Full wwPDB X-ray Structure Validation Report (i)

Feb 1, 2016 – 05:05 PM GMT

PDB ID	:	4H4O
Title	:	Crystal Structure of HIV-1 Reverse Transcriptase (RT) in Complex with (E)-3-(3-(2-(2-(2,4-dioxo-3,4-dihydropyrimidin-1(2H)-yl)ethoxy)- 4-fluorophenoxy)-5-fluorophenyl)acrylonitrile (JLJ506), A Non-nucleoside inhibitor
Authors	:	Frey, K.M.; Anderson, K.S.
Deposited on	:	2012-09-17
Resolution	:	2.90 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
A user guide is available at
http://wwpdb.org/validation/2016/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The following versions of software and data (see references (1)) were used in the production of this report:

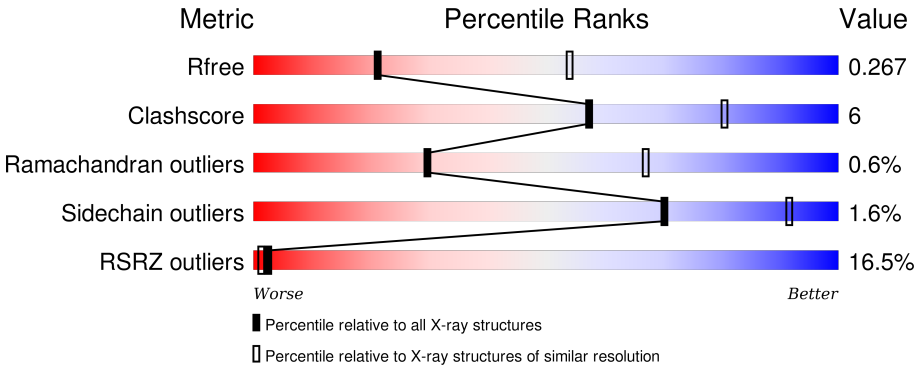
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	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 2.90 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	1451 (2.90-2.90)
Clashscore	102246	1668 (2.90-2.90)
Ramachandran outliers	100387	1630 (2.90-2.90)
Sidechain outliers	100360	1632 (2.90-2.90)
RSRZ outliers	91569	1456 (2.90-2.90)

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 >=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 <=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	17% 85% 13%
2	B	428	16% 82% 17%

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 8082 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 Reverse transcriptase/ribonuclease H, Exoribonuclease H, p66 RT.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	549	4465	2891	742	825	7	0	0	0

There are 5 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-1	MET	-	INITIATING METHIONINE	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

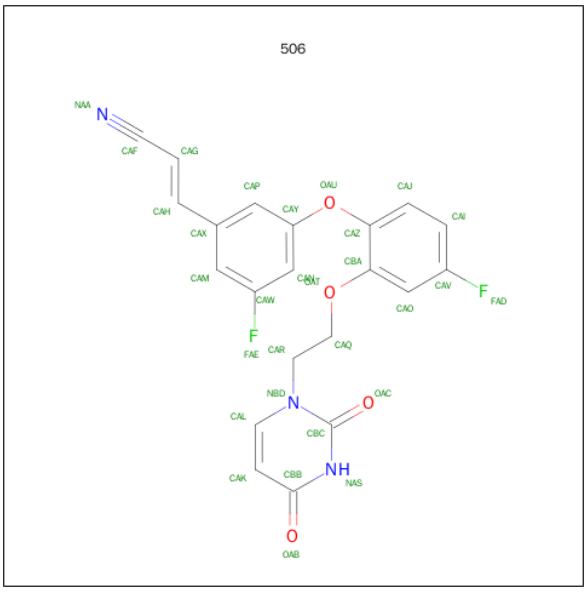
- Molecule 2 is a protein called Reverse transcriptase/ribonuclease H, Exoribonuclease H, p51 RT.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	B	428	3538	2305	586	640	7	0	0	0

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 (2E)-3-(3-{2-[2-(2,4-DIOXO-3,4-DIHYDROPYRIMIDIN-1(2H)-YL)ETHOXY]-4-FLUOROPHENOXY}-5-FLUOROPHENYL)PROP-2-ENENITRILE (three-letter code: 506) (formula: $C_{21}H_{15}F_2N_3O_4$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total C F N O 30 21 2 3 4	0	0

- Molecule 4 is water.

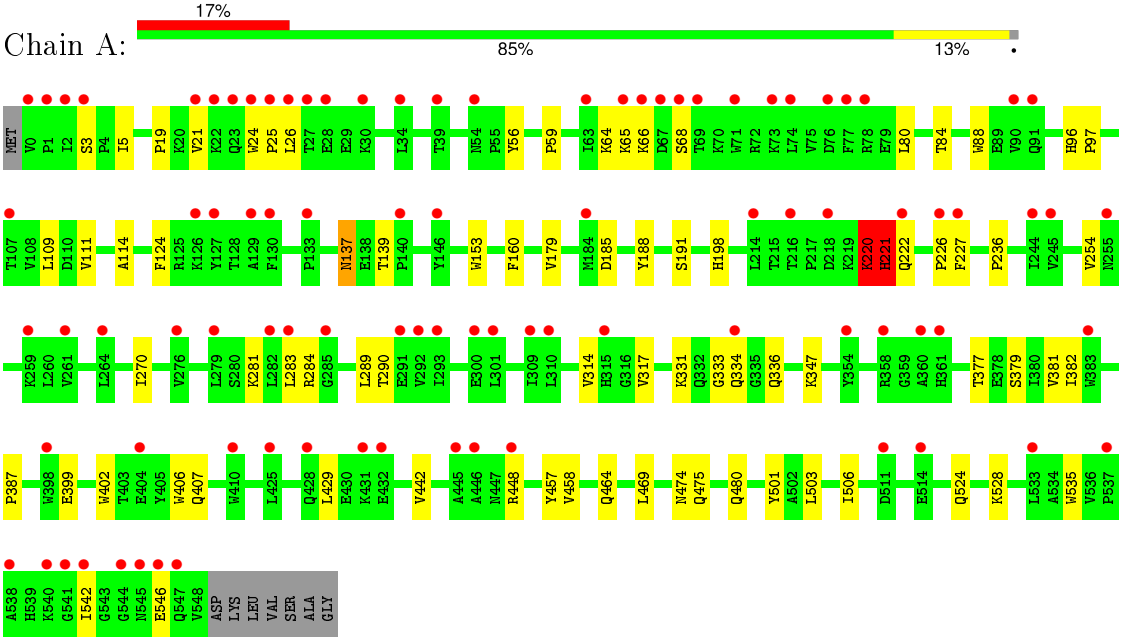
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	22	Total O 22 22	0	0
4	B	27	Total O 27 27	0	0

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.

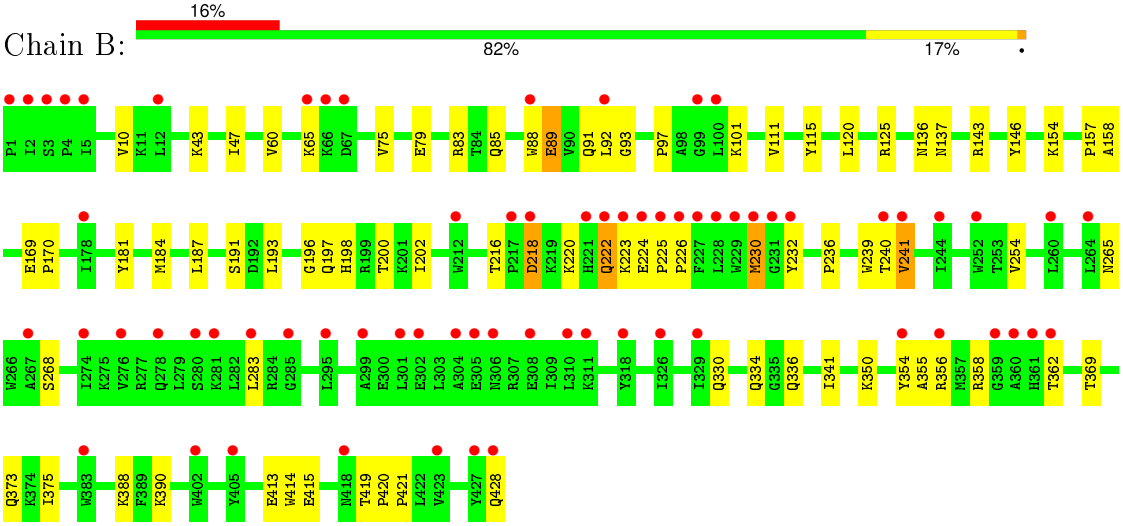
- Molecule 1: Reverse transcriptase/ribonuclease H, Exoribonuclease H, p66 RT

Chain A:



- Molecule 2: Reverse transcriptase/ribonuclease H, Exoribonuclease H, p51 RT

Chain B:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α, β, γ	225.45Å 69.58Å 104.40Å 90.00° 106.21° 90.00°	Depositor
Resolution (Å)	41.72 – 2.90 41.72 – 2.90	Depositor EDS
% Data completeness (in resolution range)	99.8 (41.72-2.90) 99.8 (41.72-2.90)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	0.07	Depositor
$< I/\sigma(I) >$ [1]	2.27 (at 2.90Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.8_1069)	Depositor
R, R_{free}	0.232 , 0.265 0.238 , 0.267	Depositor DCC
R_{free} test set	1998 reflections (6.10%)	DCC
Wilson B-factor (Å^2)	79.0	Xtriage
Anisotropy	0.256	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.27 , 113.0	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.33$	Xtriage
Outliers	0 of 34776 reflections	Xtriage
F_o,F_c correlation	0.93	EDS
Total number of atoms	8082	wwPDB-VP
Average B, all atoms (Å^2)	164.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.13% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ 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: 506

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	0.23	0/4583	0.45	0/6231
2	B	0.24	0/3643	0.48	1/4952 (0.0%)
All	All	0.24	0/8226	0.46	1/11183 (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
1	A	0	1
2	B	0	1
All	All	0	2

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	89	GLU	N-CA-C	-5.05	97.36	111.00

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	220	LYS	Peptide
2	B	419	THR	Peptide

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	4465	0	4516	49	0
2	B	3538	0	3576	52	0
3	A	30	0	15	2	0
4	A	22	0	0	0	1
4	B	27	0	0	1	0
All	All	8082	0	8107	96	1

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 6.

All (96) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:220:LYS:HB3	1:A:222:GLN:H	1.51	0.76
1:A:331:LYS:HE2	1:A:333:GLY:HA2	1.68	0.76
1:A:191:SER:OG	1:A:198:HIS:ND1	2.23	0.68
1:A:64:LYS:HD2	1:A:68:SER:HA	1.75	0.67
1:A:226:PRO:HA	1:A:227:PHE:HB2	1.77	0.66
1:A:317:VAL:HG11	1:A:347:LYS:HD3	1.79	0.65
2:B:137:ASN:O	4:B:505:HOH:O	2.15	0.64
2:B:336:GLN:HG2	2:B:355:ALA:HB2	1.80	0.63
1:A:84:THR:HG21	1:A:153:TRP:HE1	1.61	0.63
2:B:390:LYS:NZ	2:B:415:GLU:OE2	2.34	0.61
1:A:88:TRP:CE2	2:B:143:ARG:HD2	2.37	0.59
1:A:334:GLN:HB2	1:A:336:GLN:HE21	1.68	0.58
2:B:157:PRO:HG3	2:B:184:MET:HA	1.86	0.58
2:B:354:TYR:HB3	2:B:356:ARG:HH12	1.71	0.56
1:A:220:LYS:O	1:A:221:HIS:HB2	2.04	0.55
2:B:191:SER:OG	2:B:198:HIS:ND1	2.30	0.54
1:A:220:LYS:CB	1:A:222:GLN:H	2.20	0.54
1:A:270:ILE:HG13	1:A:314:VAL:HG13	1.90	0.54
2:B:91:GLN:HG2	2:B:92:LEU:HD12	1.88	0.53
2:B:111:VAL:HG11	2:B:187:LEU:HD22	1.90	0.52
1:A:399:GLU:HA	1:A:402:TRP:CD1	2.45	0.52
1:A:84:THR:HG22	1:A:124:PHE:HZ	1.75	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:236:PRO:HA	2:B:239:TRP:CG	2.46	0.51
1:A:88:TRP:CD2	2:B:143:ARG:HD2	2.46	0.51
2:B:79:GLU:OE2	2:B:83:ARG:NH1	2.44	0.50
1:A:281:LYS:HG3	1:A:284:ARG:HE	1.76	0.50
2:B:89:GLU:O	2:B:93:GLY:HA3	2.12	0.50
2:B:47:ILE:HG22	2:B:146:TYR:HA	1.93	0.50
2:B:97:PRO:HG3	2:B:181:TYR:HB2	1.94	0.49
2:B:239:TRP:O	2:B:350:LYS:HE2	2.13	0.49
2:B:92:LEU:HB3	2:B:158:ALA:HB1	1.95	0.48
1:A:220:LYS:HD2	1:A:220:LYS:HA	1.55	0.48
2:B:336:GLN:OE1	2:B:428:GLN:NE2	2.46	0.48
1:A:114:ALA:HB1	1:A:160:PHE:CE1	2.49	0.48
2:B:240:THR:OG1	2:B:241:VAL:N	2.46	0.48
2:B:254:VAL:HG13	2:B:283:LEU:HD22	1.96	0.48
2:B:334:GLN:O	2:B:358:ARG:NH1	2.47	0.47
1:A:19:PRO:O	1:A:56:TYR:HB3	2.14	0.47
1:A:475:GLN:HB3	1:A:501:TYR:CE2	2.49	0.47
1:A:254:VAL:HG13	1:A:283:LEU:HD11	1.96	0.47
1:A:236:PRO:HA	3:A:601:506:CBB	2.44	0.47
1:A:399:GLU:HA	1:A:402:TRP:NE1	2.29	0.47
2:B:120:LEU:HD23	2:B:125:ARG:HG2	1.98	0.46
2:B:88:TRP:N	2:B:88:TRP:CD1	2.84	0.46
2:B:354:TYR:HB3	2:B:356:ARG:NH1	2.29	0.46
1:A:111:VAL:HG23	1:A:114:ALA:HB2	1.98	0.46
1:A:65:LYS:HG2	1:A:66:LYS:H	1.80	0.46
2:B:193:LEU:HB3	2:B:197:GLN:HG3	1.98	0.45
2:B:222:GLN:HB3	2:B:223:LYS:H	1.59	0.45
2:B:420:PRO:HA	2:B:421:PRO:HD3	1.65	0.45
1:A:21:VAL:HB	1:A:59:PRO:HD3	1.98	0.45
1:A:448:ARG:HE	1:A:474:ASN:ND2	2.15	0.45
1:A:25:PRO:HA	1:A:26:LEU:HA	1.72	0.45
1:A:442:VAL:HG12	1:A:457:TYR:HB3	1.99	0.45
1:A:406:TRP:CH2	2:B:420:PRO:HD2	2.52	0.45
2:B:115:TYR:OH	2:B:184:MET:O	2.33	0.45
1:A:406:TRP:CZ3	1:A:407:GLN:HG3	2.52	0.45
1:A:379:SER:CB	1:A:387:PRO:HD3	2.47	0.44
1:A:377:THR:O	1:A:381:VAL:HG23	2.17	0.44
1:A:111:VAL:HG22	1:A:185:ASP:O	2.17	0.44
1:A:254:VAL:HB	1:A:289:LEU:O	2.17	0.44
2:B:220:LYS:HD3	2:B:220:LYS:HA	1.68	0.44
2:B:265:ASN:O	2:B:268:SER:OG	2.27	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:19:PRO:HG3	1:A:80:LEU:HB2	1.98	0.44
2:B:236:PRO:HA	2:B:239:TRP:CD2	2.53	0.44
2:B:10:VAL:HG22	2:B:88:TRP:CH2	2.52	0.44
2:B:220:LYS:C	2:B:222:GLN:H	2.21	0.44
2:B:101:LYS:O	2:B:236:PRO:HB2	2.17	0.44
2:B:43:LYS:HE3	2:B:43:LYS:HB2	1.86	0.44
1:A:3:SER:HB3	1:A:5:ILE:HG13	2.00	0.43
1:A:188:TYR:CZ	3:A:601:506:H14	2.53	0.43
1:A:96:HIS:HA	1:A:97:PRO:HD3	1.92	0.43
2:B:341:ILE:HD11	2:B:375:ILE:HG23	2.00	0.43
1:A:469:LEU:HD11	1:A:480:GLN:HG2	2.00	0.43
2:B:60:VAL:HG12	2:B:75:VAL:HG22	1.99	0.43
2:B:369:THR:HG22	2:B:373:GLN:NE2	2.34	0.43
1:A:524:GLN:O	1:A:528:LYS:HG2	2.19	0.42
2:B:198:HIS:O	2:B:202:ILE:HG12	2.20	0.42
1:A:458:VAL:HA	1:A:464:GLN:HB3	2.01	0.42
1:A:429:LEU:HD11	1:A:506:ILE:HG22	2.02	0.42
1:A:24:TRP:N	1:A:25:PRO:HD2	2.35	0.42
1:A:503:LEU:HD22	1:A:535:TRP:HB2	2.01	0.42
2:B:224:GLU:HA	2:B:225:PRO:HD2	1.96	0.42
2:B:187:LEU:HA	2:B:187:LEU:HD12	1.90	0.41
1:A:382:ILE:O	2:B:136:ASN:HB2	2.20	0.41
1:A:458:VAL:HG22	1:A:464:GLN:HB3	2.01	0.41
1:A:406:TRP:CZ3	2:B:420:PRO:HD2	2.56	0.41
2:B:85:GLN:HG3	2:B:154:LYS:HB3	2.02	0.41
2:B:388:LYS:HD2	2:B:413:GLU:HB2	2.02	0.41
2:B:216:THR:O	2:B:218:ASP:N	2.49	0.41
2:B:169:GLU:HB3	2:B:170:PRO:HD3	2.03	0.41
2:B:196:GLY:O	2:B:200:THR:HG23	2.21	0.40
2:B:236:PRO:O	2:B:239:TRP:HB2	2.21	0.40
1:A:109:LEU:HD21	1:A:221:HIS:HE1	1.87	0.40
2:B:369:THR:HG22	2:B:373:GLN:HE21	1.85	0.40
2:B:220:LYS:HG3	2:B:230:MET:HG3	2.04	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:718:HOH:O	4:A:718:HOH:O[2_756]	2.16	0.04

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	547/557 (98%)	519 (95%)	24 (4%)	4 (1%)	26 63
2	B	426/428 (100%)	397 (93%)	27 (6%)	2 (0%)	34 71
All	All	973/985 (99%)	916 (94%)	51 (5%)	6 (1%)	30 67

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	221	HIS
1	A	220	LYS
1	A	137	ASN
2	B	226	PRO
1	A	542	ILE
2	B	65	LYS

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	489/495 (99%)	483 (99%)	6 (1%)	78 94
2	B	390/390 (100%)	382 (98%)	8 (2%)	61 88
All	All	879/885 (99%)	865 (98%)	14 (2%)	70 91

All (14) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	137	ASN
1	A	139	THR
1	A	179	VAL
1	A	221	HIS
1	A	290	THR
1	A	546	GLU
2	B	218	ASP
2	B	222	GLN
2	B	230	MET
2	B	232	TYR
2	B	241	VAL
2	B	330	GLN
2	B	362	THR
2	B	414	TRP

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

Mol	Chain	Res	Type
1	A	361	HIS
1	A	474	ASN
2	B	197	GLN
2	B	278	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 carbohydrates in this entry.

5.6 Ligand geometry (i)

1 ligand is modelled in this entry.

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	506	A	601	-	28,32,32	1.69	5 (17%)	35,43,43	2.55	11 (31%)

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	506	A	601	-	-	0/13/14/14	0/3/3/3

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	601	506	CAM-CAW	2.16	1.41	1.37
3	A	601	506	CAZ-CBA	2.47	1.45	1.40
3	A	601	506	CAR-CAQ	2.54	1.56	1.51
3	A	601	506	CAL-NBD	2.65	1.40	1.36
3	A	601	506	CBB-NAS	4.87	1.42	1.33

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	A	601	506	OAT-CBA-CAO	-3.90	114.45	123.72
3	A	601	506	CAK-CBB-NAS	-3.30	114.66	123.12
3	A	601	506	CAI-CAV-CAO	-2.14	120.59	123.35
3	A	601	506	CAI-CAJ-CAZ	2.06	124.00	120.03
3	A	601	506	CAQ-CAR-NBD	2.51	114.64	110.94
3	A	601	506	OAU-CAZ-CBA	2.54	124.08	117.53
3	A	601	506	CAL-CAK-CBB	2.54	122.04	117.28
3	A	601	506	CBA-CAO-CAV	2.72	122.31	116.24
3	A	601	506	CAX-CAP-CAY	3.27	122.62	119.88
3	A	601	506	OAT-CBA-CAZ	5.69	127.74	115.78
3	A	601	506	CBB-NAS-CBC	9.98	124.02	114.14

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	601	506	2	0

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^{th} 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	549/557 (98%)	1.07	92 (16%)	2 1	112, 157, 242, 303	1 (0%)
2	B	428/428 (100%)	1.26	69 (16%)	3 1	114, 148, 248, 369	1 (0%)
All	All	977/985 (99%)	1.16	161 (16%)	2 1	112, 154, 246, 369	2 (0%)

All (161) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	1	PRO	40.9
2	B	2	ILE	19.0
1	A	541	GLY	18.2
2	B	224	GLU	16.7
2	B	231	GLY	16.2
1	A	25	PRO	15.2
2	B	4	PRO	12.9
1	A	24	TRP	12.8
1	A	545	ASN	12.3
2	B	67	ASP	10.9
1	A	67	ASP	10.0
1	A	2	ILE	9.1
1	A	542	ILE	9.0
2	B	226	PRO	8.9
2	B	217	PRO	8.4
2	B	225	PRO	7.7
2	B	3	SER	7.5
2	B	229	TRP	7.3
2	B	66	LYS	7.1
2	B	221	HIS	7.1
2	B	228	LEU	6.9
2	B	227	PHE	6.7
2	B	428	GLN	6.5
2	B	361	HIS	6.4

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Mol	Chain	Res	Type	RSRZ
2	B	418	ASN	6.1
2	B	360	ALA	6.0
1	A	546	GLU	6.0
2	B	230	MET	5.9
1	A	448	ARG	5.7
1	A	26	LEU	5.7
2	B	310	LEU	5.7
2	B	301	LEU	5.5
2	B	354	TYR	5.4
1	A	22	LYS	5.1
1	A	264	LEU	5.0
1	A	68	SER	5.0
1	A	107	THR	4.9
2	B	88	TRP	4.8
2	B	5	ILE	4.8
1	A	28	GLU	4.8
1	A	227	PHE	4.7
2	B	283	LEU	4.6
2	B	218	ASP	4.6
1	A	226	PRO	4.6
1	A	21	VAL	4.6
1	A	360	ALA	4.6
2	B	299	ALA	4.6
1	A	354	TYR	4.5
1	A	54	ASN	4.5
1	A	133	PRO	4.5
2	B	311	LYS	4.5
1	A	255	ASN	4.4
1	A	77	PHE	4.4
1	A	283	LEU	4.4
1	A	63	ILE	4.4
1	A	129	ALA	4.3
1	A	130	PHE	4.3
1	A	0	VAL	4.3
1	A	261	VAL	4.0
1	A	514	GLU	4.0
1	A	309	ILE	3.9
1	A	358	ARG	3.9
2	B	304	ALA	3.9
2	B	295	LEU	3.9
2	B	326	ILE	3.9
1	A	291	GLU	3.7

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Mol	Chain	Res	Type	RSRZ
1	A	540	LYS	3.7
1	A	74	LEU	3.7
1	A	71	TRP	3.6
2	B	285	GLY	3.5
1	A	446	ALA	3.5
2	B	329	ILE	3.5
2	B	318	TYR	3.5
1	A	361	HIS	3.5
2	B	65	LYS	3.5
2	B	302	GLU	3.4
1	A	222	GLN	3.4
2	B	305	GLU	3.4
2	B	306	ASN	3.4
1	A	216	THR	3.4
1	A	282	LEU	3.3
1	A	30	LYS	3.3
2	B	232	TYR	3.3
1	A	245	VAL	3.2
1	A	431	LYS	3.2
1	A	91	GLN	3.2
2	B	359	GLY	3.1
1	A	78	ARG	3.1
1	A	140	PRO	3.0
1	A	538	ALA	3.0
1	A	293	ILE	3.0
1	A	410	TRP	3.0
1	A	3	SER	3.0
1	A	445	ALA	2.9
1	A	127	TYR	2.9
1	A	544	GLY	2.9
1	A	334	GLN	2.9
1	A	218	ASP	2.9
2	B	427	TYR	2.9
2	B	362	THR	2.8
2	B	264	LEU	2.8
1	A	300	GLU	2.8
2	B	423	VAL	2.7
2	B	405	TYR	2.7
1	A	126	LYS	2.7
1	A	404	GLU	2.7
1	A	279	LEU	2.7
1	A	511	ASP	2.7

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Mol	Chain	Res	Type	RSRZ
1	A	90	VAL	2.7
1	A	76	ASP	2.7
1	A	34	LEU	2.7
2	B	100	LEU	2.7
1	A	69	THR	2.7
2	B	276	VAL	2.7
2	B	356	ARG	2.7
1	A	292	VAL	2.6
1	A	285	GLY	2.6
2	B	241	VAL	2.6
1	A	398	TRP	2.6
1	A	315	HIS	2.6
1	A	244	ILE	2.6
2	B	281	LYS	2.5
1	A	276	VAL	2.5
1	A	259	LYS	2.5
2	B	280	SER	2.5
1	A	428	GLN	2.5
1	A	1	PRO	2.5
1	A	73	LYS	2.4
2	B	308	GLU	2.4
2	B	383	TRP	2.4
2	B	278	GLN	2.4
1	A	310	LEU	2.4
1	A	432	GLU	2.4
1	A	533	LEU	2.3
2	B	274	ILE	2.3
1	A	27	THR	2.3
2	B	222	GLN	2.3
1	A	65	LYS	2.3
1	A	66	LYS	2.3
1	A	425	LEU	2.3
2	B	178	ILE	2.2
1	A	184	MET	2.2
2	B	12	LEU	2.2
1	A	146	TYR	2.2
1	A	214	LEU	2.2
1	A	383	TRP	2.2
2	B	99	GLY	2.1
2	B	212	TRP	2.1
2	B	402	TRP	2.1
2	B	92	LEU	2.1

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Mol	Chain	Res	Type	RSRZ
2	B	240	THR	2.1
1	A	547	GLN	2.1
2	B	260	LEU	2.1
2	B	252	TRP	2.1
1	A	39	THR	2.1
1	A	23	GLN	2.1
1	A	301	LEU	2.1
1	A	537	PRO	2.0
2	B	244	ILE	2.0
2	B	223	LYS	2.0
2	B	267	ALA	2.0

6.2 Non-standard residues in protein, DNA, RNA chains (i)

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

6.3 Carbohydrates (i)

There are no carbohydrates in this entry.

6.4 Ligands (i)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95^{th} 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
3	506	A	601	30/30	0.79	0.39	1.47	125,145,153,160	0

6.5 Other polymers (i)

There are no such residues in this entry.