Full wwPDB X-ray Structure Validation Report ⓘ

Aug 30, 2017 – 03:18 PM EDT

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PDB ID	:	4WE1
Title	:	Crystal Structure of HIV-1 Reverse Transcriptase in Complex with 5-(2-(2-(2 ,4-dioxo-3,4-dihydropyrimidin-1(2H)-yl)ethoxy)phenoxy)-2-naphthonitrile (JLJ600)
Authors	:	Frey, K.M.; Anderson, K.S.
Deposited on	:	unknown
Resolution	:	2.49 Å(reported)

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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 2.49 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	Percentile Ranks	Value
Rfree		0.286
Clashscore		5
Ramachandran outliers		0
Sidechain outliers		5.1%
RSRZ outliers		9.1%

Worse   Better

■ Percentile relative to all X-ray structures

▯ Percentile relative to X-ray structures of similar resolution
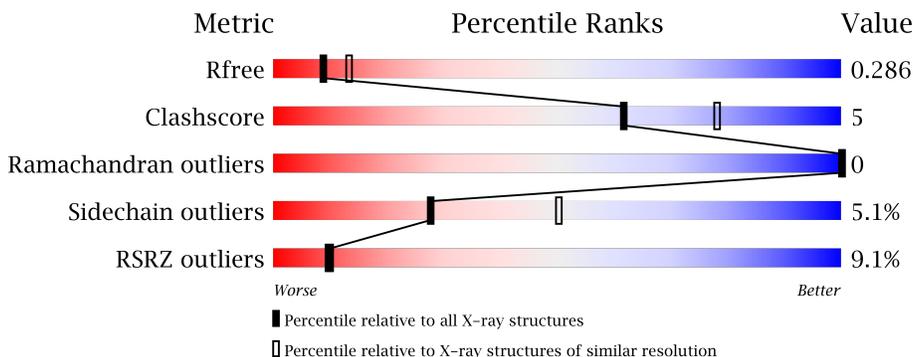
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R$_{free}$	100719	3846 (2.50-2.50)
Clashscore	112137	4554 (2.50-2.50)
Ramachandran outliers	110173	4463 (2.50-2.50)
Sidechain outliers	110143	4465 (2.50-2.50)
RSRZ outliers	101464	3876 (2.50-2.50)

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 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	10% / 79% / 17% / · ·
2	B	428	7% / 81% / 11% / · 6%

2 Entry composition (i)

There are 6 unique types of molecules in this entry. The entry contains 7807 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called Gag-Pol polyprotein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	542	Total	C	N	O	S	0	0	0
			4375	2832	728	808	7			

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 Gag-Pol polyprotein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	402	Total	C	N	O	S	0	1	0
			3296	2145	545	600	6			

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 5-{2-[2-(2,4-dioxo-3,4-dihydropyrimidin-1(2H)-yl)ethoxy]phenoxy}naphthalene-2-carbonitrile (three-letter code: 3LQ) (formula: $C_{23}H_{17}N_3O_4$).
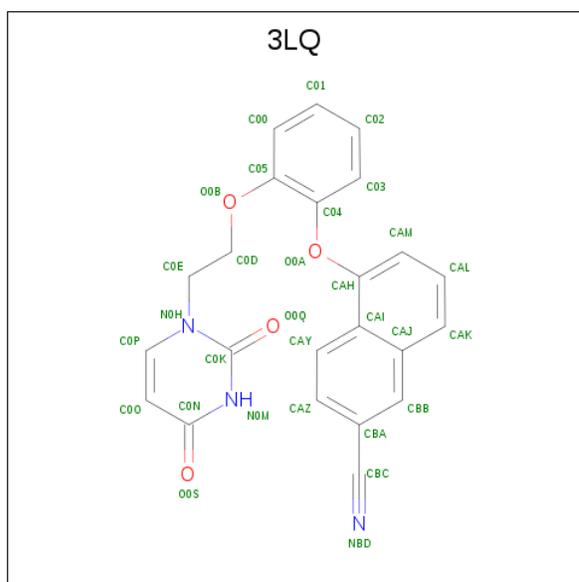
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	N	O		
3	A	1	30	23	3	4	0	0

- Molecule 4 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Mg		
4	A	2	2	2	0	0

- Molecule 5 is SULFATE ION (three-letter code: SO4) (formula: O_4S).
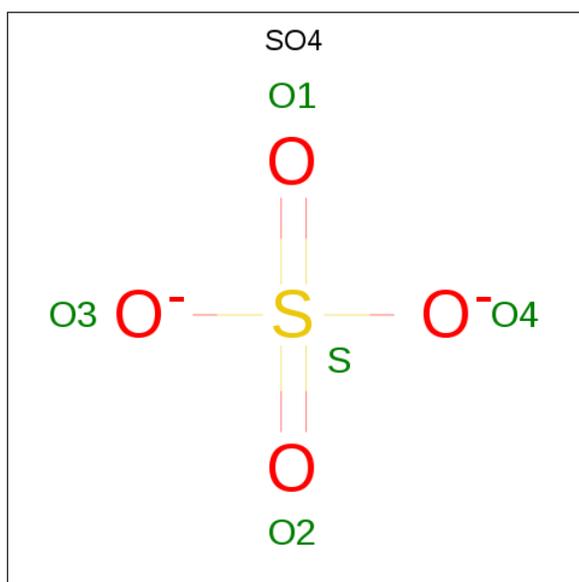
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total 5	O 4	S 1	0	0
5	A	1	Total 5	O 4	S 1	0	0
5	A	1	Total 5	O 4	S 1	0	0
5	A	1	Total 5	O 4	S 1	0	0

- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	44	Total 44	O 44	0	0
6	B	40	Total 40	O 40	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 the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density (RSRZ > 2). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

• Molecule 1: Gag-Pol polyprotein

Chain A:
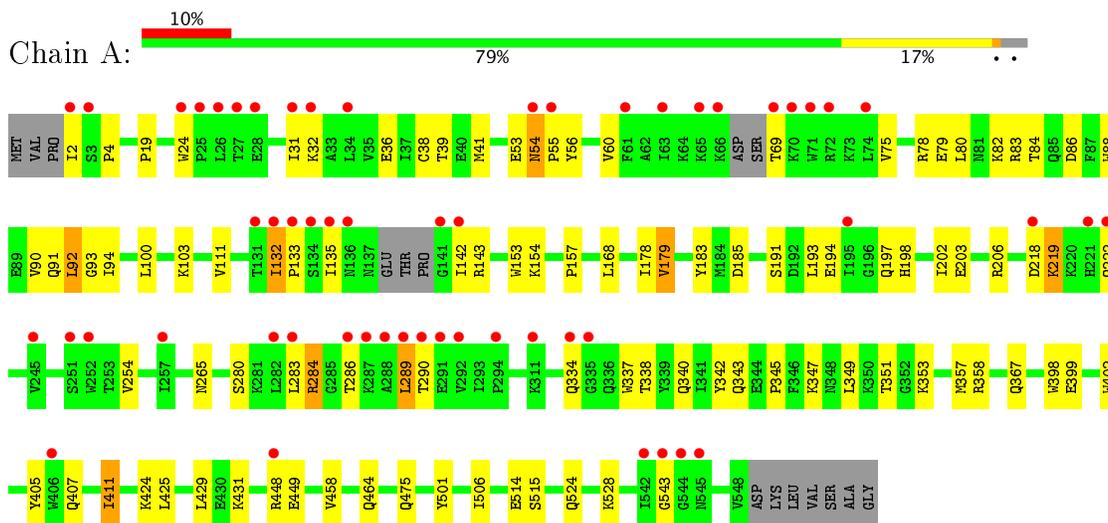
• Molecule 2: Gag-Pol polyprotein

Chain B:
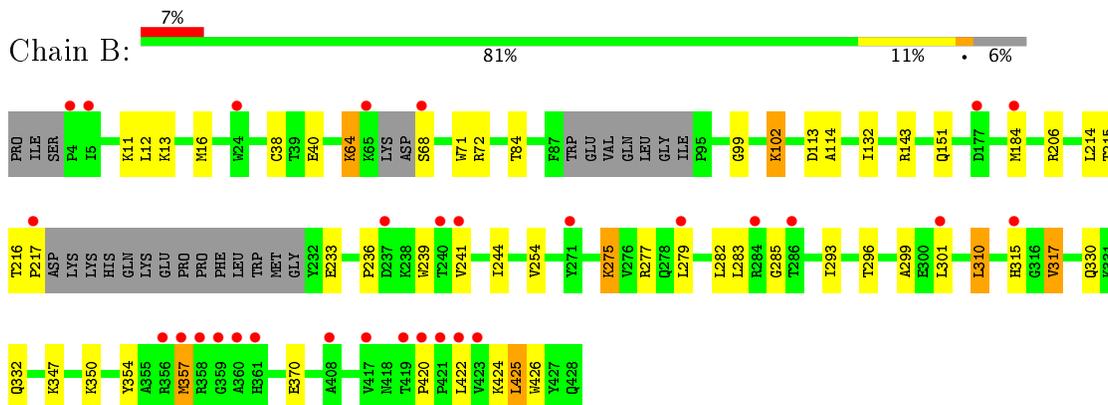
4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α, β, γ	220.27Å 67.22Å 102.48Å 90.00° 108.08° 90.00°	Depositor
Resolution (Å)	38.77 – 2.49 38.76 – 2.49	Depositor EDS
% Data completeness (in resolution range)	98.5 (38.77-2.49) 98.6 (38.76-2.49)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.07	Depositor
$<I/\sigma(I)>$ [1]	3.62 (at 2.48Å)	Xtriage
Refinement program	PHENIX	Depositor
R, R_{free}	0.238 , 0.287 0.235 , 0.286	Depositor DCC
R_{free} test set	1998 reflections (4.04%)	DCC
Wilson B-factor (Å^2)	50.9	Xtriage
Anisotropy	0.284	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.34 , 51.8	EDS
L-test for twinning[2]	$<|L|> = 0.49$, $<L^2> = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.92	EDS
Total number of atoms	7807	wwPDB-VP
Average B, all atoms (Å^2)	60.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.81% of the height of the origin peak. No significant pseudotranslation is detected.*

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[1] Intensities estimated from amplitudes.

[2] Theoretical values of $<|L|>$, $<L^2>$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: MG, SO4, 3LQ

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	0.24	0/4489	0.45	1/6106 (0.0%)
2	B	0.23	0/3391	0.45	0/4609
All	All	0.24	0/7880	0.45	1/10715 (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})
1	A	289	LEU	CA-CB-CG	5.12	127.07	115.30

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	54	ASN	Peptide
2	B	420	PRO	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	4375	0	4369	54	0
2	B	3296	0	3309	26	0
3	A	30	0	17	3	0
4	A	2	0	0	0	0
5	A	20	0	0	1	0
6	A	44	0	0	0	0
6	B	40	0	0	0	0
All	All	7807	0	7695	78	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 5.

All (78) 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:543:GLY:HA2	2:B:285:GLY:HA2	1.71	0.73
2:B:12:LEU:HG	2:B:84:THR:HG22	1.71	0.71
1:A:265:ASN:OD1	1:A:353:LYS:NZ	2.24	0.69
1:A:191:SER:OG	1:A:198:HIS:ND1	2.26	0.66
2:B:114:ALA:HB2	2:B:214:LEU:HG	1.80	0.64
1:A:90:VAL:HG21	1:A:157:PRO:HB2	1.80	0.63
1:A:194:GLU:H	1:A:197:GLN:HE21	1.47	0.62
1:A:54:ASN:HD22	1:A:56:TYR:HB2	1.65	0.62
2:B:357:MET:SD	2:B:357:MET:N	2.73	0.61
2:B:279:LEU:HD23	2:B:299:ALA:HB1	1.86	0.58
2:B:254:VAL:HG13	2:B:283:LEU:HD22	1.86	0.57
2:B:241:VAL:HG22	2:B:350:LYS:HA	1.86	0.57
1:A:219:LYS:HD2	1:A:222:GLN:HG2	1.87	0.57
2:B:244:ILE:HB	2:B:310:LEU:HG	1.88	0.56
2:B:72:ARG:NH2	2:B:151:GLN:OE1	2.38	0.56
2:B:296:THR:HG23	2:B:299:ALA:H	1.70	0.56
1:A:193:LEU:HB3	1:A:197:GLN:HG3	1.88	0.55
1:A:448:ARG:NH1	5:A:604:SO4:O2	2.39	0.55
1:A:31:ILE:HG23	1:A:132:ILE:HD11	1.89	0.55
2:B:99:GLY:HA2	2:B:102:LYS:HD3	1.89	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:19:PRO:HG3	1:A:80:LEU:HB2	1.90	0.54
1:A:84:THR:HG21	1:A:153:TRP:HE1	1.73	0.53
2:B:13:LYS:HB2	2:B:16:MET:HE2	1.91	0.53
1:A:343:GLN:HG3	1:A:349:LEU:HD21	1.91	0.52
1:A:132:ILE:HD12	1:A:133:PRO:HD2	1.92	0.52
1:A:337:TRP:HE1	1:A:367:GLN:NE2	2.08	0.51
2:B:206:ARG:NH1	2:B:216:THR:O	2.43	0.51
2:B:275:LYS:HD3	2:B:277:ARG:H	1.74	0.51
1:A:218:ASP:N	1:A:218:ASP:OD1	2.33	0.50
2:B:236:PRO:HA	2:B:239:TRP:CD2	2.47	0.50
1:A:203:GLU:OE2	1:A:206:ARG:NH1	2.45	0.49
1:A:60:VAL:HG23	1:A:75:VAL:HG22	1.95	0.49
1:A:405:TYR:CE2	1:A:407:GLN:HB3	2.47	0.49
1:A:38:CYS:HA	1:A:41:MET:HE2	1.95	0.49
2:B:354:TYR:OH	2:B:370:GLU:OE1	2.30	0.48
1:A:340:GLN:HG3	1:A:351:THR:HG22	1.94	0.48
1:A:78:ARG:O	1:A:82:LYS:HG3	2.13	0.48
1:A:342:TYR:HA	1:A:349:LEU:HD23	1.95	0.48
1:A:36:GLU:O	1:A:39:THR:OG1	2.22	0.48
1:A:132:ILE:HG23	1:A:142:ILE:HB	1.97	0.47
1:A:179:VAL:HG13	3:A:601:3LQ:H2	1.97	0.47
1:A:357:MET:O	1:A:358:ARG:HG2	2.16	0.46
1:A:86:ASP:OD1	1:A:154:LYS:NZ	2.33	0.46
1:A:284:ARG:NH2	1:A:514:GLU:OE1	2.48	0.46
1:A:280:SER:HA	1:A:283:LEU:HB2	1.97	0.46
2:B:425:LEU:HD12	2:B:426:TRP:CD1	2.51	0.46
1:A:54:ASN:ND2	1:A:56:TYR:HB2	2.29	0.46
1:A:342:TYR:CE1	1:A:345:PRO:HA	2.51	0.46
1:A:458:VAL:HG13	1:A:464:GLN:HG2	1.98	0.45
1:A:55:PRO:O	1:A:56:TYR:CG	2.70	0.45
1:A:79:GLU:OE2	1:A:83:ARG:NH1	2.44	0.45
1:A:32:LYS:HA	1:A:32:LYS:HD3	1.75	0.45
2:B:215:THR:HG22	2:B:217:PRO:HD3	1.98	0.44
1:A:100:LEU:HB3	3:A:601:3LQ:H6	1.98	0.44
1:A:103:LYS:HE3	1:A:179:VAL:HG11	2.00	0.44
2:B:282:LEU:HB3	2:B:293:ILE:HG21	2.00	0.44
1:A:429:LEU:HD11	1:A:506:ILE:HG22	1.99	0.43
1:A:88:TRP:CE2	2:B:143:ARG:HD2	2.53	0.43
1:A:2:ILE:C	1:A:4:PRO:HD2	2.39	0.43
2:B:317:VAL:HG12	2:B:347:LYS:HB3	2.00	0.43
1:A:424:LYS:NZ	1:A:425:LEU:H	2.16	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:332:GLN:HA	2:B:424:LYS:HE3	2.01	0.43
1:A:79:GLU:O	1:A:83:ARG:HG3	2.19	0.42
1:A:399:GLU:HA	1:A:402:TRP:CE2	2.54	0.42
2:B:38:CYS:SG	2:B:132:ILE:HD11	2.59	0.42
1:A:402:TRP:CE3	1:A:411:ILE:HG21	2.55	0.41
1:A:56:TYR:O	1:A:143:ARG:NH2	2.52	0.41
2:B:422:LEU:HA	2:B:422:LEU:HD23	1.84	0.41
1:A:92:LEU:HD12	1:A:93:GLY:H	1.86	0.41
1:A:94:ILE:HG22	1:A:183:TYR:CE1	2.56	0.41
2:B:64:LYS:HE2	2:B:71:TRP:CZ2	2.56	0.41
1:A:475:GLN:HB3	1:A:501:TYR:CE2	2.56	0.40
2:B:310:LEU:HD12	2:B:310:LEU:HA	1.84	0.40
1:A:202:ILE:O	1:A:206:ARG:HG3	2.21	0.40
1:A:524:GLN:O	1:A:528:LYS:HG2	2.21	0.40
1:A:132:ILE:HA	1:A:133:PRO:HD3	1.77	0.40
1:A:179:VAL:CG1	3:A:601:3LQ:H2	2.51	0.40
1:A:80:LEU:O	1:A:84:THR:HG23	2.22	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	536/557 (96%)	525 (98%)	11 (2%)	0	100	100
2	B	395/428 (92%)	389 (98%)	6 (2%)	0	100	100
All	All	931/985 (94%)	914 (98%)	17 (2%)	0	100	100

There are no Ramachandran outliers to report.

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	471/495 (95%)	445 (94%)	26 (6%)	25	46
2	B	360/390 (92%)	343 (95%)	17 (5%)	30	54
All	All	831/885 (94%)	788 (95%)	43 (5%)	28	49

All (43) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	24	TRP
1	A	53	GLU
1	A	69	THR
1	A	91	GLN
1	A	92	LEU
1	A	111	VAL
1	A	132	ILE
1	A	135	ILE
1	A	168	LEU
1	A	178	ILE
1	A	179	VAL
1	A	185	ASP
1	A	219	LYS
1	A	254	VAL
1	A	284	ARG
1	A	286	THR
1	A	289	LEU
1	A	290	THR
1	A	334	GLN
1	A	338	THR
1	A	347	LYS
1	A	398	TRP
1	A	411	ILE
1	A	431	LYS
1	A	449	GLU
1	A	515	SER
2	B	11	LYS

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Mol	Chain	Res	Type
2	B	40	GLU
2	B	64	LYS
2	B	68	SER
2	B	102	LYS
2	B	113	ASP
2	B	184	MET
2	B	233[A]	GLU
2	B	233[B]	GLU
2	B	275	LYS
2	B	301	LEU
2	B	310	LEU
2	B	315	HIS
2	B	317	VAL
2	B	330	GLN
2	B	357	MET
2	B	425	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (12) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	57	ASN
1	A	147	ASN
1	A	197	GLN
1	A	208	HIS
1	A	340	GLN
1	A	361	HIS
1	A	367	GLN
1	A	500	GLN
2	B	161	GLN
2	B	197	GLN
2	B	255	ASN
2	B	418	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 carbohydrates in this entry.

5.6 Ligand geometry (i)

Of 7 ligands modelled in this entry, 2 are monoatomic - leaving 5 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	3LQ	A	601	-	30,33,33	1.63	5 (16%)	37,45,45	2.89	4 (10%)
5	SO4	A	604	-	4,4,4	0.16	0	6,6,6	0.05	0
5	SO4	A	605	-	4,4,4	0.15	0	6,6,6	0.07	0
5	SO4	A	606	-	4,4,4	0.14	0	6,6,6	0.07	0
5	SO4	A	607	-	4,4,4	0.16	0	6,6,6	0.06	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	3LQ	A	601	-	-	0/12/12/12	0/4/4/4
5	SO4	A	604	-	-	0/0/0/0	0/0/0/0
5	SO4	A	605	-	-	0/0/0/0	0/0/0/0
5	SO4	A	606	-	-	0/0/0/0	0/0/0/0
5	SO4	A	607	-	-	0/0/0/0	0/0/0/0

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	601	3LQ	CAI-CAJ	-2.11	1.39	1.43
3	A	601	3LQ	CAZ-CBA	2.62	1.44	1.39
3	A	601	3LQ	CBA-CBC	3.13	1.52	1.44
3	A	601	3LQ	O0A-CAH	3.42	1.45	1.38
3	A	601	3LQ	C0P-N0H	3.99	1.42	1.36

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	A	601	3LQ	C0O-C0N-N0M	-3.44	114.90	123.12
3	A	601	3LQ	C0E-N0H-C0P	-2.06	114.41	118.22
3	A	601	3LQ	C0D-O0B-C05	2.90	124.77	117.70
3	A	601	3LQ	C0N-N0M-C0K	16.22	128.06	114.13

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	601	3LQ	3	0
5	A	604	SO4	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 (i)

6.1 Protein, DNA and RNA chains (i)

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	542/557 (97%)	0.56	56 (10%)	7	6	34, 59, 96, 115	0
2	B	402/428 (93%)	0.55	30 (7%)	15	15	36, 56, 85, 130	0
All	All	944/985 (95%)	0.56	86 (9%)	10	10	34, 58, 92, 130	0

All (86) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	360	ALA	10.4
2	B	359	GLY	9.7
1	A	69	THR	8.6
1	A	133	PRO	6.5
1	A	32	LYS	5.9
1	A	132	ILE	5.7
1	A	286	THR	5.6
1	A	54	ASN	5.4
1	A	542	ILE	5.0
2	B	241	VAL	4.9
1	A	71	TRP	4.9
1	A	61	PHE	4.5
1	A	24	TRP	4.4
2	B	237	ASP	4.2
2	B	358	ARG	4.0
2	B	361	HIS	3.9
1	A	311	LYS	3.9
2	B	5	ILE	3.7
1	A	222	GLN	3.6
2	B	357	MET	3.6
1	A	290	THR	3.6
1	A	218	ASP	3.5
2	B	4	PRO	3.4
1	A	289	LEU	3.4

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Mol	Chain	Res	Type	RSRZ
1	A	2	ILE	3.3
2	B	240	THR	3.3
1	A	134	SER	3.3
1	A	282	LEU	3.2
1	A	31	ILE	3.2
1	A	63	ILE	3.2
1	A	135	ILE	3.1
2	B	419	THR	3.1
1	A	545	ASN	3.1
2	B	423	VAL	3.0
2	B	315	HIS	3.0
1	A	27	THR	3.0
1	A	65	LYS	2.9
1	A	142	ILE	2.9
1	A	288	ALA	2.9
1	A	335	GLY	2.8
2	B	68	SER	2.8
1	A	544	GLY	2.8
1	A	221	HIS	2.8
2	B	284	ARG	2.7
1	A	543	GLY	2.7
2	B	301	LEU	2.7
1	A	141	GLY	2.7
1	A	66	LYS	2.6
1	A	26	LEU	2.6
2	B	217	PRO	2.5
1	A	195	ILE	2.5
1	A	291	GLU	2.5
1	A	283	LEU	2.5
1	A	292	VAL	2.5
1	A	257	ILE	2.5
2	B	184	MET	2.4
1	A	25	PRO	2.4
1	A	34	LEU	2.4
1	A	72	ARG	2.4
1	A	245	VAL	2.4
2	B	420	PRO	2.4
2	B	177	ASP	2.3
1	A	136	ASN	2.3
1	A	287	LYS	2.3
1	A	3	SER	2.3
1	A	74	LEU	2.3

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Mol	Chain	Res	Type	RSRZ
2	B	408	ALA	2.3
1	A	251	SER	2.3
1	A	334	GLN	2.2
1	A	131	THR	2.2
2	B	356	ARG	2.2
1	A	252	TRP	2.2
1	A	406	TRP	2.2
2	B	286	THR	2.2
2	B	271	TYR	2.2
1	A	70	LYS	2.2
2	B	279	LEU	2.1
1	A	294	PRO	2.1
2	B	65	LYS	2.1
2	B	417	VAL	2.1
2	B	24	TRP	2.1
2	B	421	PRO	2.1
1	A	55	PRO	2.1
2	B	422	LEU	2.0
1	A	448	ARG	2.0
1	A	28	GLU	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
4	MG	A	603	1/1	0.91	0.30	1.85	58,58,58,58	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
5	SO4	A	604	5/5	0.93	0.26	-0.41	75,79,99,99	0
3	3LQ	A	601	30/30	0.95	0.14	-1.04	38,47,52,56	0
5	SO4	A	606	5/5	0.97	0.12	-1.06	58,64,72,75	0
5	SO4	A	607	5/5	0.97	0.13	-	61,64,69,70	0
4	MG	A	602	1/1	0.96	0.14	-	75,75,75,75	0
5	SO4	A	605	5/5	0.94	0.08	-	69,74,85,88	0

6.5 Other polymers (i)

There are no such residues in this entry.