1:E:25:LYS:HD2	1:E:29:GLU:OE2	2.06	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:170:LYS:HD2	2:E:232:IOD:I	2.75	0.55
1:B:7:GLN:O	1:B:7:GLN:HG2	2.05	0.55
1:A:161:PHE:O	1:A:165:VAL:HG23	2.08	0.54
1:B:10:MET:CB	1:B:119:THR:HG22	2.36	0.54
1:C:34:PRO:HG3	1:C:174:ALA:HA	1.90	0.54
1:A:13:GLN:HA	1:A:13:GLN:OE1	2.09	0.53
1:A:162:ARG:HG3	1:A:215:MET:HE1	1.89	0.53
1:C:13:GLN:HA	1:C:13:GLN:OE1	2.08	0.53
1:B:25:LYS:HD2	1:B:29:GLU:OE2	2.09	0.53
1:B:162:ARG:HG3	1:B:215:MET:HE1	1.91	0.53
1:E:13:GLN:HA	1:E:13:GLN:OE1	2.08	0.53
1:C:79:GLU:OE1	1:C:82:ARG:NH1	2.42	0.52
1:B:169:TYR:CZ	1:C:67:GLN:HG2	2.45	0.52
1:C:215:MET:SD	1:D:68:MET:HE2	2.50	0.51
1:E:79:GLU:OE1	1:E:82:ARG:NH1	2.44	0.51
1:B:150:ILE:CA	1:B:175:GLU:OE2	2.59	0.51
1:E:118:MET:HG3	1:E:126:VAL:HG22	1.91	0.51
1:B:170:LYS:HD2	2:B:232:IOD:I	2.81	0.50
1:B:161:PHE:O	1:B:165:VAL:HG23	2.10	0.50
1:B:26:VAL:HG13	1:B:30:LYS:HD2	1.93	0.49
1:A:93:PRO:C	1:A:95:GLN:H	2.20	0.49
1:B:143:ARG:HH12	1:B:176:GLN:HB2	1.78	0.49
1:E:26:VAL:HG13	1:E:30:LYS:HD2	1.95	0.49
1:A:28:GLU:OE1	1:A:28:GLU:CA	2.57	0.49
1:D:26:VAL:HG13	1:D:30:LYS:HD2	1.95	0.49
1:A:92:ALA:O	1:A:95:GLN:HB2	2.13	0.48
1:B:144:MET:HE2	1:B:144:MET:HB3	1.66	0.48
1:A:198:CYS:O	1:A:202:LEU:HG	2.13	0.48
1:D:2:ILE:HD12	1:D:118:MET:HE2	1.95	0.48
1:E:44:SER:OG	1:E:131:LYS:HE3	2.13	0.48
1:C:17:PRO:O	1:C:21:CYS:SG	2.72	0.48
1:E:161:PHE:O	1:E:165:VAL:HG23	2.13	0.48
1:E:143:ARG:NH1	1:E:176:GLN:OE1	2.47	0.47
1:D:70:LYS:HE3	1:D:70:LYS:HB2	1.58	0.47
1:D:17:PRO:O	1:D:21:CYS:SG	2.73	0.47
1:A:70:LYS:HE3	1:A:70:LYS:HB2	1.68	0.46
1:D:110:THR:HB	1:D:112:GLN:OE1	2.15	0.46
1:A:85:PRO:HA	1:A:100:ARG:CZ	2.45	0.46
1:D:162:ARG:HG3	1:D:215:MET:HE1	1.97	0.46
1:B:2:ILE:HG22	1:B:10:MET:HE3	1.98	0.46
1:B:10:MET:HB3	1:B:119:THR:CG2	2.41	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:26:VAL:HG11	1:D:39:MET:HG2	1.97	0.46
1:A:25:LYS:HD2	1:A:29:GLU:OE2	2.16	0.46
1:A:26:VAL:HG13	1:A:30:LYS:HD2	1.96	0.46
1:A:68:MET:HE2	1:E:215:MET:SD	2.55	0.46
1:B:39:MET:HE1	1:C:24:VAL:CG2	2.27	0.45
1:E:2:ILE:HD12	1:E:118:MET:HE2	1.97	0.45
1:B:65:ALA:HB1	1:B:141:ILE:HD13	1.98	0.45
1:D:25:LYS:HD2	1:D:29:GLU:OE2	2.17	0.45
1:B:212:GLU:OE1	1:C:140:LYS:HE3	2.16	0.45
1:B:104:ILE:HG12	1:B:126:VAL:HG12	1.99	0.45
1:C:70:LYS:HE3	1:C:70:LYS:HB2	1.61	0.44
1:A:169:TYR:CZ	1:B:67:GLN:HG2	2.51	0.44
1:B:189:LEU:HD22	1:B:193:ASN:HD21	1.81	0.44
1:D:112:GLN:H	1:D:112:GLN:CD	2.24	0.44
1:A:92:ALA:HB3	1:A:95:GLN:HG3	1.99	0.44
1:B:171:THR:O	1:B:175:GLU:HG3	2.17	0.44
1:C:26:VAL:HG13	1:C:30:LYS:HD2	1.99	0.43
1:E:72:THR:O	1:E:76:GLU:HG2	2.19	0.43
1:D:104:ILE:HG12	1:D:126:VAL:HG12	2.00	0.43
1:E:155:GLN:HG2	1:E:156:GLY:O	2.18	0.43
1:B:28:GLU:HG2	1:B:29:GLU:N	2.34	0.42
1:A:39:MET:HE2	1:B:58:THR:HB	2.01	0.42
1:A:170:LYS:HD2	2:A:234:IOD:I	2.89	0.42
1:B:111:LEU:O	1:B:115:ILE:HG13	2.19	0.42
1:E:144:MET:HB3	1:E:144:MET:HE2	1.60	0.42
1:B:39:MET:HE2	1:B:39:MET:HB2	1.91	0.42
1:C:39:MET:CE	1:D:58:THR:HB	2.49	0.42
1:A:210:THR:O	1:A:214:MET:HG3	2.19	0.42
1:C:104:ILE:HG12	1:C:126:VAL:HG12	2.01	0.42
1:C:144:MET:HE2	1:C:144:MET:HB3	1.56	0.42
1:E:30:LYS:HE2	1:E:35:GLU:OE2	2.19	0.42
1:D:4:GLN:HA	1:D:9:GLN:O	2.19	0.42
1:B:11:VAL:CG1	1:B:12:HIS:H	2.17	0.42
1:C:161:PHE:O	1:C:165:VAL:HG23	2.19	0.42
1:D:30:LYS:HE2	1:D:35:GLU:OE2	2.20	0.42
1:D:198:CYS:O	1:D:202:LEU:HG	2.19	0.42
1:E:104:ILE:HG12	1:E:126:VAL:HG12	2.02	0.42
1:D:39:MET:HB2	1:D:39:MET:HE2	1.83	0.41
1:E:162:ARG:HG3	1:E:215:MET:HE1	2.02	0.41
1:B:169:TYR:CE2	1:C:67:GLN:HG2	2.55	0.41
1:B:198:CYS:O	1:B:202:LEU:HG	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:11:VAL:HG12	1:D:12:HIS:N	2.35	0.41
1:B:72:THR:O	1:B:76:GLU:HG2	2.20	0.41
1:D:44:SER:OG	1:D:131:LYS:HE3	2.19	0.41
1:A:155:GLN:HG2	1:A:156:GLY:O	2.21	0.41
1:E:151:LEU:HD23	1:E:189:LEU:HD11	2.03	0.41
1:C:170:LYS:HD2	2:C:232:IOD:I	2.91	0.41
1:C:198:CYS:O	1:C:202:LEU:HG	2.21	0.41
1:C:162:ARG:HG3	1:C:215:MET:HE1	2.03	0.41
1:E:157:PRO:HD2	2:E:233:IOD:I	2.91	0.41
1:B:30:LYS:HE2	1:B:35:GLU:OE2	2.21	0.40
1:B:155:GLN:HG2	1:B:156:GLY:O	2.21	0.40
1:D:170:LYS:CD	2:D:233:IOD:I	3.40	0.40
1:A:85:PRO:O	1:A:86:VAL:C	2.57	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	206/231 (89%)	200 (97%)	6 (3%)	0	100	100
1	B	205/231 (89%)	196 (96%)	8 (4%)	1 (0%)	24	43
1	C	205/231 (89%)	199 (97%)	6 (3%)	0	100	100
1	D	200/231 (87%)	195 (98%)	5 (2%)	0	100	100
1	E	193/231 (84%)	187 (97%)	6 (3%)	0	100	100
All	All	1009/1155 (87%)	977 (97%)	31 (3%)	1 (0%)	48	68

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	11	VAL

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	172/193 (89%)	168 (98%)	4 (2%)	44	72
1	B	170/193 (88%)	166 (98%)	4 (2%)	43	70
1	C	170/193 (88%)	168 (99%)	2 (1%)	63	83
1	D	171/193 (89%)	168 (98%)	3 (2%)	51	77
1	E	166/193 (86%)	162 (98%)	4 (2%)	43	70
All	All	849/965 (88%)	832 (98%)	17 (2%)	48	75

All (17) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	16	SER
1	A	21	CYS
1	A	28	GLU
1	A	124	ILE
1	B	4	GLN
1	B	16	SER
1	B	83	LEU
1	B	124	ILE
1	C	16	SER
1	C	124	ILE
1	D	16	SER
1	D	28	GLU
1	D	124	ILE
1	E	16	SER
1	E	124	ILE
1	E	131	LYS
1	E	192	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (6) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	12	HIS

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Mol	Chain	Res	Type
1	B	67	GLN
1	C	12	HIS
1	C	50	GLN
1	C	192	GLN
1	E	193	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 10 ligands modelled in this entry, 10 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

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, 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	210/231 (90%)	0.70	22 (10%)	11 10	38, 64, 99, 136	0
1	B	209/231 (90%)	0.79	27 (12%)	7 6	39, 64, 95, 106	0
1	C	209/231 (90%)	0.62	15 (7%)	21 19	36, 63, 94, 107	0
1	D	206/231 (89%)	0.72	18 (8%)	16 14	38, 63, 93, 105	0
1	E	199/231 (86%)	0.62	10 (5%)	34 30	39, 62, 94, 106	0
All	All	1033/1155 (89%)	0.69	92 (8%)	15 13	36, 63, 96, 136	0

All (92) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	E	177	ALA	5.7
1	A	86	VAL	5.6
1	B	157	PRO	5.6
1	B	175	GLU	4.8
1	A	88	ALA	3.9
1	B	124	ILE	3.8
1	C	85	PRO	3.6
1	A	209	ALA	3.6
1	E	181	VAL	3.6
1	C	15	ILE	3.5
1	B	6	LEU	3.5
1	D	157	PRO	3.4
1	D	198	CYS	3.4
1	B	158	LYS	3.4
1	C	12	HIS	3.3
1	A	15	ILE	3.1
1	C	176	GLN	3.1
1	D	178	SER	3.0
1	B	12	HIS	3.0
1	B	156	GLY	3.0

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Mol	Chain	Res	Type	RSRZ
1	D	188	THR	3.0
1	B	219	GLN	2.9
1	A	207	PRO	2.9
1	E	85	PRO	2.9
1	B	181	VAL	2.9
1	B	85	PRO	2.9
1	A	157	PRO	2.8
1	E	144	MET	2.8
1	A	79	GLU	2.8
1	D	181	VAL	2.8
1	D	85	PRO	2.8
1	D	143	ARG	2.8
1	D	156	GLY	2.7
1	D	177	ALA	2.7
1	B	96	MET	2.7
1	E	2	ILE	2.7
1	A	202	LEU	2.7
1	B	3	VAL	2.7
1	D	176	GLN	2.7
1	A	2	ILE	2.6
1	A	187	GLU	2.6
1	B	178	SER	2.6
1	E	151	LEU	2.6
1	D	203	LYS	2.6
1	A	145	TYR	2.6
1	B	207	PRO	2.5
1	B	205	LEU	2.5
1	C	177	ALA	2.5
1	A	83	LEU	2.5
1	B	122	PRO	2.5
1	B	197	ASP	2.5
1	E	180	GLU	2.4
1	A	168	PHE	2.4
1	E	178	SER	2.4
1	B	180	GLU	2.4
1	B	177	ALA	2.4
1	A	85	PRO	2.4
1	E	147	PRO	2.4
1	C	178	SER	2.4
1	C	2	ILE	2.4
1	C	11	VAL	2.4
1	B	188	THR	2.3

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Mol	Chain	Res	Type	RSRZ
1	B	11	VAL	2.3
1	D	121	ASN	2.3
1	A	87	HIS	2.3
1	B	145	TYR	2.3
1	C	154	ARG	2.3
1	C	180	GLU	2.3
1	D	29	GLU	2.3
1	B	2	ILE	2.2
1	C	181	VAL	2.2
1	A	188	THR	2.2
1	B	186	THR	2.2
1	D	31	ALA	2.2
1	A	219	GLN	2.2
1	B	202	LEU	2.2
1	C	96	MET	2.2
1	A	181	VAL	2.1
1	D	11	VAL	2.1
1	C	208	GLY	2.1
1	A	93	PRO	2.1
1	D	207	PRO	2.1
1	D	206	GLY	2.1
1	C	187	GLU	2.1
1	A	153	ILE	2.1
1	C	158	LYS	2.1
1	A	189	LEU	2.0
1	A	203	LYS	2.0
1	E	176	GLN	2.0
1	B	184	ALA	2.0
1	B	101	GLY	2.0
1	D	186	THR	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(Å ²)	Q<0.9
2	IOD	E	233	1/1	0.76	0.19	189,189,189,189	0
2	IOD	A	235	1/1	0.88	0.15	173,173,173,173	0
2	IOD	D	232	1/1	0.89	0.14	162,162,162,162	0
2	IOD	A	233	1/1	0.93	0.17	170,170,170,170	0
2	IOD	A	232	1/1	0.96	0.24	133,133,133,133	0
2	IOD	C	232	1/1	0.96	0.22	130,130,130,130	0
2	IOD	A	234	1/1	0.98	0.10	76,76,76,76	0
2	IOD	D	233	1/1	0.99	0.05	67,67,67,67	0
2	IOD	E	232	1/1	0.99	0.12	80,80,80,80	0
2	IOD	B	232	1/1	0.99	0.06	58,58,58,58	0

6.5 Other polymers [i](#)

There are no such residues in this entry.