Full wwPDB X-ray Structure Validation Report (i)

Feb 1, 2016 – 06:08 PM GMT

PDB ID	:	4KO0
Title	:	CRYSTAL STRUCTURE OF HIV-1 REVERSE TRANSCRIPTASE (RT) IN COMPLEX WITH an anilinylpyrimidine derivative (JLJ-135)
Authors	:	Das, K.; Bauman, J.D.; Arnold, E.
Deposited on	:	2013-05-10
Resolution	:	1.95 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:

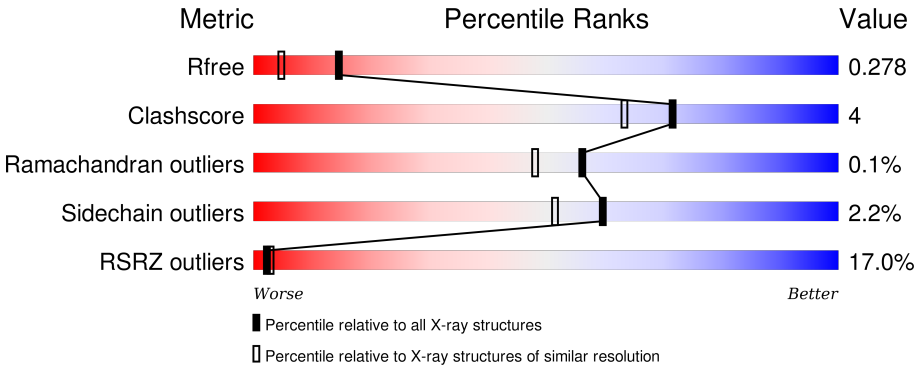
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	trunk26865

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 1.95 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	1833 (1.96-1.96)
Clashscore	102246	1953 (1.96-1.96)
Ramachandran outliers	100387	1936 (1.96-1.96)
Sidechain outliers	100360	1936 (1.96-1.96)
RSRZ outliers	91569	1835 (1.96-1.96)

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% 89% 10%
2	B	428	17% 86% 9%

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 8309 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 reverse transcriptase, p66 subunit.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	556	Total	C	N	O	S	0	2	0
			4521	2926	751	836	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

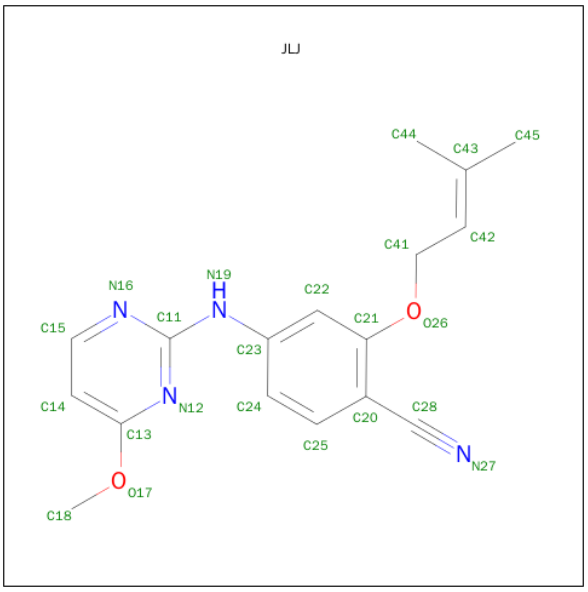
- Molecule 2 is a protein called HIV-1 reverse transcriptase, p51 subunit.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	410	Total	C	N	O	S	0	2	0
			3409	2221	564	617	7			

There is a discrepancy between the modelled and reference sequences:

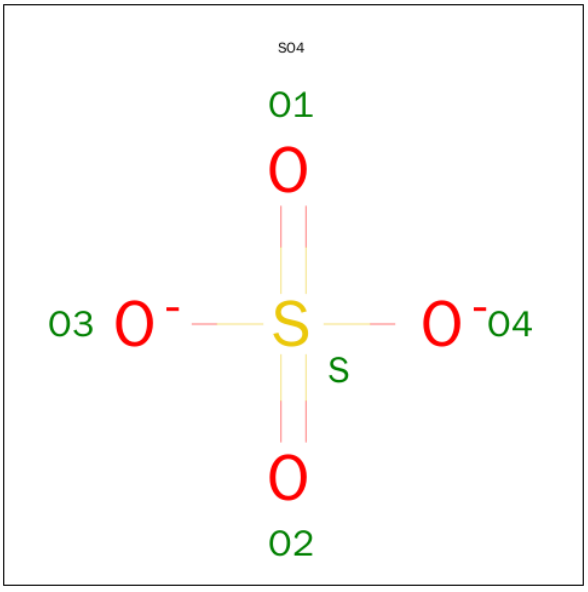
Chain	Residue	Modelled	Actual	Comment	Reference
B	280	SER	CYS	ENGINEERED MUTATION	UNP P03366

- Molecule 3 is 4-[(4-METHOXYPYRIMIDIN-2-YL)AMINO]-2-[(3-METHYLBUT-2-EN-1-YL)OXY]BENZONITRILE (three-letter code: JLJ) (formula: $C_{17}H_{18}N_4O_2$).



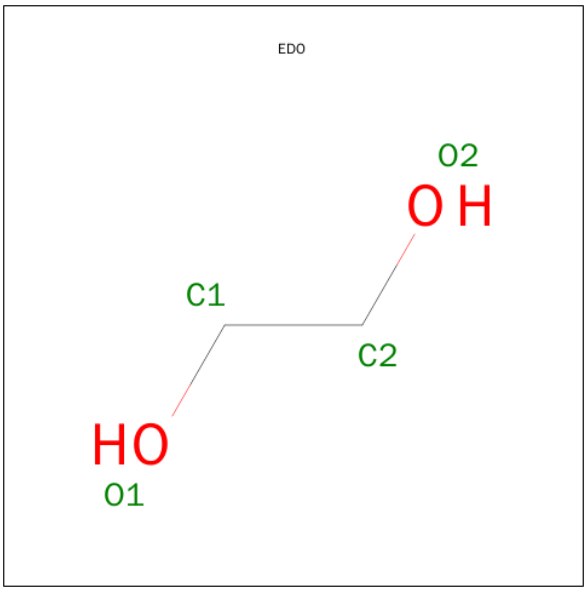
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	N	O	0	0
			23	17	4	2		

- Molecule 4 is SULFATE ION (three-letter code: SO4) (formula: O_4S).



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		

- 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 O 4 2 2	0	0
5	B	1	Total C O 4 2 2	0	0

- Molecule 6 is water.

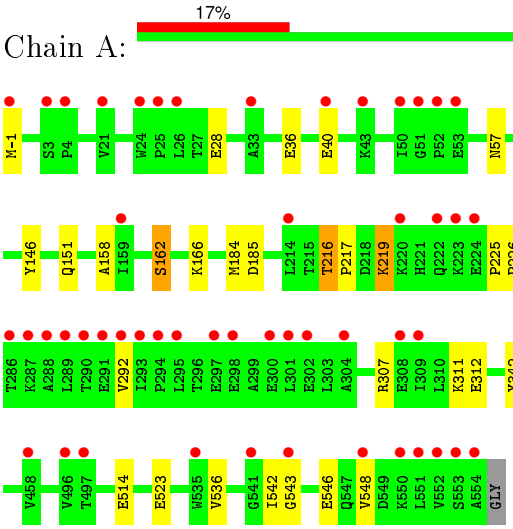
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	190	Total O 190 190	0	0
6	B	148	Total O 148 148	0	0

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.

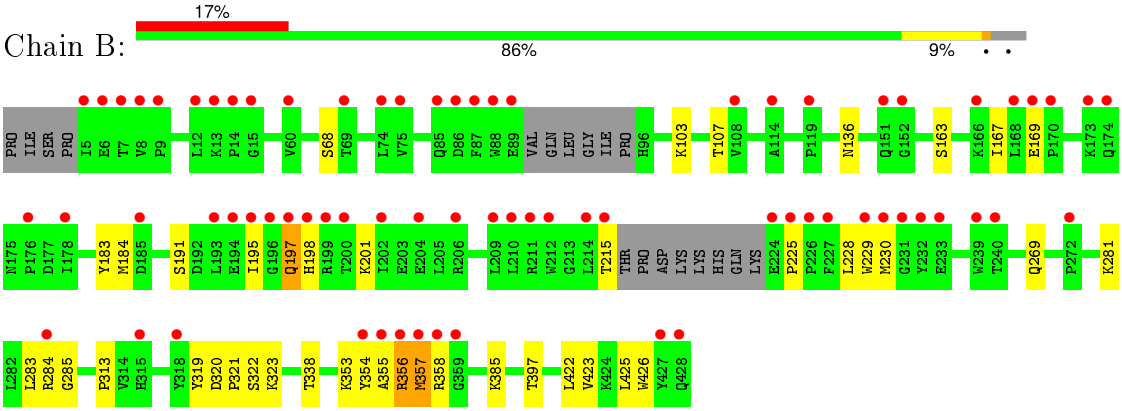
- Molecule 1: HIV-1 reverse transcriptase, p66 subunit

Chain A:



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

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	162.21Å 73.95Å 109.20Å 90.00° 100.23° 90.00°	Depositor
Resolution (Å)	29.31 – 1.95 29.46 – 1.95	Depositor EDS
% Data completeness (in resolution range)	98.8 (29.31-1.95) 98.7 (29.46-1.95)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.48 (at 1.95Å)	Xtriage
Refinement program	PHENIX (PHENIX.REFINE: 1.7.3_928)	Depositor
R, R_{free}	0.237 , 0.275 0.236 , 0.278	Depositor DCC
R_{free} test set	1863 reflections (2.08%)	DCC
Wilson B-factor (Å^2)	40.1	Xtriage
Anisotropy	0.145	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.37 , 55.5	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.33$	Xtriage
Outliers	0 of 91731 reflections	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	8309	wwPDB-VP
Average B, all atoms (Å^2)	56.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.67% 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: EDO, SO4, JLJ

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	0.45	0/4643	0.55	0/6311
2	B	0.40	0/3511	0.55	0/4768
All	All	0.43	0/8154	0.55	0/11079

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

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	4521	0	4576	40	0
2	B	3409	0	3427	35	0
3	A	23	0	18	2	0
4	A	10	0	0	0	0
5	A	4	0	6	0	0
5	B	4	0	6	0	0
6	A	190	0	0	3	0
6	B	148	0	0	2	0
All	All	8309	0	8033	69	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 (69) 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:356:ARG:H	2:B:356:ARG:HD2	1.17	1.08
1:A:543:GLY:HA3	2:B:285:GLY:H	1.43	0.82
2:B:356:ARG:N	2:B:356:ARG:HD2	1.98	0.79
2:B:355:ALA:H	2:B:356:ARG:HD2	1.51	0.76
2:B:320:ASP:HB3	2:B:323:LYS:HE2	1.76	0.68
1:A:253:THR:HG22	1:A:292:VAL:HG22	1.76	0.67
2:B:356:ARG:CD	2:B:356:ARG:H	1.98	0.67
2:B:323:LYS:O	2:B:385:LYS:NZ	2.29	0.66
1:A:404:GLU:HG3	6:A:849:HOH:O	1.96	0.65
1:A:373[A]:GLN:NE2	2:B:397:THR:OG1	2.28	0.65
1:A:73:LYS:NZ	1:A:146:TYR:OH	2.30	0.64
1:A:417:VAL:HG22	1:A:419:THR:HG23	1.81	0.62
1:A:28:GLU:HG3	1:A:135:ILE:HD12	1.82	0.59
1:A:216:THR:OG1	1:A:217:PRO:HD2	2.03	0.59
1:A:543:GLY:HA2	1:A:546:GLU:HB3	1.86	0.58
1:A:543:GLY:HA3	2:B:285:GLY:N	2.18	0.57
1:A:354:TYR:HD1	1:A:374:LYS:HE2	1.70	0.56
1:A:116:PHE:HE1	1:A:151:GLN:HE21	1.54	0.55
1:A:36:GLU:O	1:A:40:GLU:HG2	2.09	0.53
1:A:543:GLY:N	2:B:283:LEU:O	2.42	0.52
2:B:319:TYR:OH	2:B:385:LYS:HE2	2.11	0.50
2:B:358:ARG:HG2	2:B:358:ARG:O	2.11	0.50
1:A:281:LYS:HE3	1:A:284:ARG:NH2	2.27	0.50
2:B:313:PRO:O	6:B:696:HOH:O	2.20	0.49
1:A:57:ASN:OD1	1:A:143:ARG:NH1	2.44	0.49
2:B:163:SER:O	2:B:167:ILE:HG13	2.13	0.49
1:A:523:GLU:OE1	6:A:868:HOH:O	2.20	0.48
2:B:191:SER:HG	2:B:198:HIS:CE1	2.27	0.48
2:B:225:PRO:HG3	2:B:228:LEU:HD23	1.97	0.47
1:A:249:LYS:HB2	1:A:252:TRP:CE2	2.49	0.47
3:A:601:JLJ:N12	3:A:601:JLJ:H7	2.30	0.46
1:A:184:MET:O	6:A:873:HOH:O	2.20	0.46
2:B:354:TYR:HA	2:B:356:ARG:HH11	1.81	0.46
1:A:246:LEU:HD12	1:A:307:ARG:HG2	1.97	0.46
2:B:356:ARG:O	2:B:357:MET:HE3	2.16	0.45
2:B:423:VAL:HA	2:B:426:TRP:CD1	2.51	0.45
1:A:90:VAL:O	1:A:92:LEU:N	2.49	0.45
1:A:342:TYR:HA	1:A:349:LEU:HD13	1.97	0.45
1:A:255:ASN:O	1:A:259:LYS:HG3	2.17	0.45
1:A:543:GLY:HA3	2:B:284:ARG:HA	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:269:GLN:NE2	6:B:675:HOH:O	2.24	0.45
1:A:219:LYS:HB3	1:A:219:LYS:HE3	1.52	0.44
2:B:358:ARG:CG	2:B:358:ARG:O	2.65	0.44
1:A:443:ASP:HB2	1:A:548:VAL:HG13	2.00	0.44
2:B:195:ILE:HA	2:B:198:HIS:HB3	1.99	0.44
1:A:118:VAL:HA	1:A:119:PRO:HD3	1.83	0.44
2:B:107:THR:OG1	2:B:198:HIS:NE2	2.42	0.44
1:A:95:PRO:HA	2:B:136:ASN:O	2.17	0.43
2:B:68:SER:HB2	2:B:230:MET:HE1	2.01	0.43
1:A:363:ASN:OD1	1:A:363:ASN:C	2.56	0.43
1:A:225:PRO:HA	1:A:226:PRO:C	2.38	0.43
1:A:369:THR:O	1:A:373[B]:GLN:HG2	2.18	0.43
1:A:216:THR:OG1	1:A:217:PRO:CD	2.65	0.43
1:A:536:VAL:HB	1:A:542:ILE:HD13	2.00	0.43
1:A:253:THR:HA	1:A:292:VAL:HA	2.00	0.43
2:B:338:THR:HG22	2:B:353:LYS:HG3	2.01	0.43
1:A:236:PRO:HA	3:A:601:JLJ:H9	2.00	0.42
2:B:320:ASP:HA	2:B:321:PRO:HD2	1.85	0.42
2:B:197:GLN:O	2:B:201:LYS:HG2	2.21	0.41
1:A:70:LYS:HB2	1:A:70:LYS:HE3	1.94	0.41
2:B:103:LYS:HA	2:B:103:LYS:HD3	1.88	0.41
1:A:542:ILE:HG12	2:B:283:LEU:HD12	2.01	0.41
1:A:158:ALA:O	1:A:162:SER:OG	2.34	0.41
1:A:112:GLY:O	1:A:115:TYR:HB2	2.21	0.41
2:B:357:MET:HE2	2:B:357:MET:HA	2.02	0.41
2:B:183:TYR:CE2	2:B:184:MET:HG2	2.56	0.41
2:B:229:TRP:CH2	2:B:230:MET:HE3	2.55	0.40
1:A:311:LYS:HG3	1:A:312:GLU:N	2.36	0.40
2:B:355:ALA:N	2:B:356:ARG:HD2	2.25	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	555/557 (100%)	543 (98%)	11 (2%)	1 (0%)	52 43
2	B	406/428 (95%)	391 (96%)	15 (4%)	0	100 100
All	All	961/985 (98%)	934 (97%)	26 (3%)	1 (0%)	56 48

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	91	GLN

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	496/495 (100%)	486 (98%)	10 (2%)	63 55
2	B	374/390 (96%)	365 (98%)	9 (2%)	57 47
All	All	870/885 (98%)	851 (98%)	19 (2%)	60 51

All (19) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	-1	MET
1	A	115	TYR
1	A	162	SER
1	A	166	LYS
1	A	185	ASP
1	A	216	THR
1	A	219	LYS
1	A	363	ASN
1	A	374	LYS
1	A	514	GLU
2	B	169	GLU
2	B	197	GLN
2	B	215	THR
2	B	281	LYS
2	B	322	SER

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Mol	Chain	Res	Type
2	B	356	ARG
2	B	357	MET
2	B	422	LEU
2	B	425	LEU

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	151	GLN
1	A	161	GLN
1	A	182	GLN
2	B	161	GLN

5.3.3 RNA

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains

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

5.5 Carbohydrates

There are no carbohydrates in this entry.

5.6 Ligand geometry

5 ligands are 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	JLJ	A	601	-	24,24,24	1.42	3 (12%)	31,31,31	2.47	8 (25%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
4	SO4	A	602	-	4,4,4	0.06	0	6,6,6	0.14	0
4	SO4	A	603	-	4,4,4	0.04	0	6,6,6	0.23	0
5	EDO	A	604	-	3,3,3	0.45	0	2,2,2	0.87	0
5	EDO	B	501	-	3,3,3	0.23	0	2,2,2	0.63	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	JLJ	A	601	-	-	0/14/14/14	0/2/2/2
4	SO4	A	602	-	-	0/0/0/0	0/0/0/0
4	SO4	A	603	-	-	0/0/0/0	0/0/0/0
5	EDO	A	604	-	-	0/1/1/1	0/0/0/0
5	EDO	B	501	-	-	0/1/1/1	0/0/0/0

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	601	JLJ	C11-N19	2.15	1.40	1.36
3	A	601	JLJ	O26-C21	2.99	1.43	1.37
3	A	601	JLJ	C20-C28	4.49	1.51	1.44

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	A	601	JLJ	N16-C11-N12	-5.63	120.67	126.67
3	A	601	JLJ	C14-C15-N16	-3.34	120.09	123.90
3	A	601	JLJ	C41-C42-C43	-2.84	122.06	126.71
3	A	601	JLJ	O17-C13-C14	2.03	120.38	116.79
3	A	601	JLJ	C41-O26-C21	3.37	124.55	117.59
3	A	601	JLJ	C11-N12-C13	4.30	120.81	114.96
3	A	601	JLJ	C15-N16-C11	6.18	120.86	115.49
3	A	601	JLJ	O26-C41-C42	6.53	120.98	108.05

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	JLJ	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	556/557 (99%)	1.07	92 (16%) 2 3	25, 53, 93, 124	0
2	B	410/428 (95%)	1.14	72 (17%) 2 3	29, 51, 101, 120	0
All	All	966/985 (98%)	1.10	164 (16%) 2 3	25, 52, 99, 124	0

All (164) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	286	THR	10.4
2	B	89	GLU	10.1
1	A	24	TRP	10.0
1	A	69	THR	9.9
2	B	88	TRP	9.6
1	A	222	GLN	9.5
2	B	214	LEU	8.5
1	A	67	ASP	8.1
2	B	209	LEU	8.0
1	A	289	LEU	7.9
2	B	356	ARG	7.4
1	A	282	LEU	7.4
1	A	290	THR	7.2
1	A	250	ASP	7.0
1	A	257	ILE	6.9
2	B	212	TRP	6.8
1	A	68	SER	6.8
1	A	301	LEU	6.7
1	A	65	LYS	6.7
1	A	252	TRP	6.6
2	B	5	ILE	6.5
1	A	288	ALA	6.3
2	B	215	THR	6.2
2	B	193	LEU	6.1

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Mol	Chain	Res	Type	RSRZ
1	A	92	LEU	6.0
1	A	66	LYS	5.9
2	B	225	PRO	5.9
1	A	285	GLY	5.9
2	B	358	ARG	5.9
2	B	226	PRO	5.7
2	B	197	GLN	5.6
1	A	287	LYS	5.4
2	B	195	ILE	5.3
2	B	7	THR	5.2
2	B	231	GLY	5.2
1	A	70	LYS	5.1
1	A	292	VAL	5.1
1	A	64	LYS	5.1
2	B	239	TRP	5.1
1	A	254	VAL	5.0
2	B	14	PRO	5.0
1	A	116	PHE	4.9
2	B	284	ARG	4.8
2	B	357	MET	4.6
1	A	553	SER	4.6
2	B	202	ILE	4.6
1	A	294	PRO	4.5
1	A	-1	MET	4.5
2	B	230	MET	4.5
1	A	283	LEU	4.5
1	A	297	GLU	4.4
1	A	554	ALA	4.3
1	A	223	LYS	4.3
2	B	13	LYS	4.2
2	B	173	LYS	4.2
2	B	6	GLU	4.2
1	A	113	ASP	4.1
1	A	91	GLN	4.1
2	B	224	GLU	4.1
2	B	232	TYR	4.1
1	A	63	ILE	4.0
2	B	85	GLN	4.0
1	A	40	GLU	3.9
2	B	69	THR	3.8
2	B	229	TRP	3.8
1	A	256	ASP	3.8

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Mol	Chain	Res	Type	RSRZ
2	B	87	PHE	3.7
2	B	227	PHE	3.7
1	A	224	GLU	3.7
2	B	210	LEU	3.7
2	B	200	THR	3.7
1	A	295	LEU	3.7
1	A	291	GLU	3.6
1	A	50	ILE	3.5
1	A	293	ILE	3.5
1	A	279	LEU	3.5
1	A	552	VAL	3.4
2	B	9	PRO	3.4
2	B	168	LEU	3.4
1	A	244	ILE	3.4
1	A	309	ILE	3.4
2	B	178	ILE	3.3
2	B	196	GLY	3.3
2	B	198	HIS	3.3
2	B	240	THR	3.3
1	A	71	TRP	3.3
2	B	194	GLU	3.2
1	A	251	SER	3.2
1	A	53	GLU	3.2
2	B	86	ASP	3.2
1	A	52	PRO	3.2
2	B	166	LYS	3.2
1	A	4	PRO	3.2
2	B	318	TYR	3.1
1	A	284	ARG	3.1
2	B	355	ALA	3.1
1	A	298	GLU	3.1
1	A	410	TRP	3.1
2	B	170	PRO	3.0
1	A	255	ASN	3.0
1	A	550	LYS	3.0
1	A	117	SER	3.0
1	A	21	VAL	2.9
1	A	308	GLU	2.9
2	B	75	VAL	2.9
1	A	358	ARG	2.9
1	A	228	LEU	2.8
2	B	428	GLN	2.8

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Mol	Chain	Res	Type	RSRZ
2	B	12	LEU	2.8
2	B	176	PRO	2.8
2	B	8	VAL	2.8
1	A	61	PHE	2.8
1	A	214	LEU	2.8
1	A	246	LEU	2.7
2	B	359	GLY	2.7
2	B	272	PRO	2.7
1	A	496	VAL	2.6
2	B	174	GLN	2.6
2	B	206	ARG	2.6
2	B	211	ARG	2.6
1	A	247	PRO	2.6
1	A	448	ARG	2.6
1	A	458	VAL	2.6
2	B	315[A]	HIS	2.6
1	A	548	VAL	2.5
2	B	114	ALA	2.5
1	A	551	LEU	2.5
1	A	449	GLU	2.5
1	A	541	GLY	2.5
1	A	535	TRP	2.4
1	A	243	PRO	2.4
1	A	543	GLY	2.4
2	B	151	GLN	2.4
2	B	119	PRO	2.4
2	B	169	GLU	2.4
1	A	3	SER	2.4
1	A	372	VAL	2.3
2	B	204	GLU	2.3
2	B	15	GLY	2.3
1	A	304	ALA	2.3
1	A	300	GLU	2.3
2	B	427	TYR	2.3
1	A	51	GLY	2.3
1	A	220	LYS	2.3
1	A	411	ILE	2.3
1	A	33	ALA	2.2
2	B	354	TYR	2.2
2	B	108	VAL	2.2
1	A	497	THR	2.2
2	B	185	ASP	2.2

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Mol	Chain	Res	Type	RSRZ
2	B	199	ARG	2.2
1	A	442	VAL	2.2
1	A	26	LEU	2.2
1	A	346	PHE	2.1
2	B	60	VAL	2.1
1	A	302	GLU	2.1
2	B	152	GLY	2.1
1	A	263	LYS	2.1
2	B	74	LEU	2.1
1	A	412	PRO	2.1
1	A	159	ILE	2.0
2	B	233	GLU	2.0
1	A	25	PRO	2.0
1	A	43	LYS	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	JLJ	A	601	23/23	0.94	0.13	0.25	35,40,46,49	0
5	EDO	A	604	4/4	0.95	0.10	-0.63	41,43,48,50	0
4	SO4	A	602	5/5	0.93	0.08	-2.39	70,74,79,85	0
5	EDO	B	501	4/4	0.95	0.12	-	40,42,45,46	0
4	SO4	A	603	5/5	0.86	0.32	-	68,68,90,91	0

6.5 Other polymers (i)

There are no such residues in this entry.