



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 19, 2016 – 10:32 PM GMT

PDB ID : 5CYM
Title : HIV-1 reverse transcriptase complexed with 4-iodopyrazole
Authors : Bauman, J.D.; Arnold, E.
Deposited on : 2015-07-30
Resolution : 2.10 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
<http://wwpdb.org/validation/2016/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
Mogul : 1.7.1 (RC1), CSD as537be (2016)
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

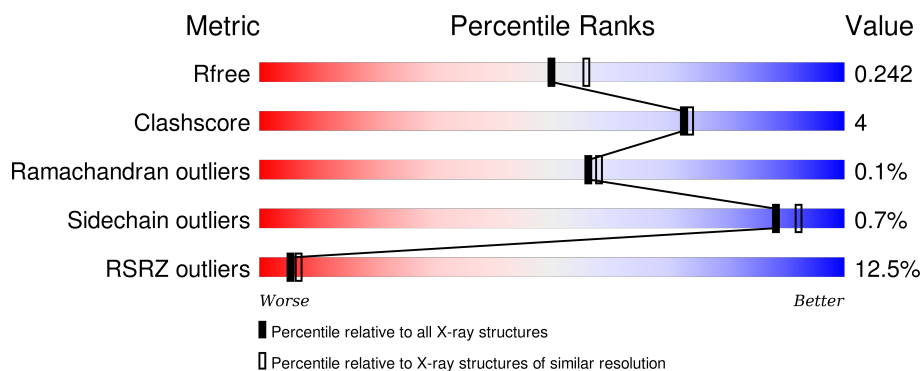
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.10 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	3939 (2.10-2.10)
Clashscore	102246	4460 (2.10-2.10)
Ramachandran outliers	100387	4413 (2.10-2.10)
Sidechain outliers	100360	4414 (2.10-2.10)
RSRZ outliers	91569	3948 (2.10-2.10)

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 ≥ 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	557	<div> <div>12%</div> <div>90%</div> <div>8%</div> <div>.</div> </div>
2	B	428	<div> <div>13%</div> <div>86%</div> <div>9%</div> <div>5%</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	SO4	B	501	-	-	-	X
5	EDO	A	605	-	-	-	X
5	EDO	A	606	-	-	-	X
5	EDO	B	502	-	-	-	X
5	EDO	B	503	-	-	-	X
6	IOD	A	608	-	-	-	X
6	IOD	A	613	-	-	X	-
6	IOD	A	614	-	-	X	-
6	IOD	A	615	-	-	X	-
6	IOD	A	616	-	-	X	-
7	PYZ	A	618	-	-	-	X
7	PYZ	B	509	-	-	-	X
7	PYZ	B	510	-	-	-	X
7	PYZ	B	511	-	-	-	X
8	DMS	A	619	-	-	-	X
8	DMS	B	512	-	-	-	X
8	DMS	B	513	-	-	-	X
8	DMS	B	514	-	-	-	X
8	DMS	B	515	-	-	-	X

2 Entry composition

There are 9 unique types of molecules in this entry. The entry contains 16183 atoms, of which 7992 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 reverse transcriptase, p66 subunit.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	546	Total	C	H	N	O	S	0	1	0
			8935	2878	4493	737	819	8			

There are 5 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-1	MET	-	expression tag	UNP P03366
A	0	VAL	-	expression tag	UNP P03366
A	172	ALA	LYS	engineered mutation	UNP P03366
A	173	ALA	LYS	engineered mutation	UNP P03366
A	280	SER	CYS	engineered mutation	UNP P03366

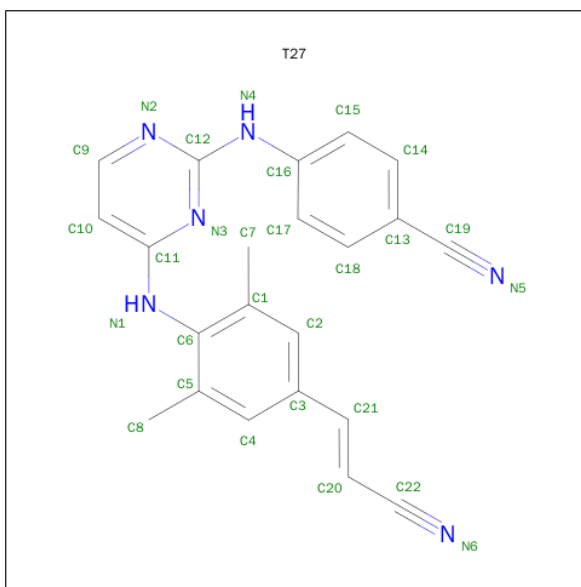
- Molecule 2 is a protein called HIV-1 reverse transcriptase, p51 subunit.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
2	B	408	Total	C	H	N	O	S	0	2	0
			6788	2201	3409	559	612	7			

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	280	SER	CYS	engineered mutation	UNP P03366

- Molecule 3 is 4-([4-([4-[(E)-2-cyanoethenyl]-2,6-dimethylphenyl]amino)pyrimidin-2-yl]amino)benzonitrile (three-letter code: T27) (formula: C₂₂H₁₈N₆).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	H	N	0	0
			46	22	18	6		

- Molecule 4 is SULFATE ION (three-letter code: SO4) (formula: O₄S).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	O	S	0	0
			5	4	1		
4	A	1	Total	O	S	0	0
			5	4	1		
4	A	1	Total	O	S	0	0
			5	4	1		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	B	1	Total	O	S	0	0
			5	4	1		

- Molecule 5 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: $C_2H_6O_2$).

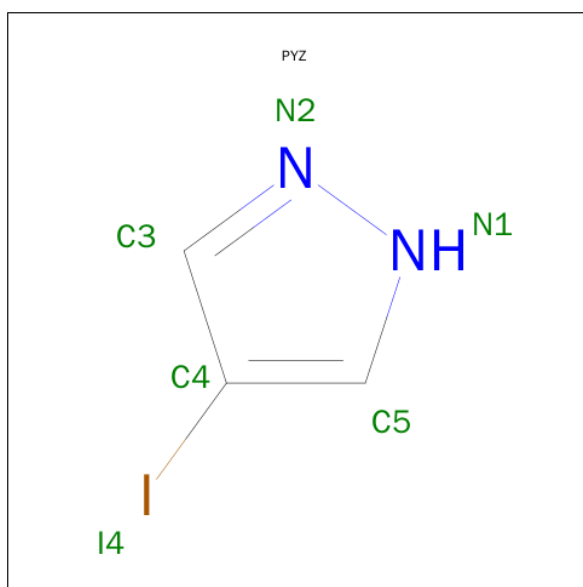


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	A	1	Total	C	H	O	0	0
			10	2	6	2		
5	A	1	Total	C	H	O	0	0
			10	2	6	2		
5	B	1	Total	C	H	O	0	0
			10	2	6	2		
5	B	1	Total	C	H	O	0	0
			10	2	6	2		

- Molecule 6 is IODIDE ION (three-letter code: IOD) (formula: I).

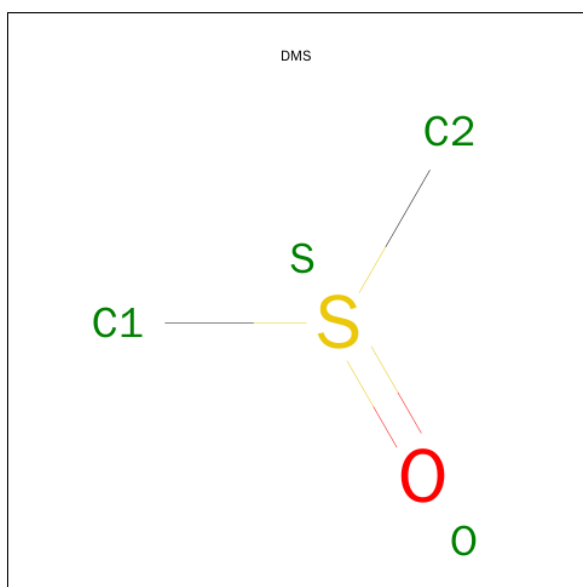
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	B	4	Total	I	0	0
			4	4		
6	A	10	Total	I	0	0
			10	10		

- Molecule 7 is 4-IODOPYRAZOLE (three-letter code: PYZ) (formula: $C_3H_3IN_2$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
7	A	1	Total	C	H	I	N	0	0
			9	3	3	1	2		
7	A	1	Total	C	H	I	N	0	0
			9	3	3	1	2		
7	B	1	Total	C	H	I	N	0	0
			9	3	3	1	2		
7	B	1	Total	C	H	I	N	0	0
			9	3	3	1	2		
7	B	1	Total	C	H	I	N	0	0
			9	3	3	1	2		

- Molecule 8 is DIMETHYL SULFOXIDE (three-letter code: DMS) (formula: C₂H₆OS).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
8	A	1	Total	C	H	O	S	0	0
			10	2	6	1	1		
8	B	1	Total	C	H	O	S	0	0
			10	2	6	1	1		
8	B	1	Total	C	H	O	S	0	0
			10	2	6	1	1		
8	B	1	Total	C	H	O	S	0	0
			10	2	6	1	1		
8	B	1	Total	C	H	O	S	0	0
			10	2	6	1	1		

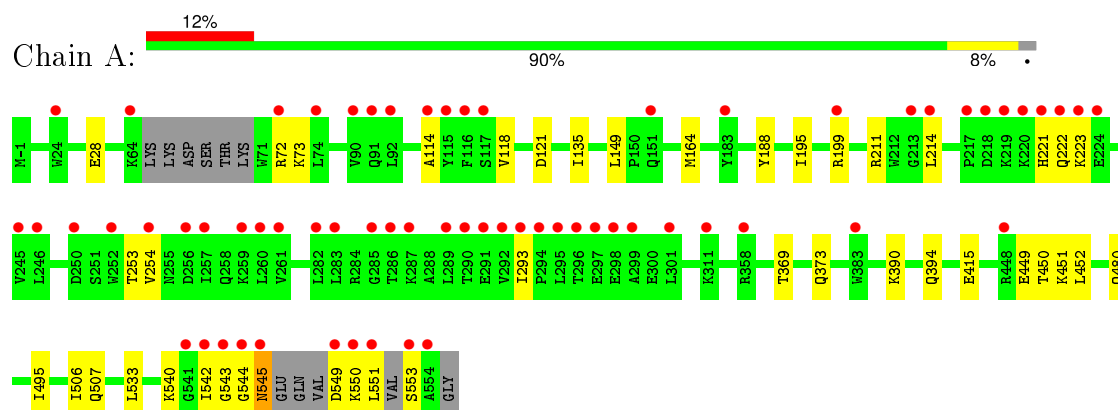
- Molecule 9 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
9	A	150	Total	O	0	0
			150	150		
9	B	86	Total	O	0	0
			86	86		

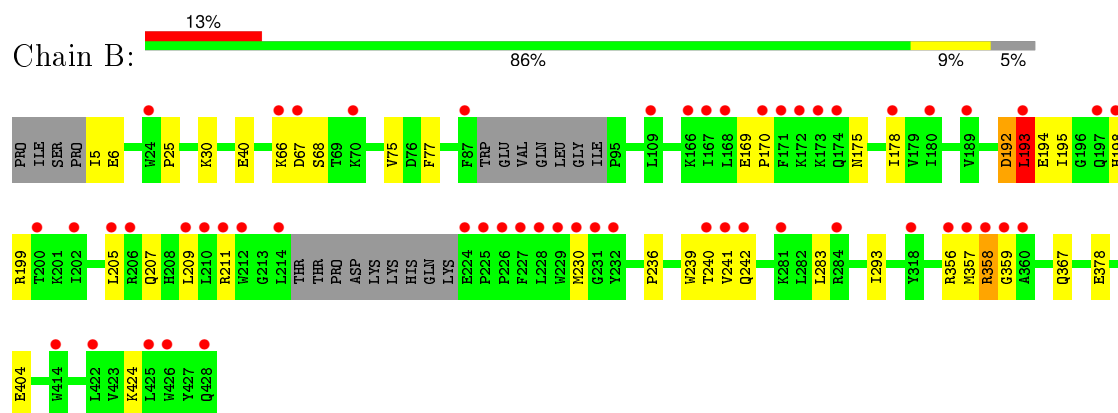
3 Residue-property plots

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: HIV-1 reverse transcriptase, p66 subunit



- Molecule 2: HIV-1 reverse transcriptase, p51 subunit



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	162.84Å 73.48Å 109.58Å 90.00° 100.67° 90.00°	Depositor
Resolution (Å)	43.17 – 2.10 43.59 – 2.10	Depositor EDS
% Data completeness (in resolution range)	98.4 (43.17-2.10) 98.2 (43.59-2.10)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.76 (at 2.10Å)	Xtriage
Refinement program	PHENIX (phenix.refine: dev_1988)	Depositor
R, R_{free}	0.195 , 0.229 0.214 , 0.242	Depositor DCC
R_{free} test set	3729 reflections (5.36%)	DCC
Wilson B-factor (Å ²)	43.9	Xtriage
Anisotropy	0.039	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.38 , 49.7	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Outliers	0 of 73508 reflections	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	16183	wwPDB-VP
Average B, all atoms (Å ²)	72.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.88% 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, 0.375 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: PYZ, EDO, DMS, SO4, IOD, T27

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	0.33	0/4560	0.46	0/6196
2	B	0.34	0/3484	0.51	3/4730 (0.1%)
All	All	0.34	0/8044	0.48	3/10926 (0.0%)

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
2	B	0	1

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	193	LEU	CB-CG-CD2	-7.78	97.77	111.00
2	B	192	ASP	N-CA-C	-6.11	94.51	111.00
2	B	193	LEU	CA-CB-CG	5.63	128.25	115.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	B	193	LEU	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	4442	4493	4490	34	0
2	B	3379	3409	3394	32	0
3	A	28	18	18	2	0
4	A	15	0	0	0	0
4	B	5	0	0	1	0
5	A	8	12	12	0	0
5	B	8	12	12	0	0
6	A	10	0	0	9	0
6	B	4	0	0	0	0
7	A	12	6	6	0	0
7	B	24	12	12	1	0
8	A	4	6	6	0	0
8	B	16	24	24	1	0
9	A	150	0	0	4	0
9	B	86	0	0	3	0
All	All	8191	7992	7974	67	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 4.

All (67) 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)
2:B:192:ASP:O	2:B:193:LEU:HB2	1.76	0.84
1:A:543:GLY:N	2:B:283:LEU:O	2.09	0.84
6:A:614:IOD:I	6:A:615:IOD:I	3.36	0.84
1:A:394:GLN:NE2	9:A:702:HOH:O	2.16	0.79
2:B:40:GLU:OE1	9:B:601:HOH:O	2.02	0.77
1:A:390:LYS:NZ	1:A:415:GLU:OE1	2.22	0.73
2:B:293:ILE:O	9:B:602:HOH:O	2.10	0.70
1:A:195:ILE:O	1:A:199:ARG:HG3	1.94	0.67
1:A:449:GLU:OE1	1:A:449:GLU:N	2.28	0.66
1:A:543:GLY:CA	2:B:283:LEU:O	2.44	0.65
2:B:193:LEU:HD22	2:B:198:HIS:HB2	1.77	0.64
2:B:193:LEU:HD23	2:B:194:GLU:C	2.20	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:121:ASP:OD1	9:A:701:HOH:O	2.16	0.61
6:A:613:IOD:I	6:A:616:IOD:I	3.59	0.60
2:B:25:PRO:HA	8:B:515:DMS:H11	1.82	0.60
1:A:506:ILE:HD11	1:A:533:LEU:HD23	1.83	0.60
1:A:222:GLN:O	1:A:222:GLN:NE2	2.34	0.60
1:A:543:GLY:HA3	2:B:283:LEU:O	2.01	0.59
1:A:506:ILE:CD1	1:A:533:LEU:HD23	2.34	0.57
2:B:240:THR:OG1	2:B:241:VAL:N	2.33	0.56
2:B:357:MET:HB3	2:B:367:GLN:HG2	1.88	0.55
1:A:549:ASP:O	6:A:616:IOD:I	2.95	0.55
1:A:544:GLY:O	6:A:615:IOD:I	2.95	0.55
2:B:30:LYS:NZ	9:B:603:HOH:O	2.39	0.54
1:A:480[B]:GLN:NE2	9:A:707:HOH:O	2.39	0.54
2:B:193:LEU:CD2	2:B:194:GLU:O	2.56	0.54
1:A:506:ILE:HG13	1:A:507:GLN:N	2.24	0.53
2:B:236:PRO:HA	2:B:239:TRP:CD2	2.45	0.52
2:B:193:LEU:CD2	2:B:198:HIS:HB2	2.40	0.51
1:A:553:SER:N	6:A:616:IOD:I	3.14	0.51
2:B:192:ASP:O	2:B:193:LEU:CB	2.55	0.51
2:B:193:LEU:HD21	2:B:194:GLU:O	2.11	0.50
1:A:450:THR:O	1:A:451:LYS:HG2	2.12	0.50
1:A:551:LEU:HD12	6:A:614:IOD:I	2.82	0.49
3:A:601:T27:H17	3:A:601:T27:N3	2.29	0.48
2:B:5:ILE:HD12	2:B:6:GLU:N	2.29	0.48
1:A:495:ILE:O	1:A:533:LEU:HD12	2.15	0.47
1:A:451:LYS:HG3	9:A:710:HOH:O	2.13	0.47
2:B:205:LEU:O	2:B:209:LEU:CD1	2.62	0.47
2:B:68:SER:HB2	2:B:230:MET:CE	2.45	0.46
2:B:207:GLN:O	2:B:211:ARG:HG3	2.15	0.46
2:B:66:LYS:NZ	2:B:67:ASP:OD1	2.49	0.46
1:A:369:THR:O	1:A:373:GLN:HG2	2.17	0.45
2:B:205:LEU:O	2:B:209:LEU:HD13	2.17	0.45
1:A:545:ASN:HA	6:A:615:IOD:I	2.87	0.45
2:B:358:ARG:HD2	2:B:359:GLY:N	2.32	0.44
1:A:450:THR:HG23	1:A:452:LEU:H	1.82	0.44
1:A:118:VAL:HG11	1:A:149:LEU:HD11	1.99	0.44
2:B:195:ILE:HD11	2:B:199:ARG:CZ	2.48	0.44
1:A:164:MET:HE2	1:A:164:MET:HB2	1.85	0.43
1:A:28:GLU:HG3	1:A:135:ILE:HD12	2.00	0.43
1:A:254:VAL:HG23	1:A:293:ILE:HD11	2.00	0.43
2:B:175:ASN:HB3	2:B:178:ILE:HG12	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:30:LYS:NZ	2:B:404:GLU:OE2	2.48	0.42
1:A:221:HIS:HD2	1:A:223:LYS:H	1.68	0.42
1:A:540:LYS:HB2	1:A:542:ILE:CD1	2.50	0.42
6:A:613:IOD:I	6:A:614:IOD:I	3.77	0.42
2:B:424:LYS:NZ	4:B:501:SO4:O3	2.52	0.42
1:A:188:TYR:CD1	3:A:601:T27:H20	2.55	0.42
2:B:75:VAL:HG11	2:B:77:PHE:CZ	2.55	0.41
2:B:169:GLU:HB3	2:B:170:PRO:HD3	2.03	0.41
1:A:549:ASP:HA	6:A:616:IOD:I	2.90	0.41
1:A:253:THR:O	1:A:254:VAL:C	2.59	0.41
1:A:72:ARG:HG3	1:A:73:LYS:N	2.36	0.41
2:B:68:SER:HB2	2:B:230:MET:HE1	2.03	0.40
2:B:378:GLU:CG	7:B:511:PYZ:HN1	2.35	0.40
1:A:114:ALA:HA	1:A:214:LEU:HD22	2.03	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	539/557 (97%)	527 (98%)	12 (2%)	0	100	100
2	B	404/428 (94%)	392 (97%)	11 (3%)	1 (0%)	52	53
All	All	943/985 (96%)	919 (98%)	23 (2%)	1 (0%)	56	58

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	193	LEU

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	486/495 (98%)	483 (99%)	3 (1%)	90	94
2	B	372/390 (95%)	369 (99%)	3 (1%)	86	91
All	All	858/885 (97%)	852 (99%)	6 (1%)	88	92

All (6) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	211	ARG
1	A	545	ASN
1	A	550	LYS
2	B	242	GLN
2	B	356	ARG
2	B	358	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

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 carbohydrates in this entry.

5.6 Ligand geometry [i](#)

Of 34 ligands modelled in this entry, 14 are monoatomic - leaving 20 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the chemical component dictionary. The Link column lists molecule types, if any, to which the group is linked. 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 $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# $ Z > 2$	Counts	RMSZ	# $ Z > 2$
3	T27	A	601	-	30,30,30	1.17	2 (6%)	39,40,40	1.84	7 (17%)
4	SO4	A	602	-	4,4,4	0.22	0	6,6,6	0.22	0
4	SO4	A	603	-	4,4,4	0.23	0	6,6,6	0.11	0
4	SO4	A	604	-	4,4,4	0.26	0	6,6,6	0.10	0
5	EDO	A	605	-	3,3,3	0.45	0	2,2,2	0.33	0
5	EDO	A	606	-	3,3,3	0.50	0	2,2,2	0.34	0
7	PYZ	A	617	-	6,6,6	2.65	3 (50%)	1,7,7	0.07	0
7	PYZ	A	618	-	6,6,6	2.46	3 (50%)	1,7,7	0.29	0
8	DMS	A	619	-	3,3,3	0.63	0	3,3,3	0.65	0
4	SO4	B	501	-	4,4,4	0.23	0	6,6,6	0.12	0
5	EDO	B	502	-	3,3,3	0.43	0	2,2,2	0.35	0
5	EDO	B	503	-	3,3,3	0.42	0	2,2,2	0.31	0
7	PYZ	B	508	-	6,6,6	2.41	3 (50%)	1,7,7	0.42	0
7	PYZ	B	509	-	6,6,6	2.41	3 (50%)	1,7,7	0.52	0
7	PYZ	B	510	-	6,6,6	2.39	3 (50%)	1,7,7	0.31	0
7	PYZ	B	511	-	6,6,6	2.40	3 (50%)	1,7,7	0.38	0
8	DMS	B	512	-	3,3,3	0.69	0	3,3,3	0.51	0
8	DMS	B	513	-	3,3,3	0.64	0	3,3,3	0.45	0
8	DMS	B	514	-	3,3,3	0.67	0	3,3,3	0.48	0
8	DMS	B	515	-	3,3,3	0.63	0	3,3,3	0.48	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the chemical component dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	T27	A	601	-	-	0/13/14/14	0/3/3/3
4	SO4	A	602	-	-	0/0/0/0	0/0/0/0
4	SO4	A	603	-	-	0/0/0/0	0/0/0/0
4	SO4	A	604	-	-	0/0/0/0	0/0/0/0
5	EDO	A	605	-	-	0/1/1/1	0/0/0/0
5	EDO	A	606	-	-	0/1/1/1	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
7	PYZ	A	617	-	-	0/0/0/0	0/1/1/1
7	PYZ	A	618	-	-	0/0/0/0	0/1/1/1
8	DMS	A	619	-	-	0/0/0/0	0/0/0/0
4	SO4	B	501	-	-	0/0/0/0	0/0/0/0
5	EDO	B	502	-	-	0/1/1/1	0/0/0/0
5	EDO	B	503	-	-	0/1/1/1	0/0/0/0
7	PYZ	B	508	-	-	0/0/0/0	0/1/1/1
7	PYZ	B	509	-	-	0/0/0/0	0/1/1/1
7	PYZ	B	510	-	-	0/0/0/0	0/1/1/1
7	PYZ	B	511	-	-	0/0/0/0	0/1/1/1
8	DMS	B	512	-	-	0/0/0/0	0/0/0/0
8	DMS	B	513	-	-	0/0/0/0	0/0/0/0
8	DMS	B	514	-	-	0/0/0/0	0/0/0/0
8	DMS	B	515	-	-	0/0/0/0	0/0/0/0

All (20) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	A	617	PYZ	C4-I4	-3.16	2.01	2.10
7	B	509	PYZ	C4-I4	-2.17	2.04	2.10
7	B	511	PYZ	C4-I4	-2.15	2.04	2.10
7	B	510	PYZ	C5-N1	2.04	1.38	1.33
7	B	508	PYZ	C5-N1	2.04	1.38	1.33
7	A	618	PYZ	C5-N1	2.10	1.38	1.33
3	A	601	T27	C11-N1	2.70	1.43	1.38
7	B	511	PYZ	C5-C4	2.97	1.43	1.37
7	B	510	PYZ	C5-C4	3.05	1.43	1.37
7	A	617	PYZ	C5-C4	3.23	1.43	1.37
7	A	618	PYZ	C5-C4	3.28	1.43	1.37
7	B	508	PYZ	C5-C4	3.41	1.44	1.37
7	B	509	PYZ	C3-N2	3.63	1.41	1.33
7	B	509	PYZ	C5-C4	3.67	1.44	1.37
3	A	601	T27	C12-N4	3.92	1.43	1.36
7	B	511	PYZ	C3-N2	4.01	1.42	1.33
7	B	508	PYZ	C3-N2	4.09	1.42	1.33
7	A	617	PYZ	C3-N2	4.11	1.42	1.33
7	B	510	PYZ	C3-N2	4.14	1.42	1.33
7	A	618	PYZ	C3-N2	4.19	1.42	1.33

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
3	A	601	T27	C10-C9-N2	-4.38	118.74	123.88
3	A	601	T27	N2-C12-N3	-4.26	122.12	126.66
3	A	601	T27	C10-C11-N3	-2.67	118.40	123.22
3	A	601	T27	C6-N1-C11	-2.57	120.36	124.35
3	A	601	T27	C3-C4-C5	-2.46	119.46	122.19
3	A	601	T27	C12-N3-C11	2.25	120.57	116.61
3	A	601	T27	C9-N2-C12	6.50	120.44	115.42

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

4 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	601	T27	2	0
4	B	501	SO4	1	0
7	B	511	PYZ	1	0
8	B	515	DMS	1	0

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	546/557 (98%)	0.76	65 (11%) 6 8	32, 56, 110, 174	0
2	B	408/428 (95%)	0.93	54 (13%) 4 6	36, 60, 114, 154	0
All	All	954/985 (96%)	0.83	119 (12%) 5 7	32, 58, 112, 174	0

All (119) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	214	LEU	11.6
1	A	219	LYS	6.4
1	A	114	ALA	6.4
1	A	116	PHE	6.3
2	B	241	VAL	6.2
1	A	295	LEU	6.1
1	A	117	SER	6.0
2	B	212	TRP	6.0
1	A	24	TRP	6.0
1	A	223	LYS	5.9
1	A	285	GLY	5.9
1	A	257	ILE	5.8
1	A	544	GLY	5.7
1	A	260	LEU	5.6
1	A	220	LYS	5.5
2	B	66	LYS	5.5
2	B	209	LEU	5.5
2	B	227	PHE	5.4
1	A	221	HIS	5.4
1	A	222	GLN	5.2
2	B	229	TRP	5.0
1	A	554	ALA	5.0
2	B	226	PRO	5.0
2	B	87	PHE	4.9

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Mol	Chain	Res	Type	RSRZ
2	B	357	MET	4.8
1	A	301	LEU	4.8
1	A	550	LYS	4.7
2	B	168	LEU	4.7
1	A	287	LYS	4.5
1	A	290	THR	4.5
1	A	293	ILE	4.5
1	A	91	GLN	4.5
2	B	67	ASP	4.4
1	A	296	THR	4.4
2	B	170	PRO	4.3
1	A	551	LEU	4.3
2	B	425	LEU	4.2
1	A	72	ARG	4.2
1	A	549	ASP	4.1
1	A	294	PRO	4.1
2	B	202	ILE	4.1
1	A	298	GLU	3.9
1	A	358	ARG	3.9
1	A	542	ILE	3.9
2	B	210	LEU	3.8
1	A	245	VAL	3.8
1	A	282	LEU	3.8
1	A	254	VAL	3.8
2	B	225	PRO	3.7
2	B	242	GLN	3.7
1	A	297	GLU	3.6
1	A	543	GLY	3.6
1	A	545	ASN	3.6
1	A	292	VAL	3.6
1	A	553	SER	3.5
1	A	92	LEU	3.5
1	A	115	TYR	3.5
1	A	217	PRO	3.4
2	B	173	LYS	3.4
2	B	167	ILE	3.4
2	B	211	ARG	3.4
2	B	224	GLU	3.4
1	A	286	THR	3.4
2	B	228	LEU	3.3
1	A	218	ASP	3.2
1	A	289	LEU	3.2

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Mol	Chain	Res	Type	RSRZ
2	B	230	MET	3.2
2	B	206	ARG	3.1
1	A	246	LEU	3.1
1	A	214	LEU	3.1
1	A	250	ASP	3.0
1	A	252	TRP	3.0
2	B	205	LEU	3.0
1	A	151	GLN	2.9
1	A	224	GLU	2.9
2	B	284	ARG	2.9
2	B	180	ILE	2.8
2	B	281	LYS	2.8
1	A	74	LEU	2.8
2	B	358	ARG	2.8
1	A	283	LEU	2.8
2	B	422	LEU	2.7
1	A	259	LYS	2.7
2	B	428	GLN	2.7
1	A	541	GLY	2.7
1	A	64	LYS	2.7
1	A	299	ALA	2.7
2	B	318	TYR	2.6
2	B	171	PHE	2.6
2	B	200	THR	2.5
1	A	311	LYS	2.5
2	B	359	GLY	2.5
2	B	109	LEU	2.5
2	B	197	GLN	2.5
2	B	166	LYS	2.4
2	B	360	ALA	2.4
2	B	189	VAL	2.4
2	B	356	ARG	2.4
1	A	261	VAL	2.4
2	B	70	LYS	2.4
1	A	213	GLY	2.3
2	B	231	GLY	2.3
2	B	232	TYR	2.3
1	A	256	ASP	2.3
2	B	174	GLN	2.3
2	B	426	TRP	2.2
2	B	198	HIS	2.2
1	A	291	GLU	2.2

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Mol	Chain	Res	Type	RSRZ
2	B	240	THR	2.2
2	B	172	LYS	2.2
2	B	178	ILE	2.1
2	B	414	TRP	2.1
1	A	448	ARG	2.1
1	A	383	TRP	2.1
1	A	183	TYR	2.1
2	B	193	LEU	2.1
1	A	90	VAL	2.0
1	A	199	ARG	2.0
2	B	24	TRP	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, 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	LLDF	B-factors(Å ²)	Q<0.9
5	EDO	B	502	4/4	0.91	0.40	19.41	67,80,97,113	0
8	DMS	B	515	4/4	0.54	0.46	12.13	118,142,143,143	0
8	DMS	B	513	4/4	0.92	0.34	9.83	132,167,168,168	0
7	PYZ	B	510	6/6	0.82	0.40	9.07	136,146,173,176	0
7	PYZ	B	509	6/6	0.67	0.36	7.80	89,102,129,326	0
8	DMS	A	619	4/4	0.82	0.26	6.47	93,112,120,120	0
8	DMS	B	512	4/4	0.90	0.26	4.59	88,106,107,107	0
7	PYZ	A	618	6/6	0.47	0.27	4.08	112,119,144,258	0
5	EDO	A	605	4/4	0.97	0.19	3.90	57,72,80,96	0
5	EDO	B	503	4/4	0.92	0.22	3.22	54,66,88,97	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
5	EDO	A	606	4/4	0.81	0.31	3.12	67,87,109,109	0
7	PYZ	B	511	6/6	0.87	0.26	2.43	93,101,121,172	0
6	IOD	A	608	1/1	0.97	0.16	2.25	162,162,162,162	0
8	DMS	B	514	4/4	0.72	0.33	2.25	119,148,148,148	0
4	SO4	B	501	5/5	0.93	0.21	2.04	122,123,126,130	0
6	IOD	A	611	1/1	-0.11	0.36	1.09	389,389,389,389	0
3	T27	A	601	28/28	0.95	0.17	1.07	34,45,63,68	0
4	SO4	A	604	5/5	0.81	0.18	0.40	133,134,136,139	0
6	IOD	A	614	1/1	-0.05	0.18	-0.07	198,198,198,198	0
7	PYZ	B	508	6/6	0.95	0.15	-0.44	97,98,117,118	0
6	IOD	A	609	1/1	0.62	0.14	-0.52	153,153,153,153	0
4	SO4	A	602	5/5	0.93	0.12	-0.54	89,95,101,103	0
7	PYZ	A	617	6/6	0.95	0.13	-0.71	47,58,74,106	0
6	IOD	A	613	1/1	0.98	0.11	-0.82	100,100,100,100	0
6	IOD	A	616	1/1	0.66	0.13	-0.85	87,87,87,87	1
6	IOD	A	610	1/1	0.75	0.09	-0.89	182,182,182,182	0
6	IOD	A	607	1/1	0.96	0.12	-1.03	132,132,132,132	0
6	IOD	A	615	1/1	0.89	0.10	-1.09	73,73,73,73	1
4	SO4	A	603	5/5	0.82	0.14	-1.15	119,121,124,135	0
6	IOD	B	506	1/1	0.68	0.12	-1.28	216,216,216,216	0
6	IOD	B	504	1/1	0.93	0.08	-1.50	112,112,112,112	0
6	IOD	B	507	1/1	0.73	0.14	-1.57	198,198,198,198	0
6	IOD	B	505	1/1	0.88	0.07	-	160,160,160,160	0
6	IOD	A	612	1/1	0.78	0.13	-	229,229,229,229	0

6.5 Other polymers [i](#)

There are no such residues in this entry.