wwPDB X-ray Structure Validation Summary Report (i)

Feb 1, 2016 – 08:12 AM GMT

PDB ID	:	3DRS
Title	:	HIV reverse transcriptase K103N mutant in complex with inhibitor R8D
Authors	:	Yan, Y.; Prasad, S.
Deposited on	:	2008-07-11
Resolution	:	3.15 Å(reported)

This is a wwPDB X-ray Structure Validation Summary 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:

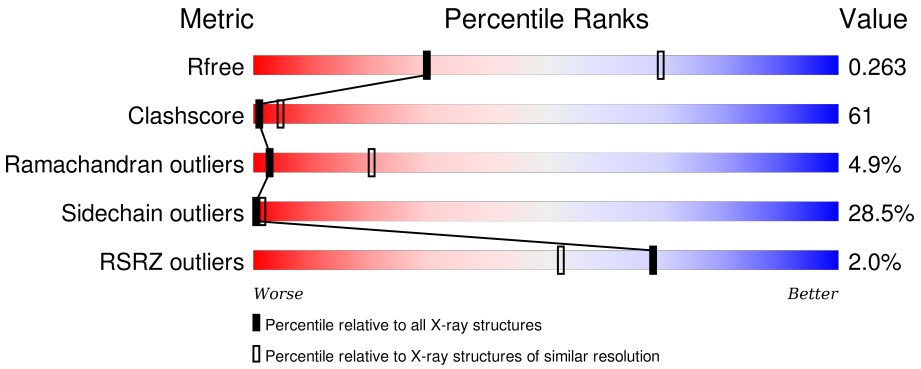
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)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

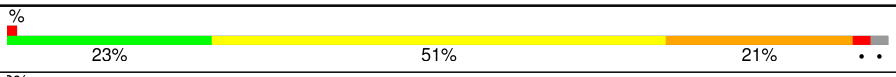
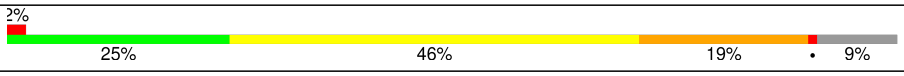
The reported resolution of this entry is 3.15 Å.

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	1112 (3.20-3.12)
Clashscore	102246	1249 (3.20-3.12)
Ramachandran outliers	100387	1222 (3.20-3.12)
Sidechain outliers	100360	1221 (3.20-3.12)
RSRZ outliers	91569	1117 (3.20-3.12)

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	563	
2	B	443	

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
3	R8D	A	601	-	-	X	-

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 7854 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.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	549	Total	C	N	O	S	0	0	0
			4475	2891	747	829	8			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-2	MET	-	EXPRESSION TAG	UNP P04585
A	-1	ASN	-	EXPRESSION TAG	UNP P04585
A	0	SER	-	EXPRESSION TAG	UNP P04585
A	103	ASN	LYS	ENGINEERED	UNP P04585

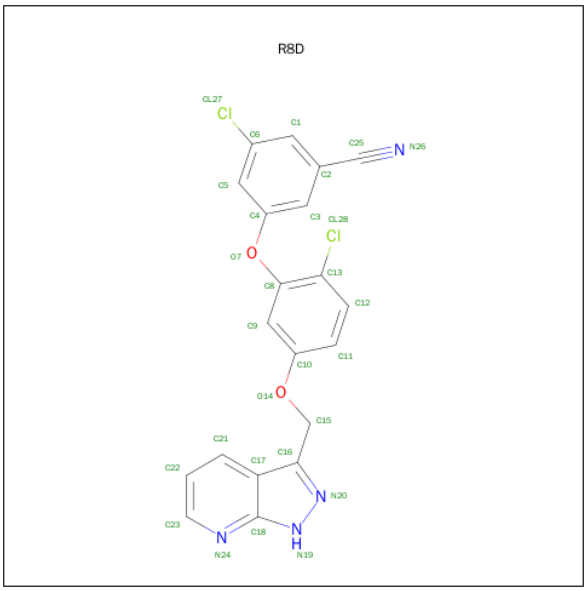
- Molecule 2 is a protein called p66 RT.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	405	Total	C	N	O	S	0	0	0
			3351	2180	555	610	6			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	-2	MET	-	EXPRESSION TAG	UNP P04585
B	-1	ASN	-	EXPRESSION TAG	UNP P04585
B	0	SER	-	EXPRESSION TAG	UNP P04585
B	103	ASN	LYS	ENGINEERED	UNP P04585

- Molecule 3 is 3-CHLORO-5-[2-CHLORO-5-(1H-PYRAZOLO[3,4-B]PYRIDIN-3-YLMETHOXY)PHENOXY]BENZONITRILE (three-letter code: R8D) (formula: $C_{20}H_{12}Cl_2N_4O_2$).



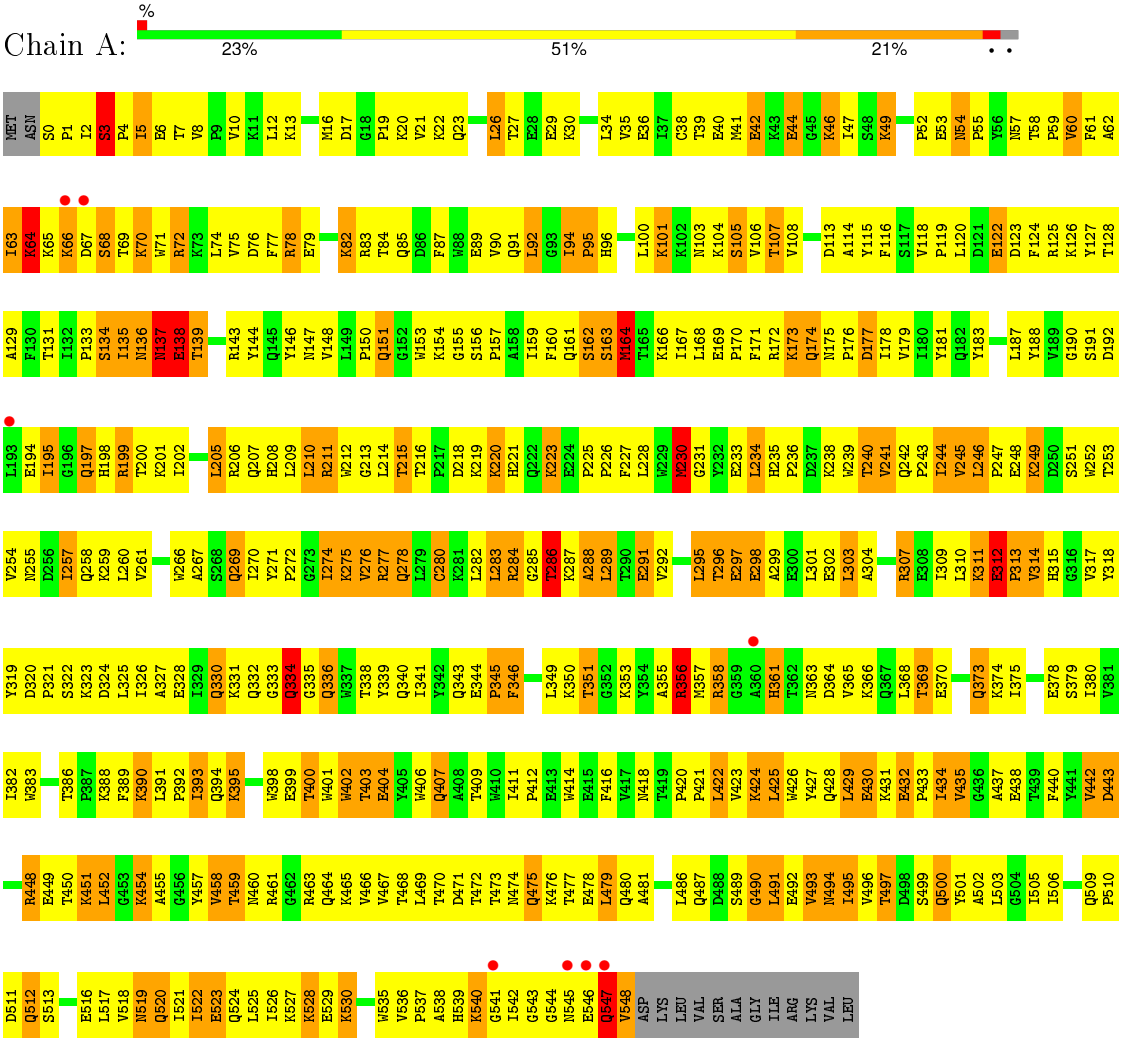
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	Cl	N	O	0	0
			28	20	2	4	2		

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.

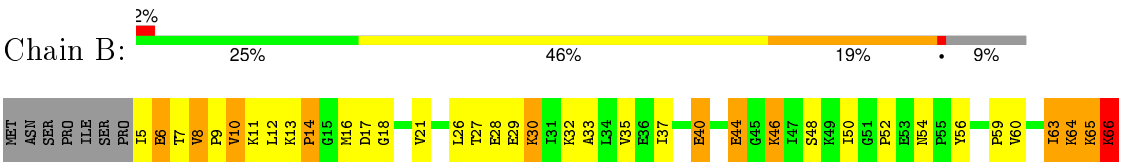
- Molecule 1: Reverse transcriptase/ribonuclease H

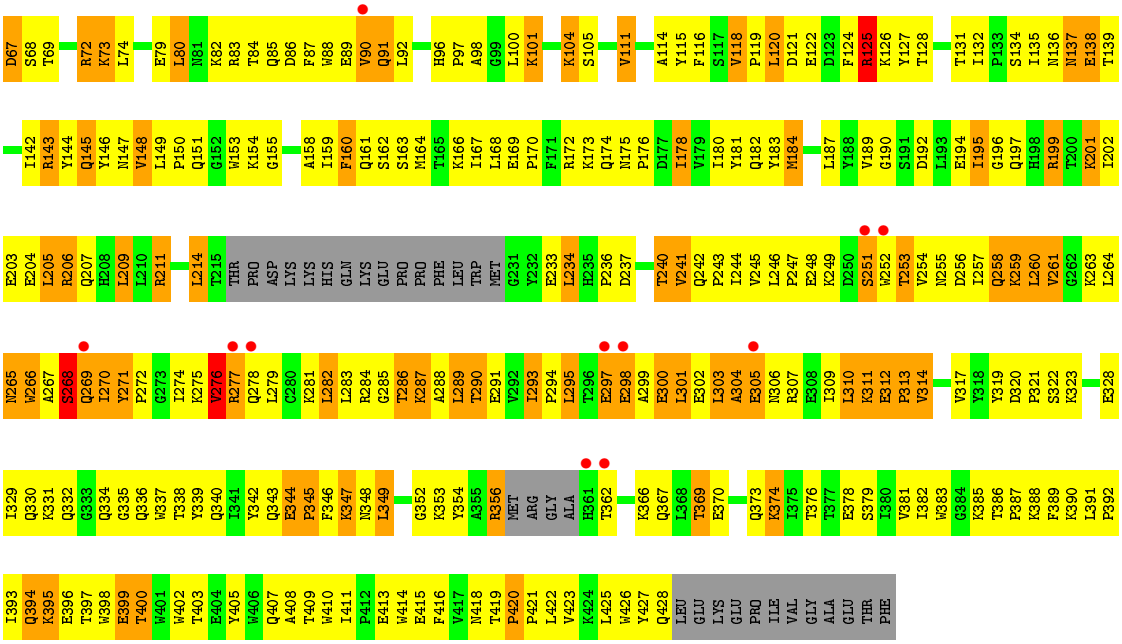
Chain A:



- Molecule 2: p66 RT

Chain B:




D67 S68 T69 R72 K73 L74 E79 L80 N81 K82 R83 T84 Q85 D86 F87 W88 E89 V90 Q91 L92 H96 P97 A98 G99 L100 K101 K104 S105 V111 A114 Y115 F116 S117 V118 P119 L120 D121 E122 D123 F124 R125 K126 Y127 T128 T131 I132 P133 S134 I135 N136 N137 E138 T139
I142 R143 Y144 Q145 Y146 N147 V148 L149 P150 Q151 G152 W153 K154 G155 A158 I159 F160 Q161 S162 S163 M164 T165 K166 I167 L168 E169 P170 F171 R172 K173 Q174 N175 P176 D177 I178 V179 I180 Y181 Q182 Y183 M184 L187 Y188 V189 G190 S191 D192 L193 E194 I195 G196 Q197 H198 R199 T200 K201 I202
E203 E204 L205 R206 Q207 HD8 L209 L210 R211 L214 T215 THR PRO ASP LYS LYS HIS GLN LYS GLU PRO PRO PHE LEU TRP MET G231 Y232 E233 L234 H235 P236 D237 T240 V241 Q242 P243 I244 V245 L246 P247 E248 K249 D250 S251 W252 T253 V254 N255 D256 I257 Q258 K259 L260 V261 G262 K263 L264
N265 W266 A267 S268 Q269 T270 Y271 P272 G273 I274 K275 V276 R277 Q278 L279 C280 K281 L282 I283 R284 G285 T286 K287 A288 L289 T290 E291 V292 I293 P294 L295 T296 E297 E298 A299 E300 L301 E302 L303 A304 E305 N306 R307 E308 I309 L310 K311 E312 P313 V314 V317 Y318 Y319 D320 P321 S322 K323 E328
I329 Q330 K331 Q332 G333 Q334 G335 Q336 W337 T338 Y339 Q340 I341 Y342 Q343 E344 P345 F346 K347 N348 L349 G352 K353 Y354 A355 R356 MET ARG GLY ALA H361 T362 K366 Q367 L368 T369 E370 Q373 K374 I375 T376 T377 E378 S379 I380 V381 I382 W383 G384 K385 T386 P387 K388 F389 K390 L391 P392
I393 Q394 K395 E396 T397 W398 E399 T400 W401 W402 T403 E404 Y405 W406 Q407 A408 T409 W410 I411 P412 E413 W414 E415 F416 V417 N418 T419 P420 P421 L422 V423 K424 L425 W426 Y427 Q428 LEU GLU LYS GLU PRO ILE VAL GLY ALA GLU THR PHE

4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α, β, γ	118.55Å 154.63Å 154.12Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	37.50 – 3.15 37.50 – 3.15	Depositor EDS
% Data completeness (in resolution range)	99.4 (37.50-3.15) 99.5 (37.50-3.15)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.09	Depositor
$< I/\sigma(I) >$ [1]	2.98 (at 3.18Å)	Xtriage
Refinement program	BUSTER-TNT 2.1.1	Depositor
R, R_{free}	0.184 , 0.250 0.192 , 0.263	Depositor DCC
R_{free} test set	1255 reflections (5.36%)	DCC
Wilson B-factor (Å^2)	68.6	Xtriage
Anisotropy	0.051	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.35 , 85.0	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.52$, $< L^2 > = 0.36$	Xtriage
Outliers	0 of 24682 reflections	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	7854	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 3.80% 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: R8D

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	0.67	0/4592	0.89	6/6242 (0.1%)
2	B	0.67	0/3445	0.95	7/4682 (0.1%)
All	All	0.67	0/8037	0.92	13/10924 (0.1%)

There are no bond length outliers.

The worst 5 of 13 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	344	GLU	C-N-CD	-19.16	78.46	120.60
2	B	312	GLU	C-N-CD	-11.88	94.47	120.60
2	B	420	PRO	C-N-CD	-10.86	96.70	120.60
1	A	312	GLU	C-N-CD	-10.29	97.96	120.60
1	A	94	ILE	C-N-CD	-8.80	101.23	120.60

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	4475	0	4514	602	1
2	B	3351	0	3373	391	0
3	A	28	0	12	16	0
All	All	7854	0	7899	967	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 61.

The worst 5 of 967 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:288:ALA:HB3	1:A:291:GLU:HB3	1.17	1.17
1:A:318:TYR:CE2	3:A:601:R8D:H15	1.82	1.14
1:A:469:LEU:HD21	1:A:480:GLN:HG2	1.32	1.12
2:B:241:VAL:HG23	2:B:243:PRO:HD3	1.16	1.08
1:A:122:GLU:HA	1:A:125:ARG:HD2	1.41	1.02

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)
1:A:448:ARG:NH2	1:A:448:ARG:NH2[3_555]	1.54	0.66

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	547/563 (97%)	427 (78%)	91 (17%)	29 (5%)	2	18
2	B	399/443 (90%)	338 (85%)	44 (11%)	17 (4%)	3	23
All	All	946/1006 (94%)	765 (81%)	135 (14%)	46 (5%)	3	20

5 of 46 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	90	VAL
1	A	138	GLU
1	A	195	ILE
1	A	230	MET

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Mol	Chain	Res	Type
1	A	286	THR

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	491/503 (98%)	344 (70%)	147 (30%)	0 1
2	B	369/403 (92%)	271 (73%)	98 (27%)	0 2
All	All	860/906 (95%)	615 (72%)	245 (28%)	0 1

5 of 245 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	422	LEU
1	A	503	LEU
2	B	310	LEU
1	A	430	GLU
1	A	454	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 32 such sidechains are listed below:

Mol	Chain	Res	Type
1	A	474	ASN
2	B	96	HIS
2	B	373	GLN
1	A	524	GLN
2	B	103	ASN

5.3.3 RNA

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	R8D	A	601	-	30,31,31	2.46	16 (53%)	32,43,43	3.21	17 (53%)

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	R8D	A	601	-	-	0/9/11/11	0/4/4/4

The worst 5 of 16 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	601	R8D	C2-C25	-5.43	1.30	1.44
3	A	601	R8D	C5-C4	-4.07	1.31	1.38
3	A	601	R8D	C6-CL27	-4.05	1.65	1.74
3	A	601	R8D	O7-C4	-3.86	1.31	1.39
3	A	601	R8D	O7-C8	-2.68	1.33	1.39

The worst 5 of 17 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	A	601	R8D	C5-C6-CL27	-6.80	110.69	119.14
3	A	601	R8D	O7-C8-C13	-5.90	106.05	119.84
3	A	601	R8D	C4-C5-C6	-5.15	111.80	118.08
3	A	601	R8D	C8-C13-CL28	-4.32	114.09	119.42
3	A	601	R8D	C22-C23-N24	-3.57	118.35	123.94

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 16 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	601	R8D	16	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, 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	549/563 (97%)	-0.16	8 (1%)	76	62	26, 58, 95, 145	0
2	B	405/443 (91%)	-0.14	11 (2%)	58	42	23, 51, 107, 124	0
All	All	954/1006 (94%)	-0.15	19 (1%)	68	52	23, 56, 105, 145	0

The worst 5 of 19 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	252	TRP	4.7
1	A	546	GLU	3.9
1	A	360	ALA	3.1
2	B	90	VAL	3.1
2	B	362	THR	3.1

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

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

6.3 Carbohydrates

There are no carbohydrates in this entry.

6.4 Ligands

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	R8D	A	601	28/28	0.92	0.30	1.49	64,69,79,79	0

6.5 Other polymers (i)

There are no such residues in this entry.