Full wwPDB X-ray Structure Validation Report (i)

Sep 5, 2023 – 04:26 AM EDT

PDB ID	:	3URQ
Title	:	Crystal Structure of PTE mutant H254G/H257W/L303T/M317L/I106C/F132I/L271I/K185R/I274N/A80V/R67H with cyclohexyl methylphosphonate inhibitor
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Deposited on	:	2011-11-22
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
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

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

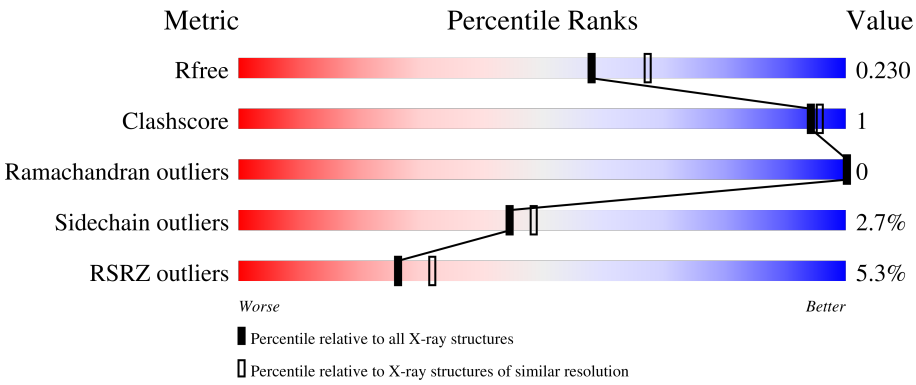
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.35
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35

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 2.10 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}	130704	5197 (2.10-2.10)
Clashscore	141614	5710 (2.10-2.10)
Ramachandran outliers	138981	5647 (2.10-2.10)
Sidechain outliers	138945	5648 (2.10-2.10)
RSRZ outliers	127900	5083 (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 of the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. 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	327	3% 95%
1	B	327	7% 94% 5%

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	QMP	A	902	-	-	X	-

2 Entry composition (i)

There are 5 unique types of molecules in this entry. The entry contains 5319 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 Parathion hydrolase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	327	2497	1576	443	471	7	0	0	0
1	B	322	2460	1555	437	461	7	0	0	0

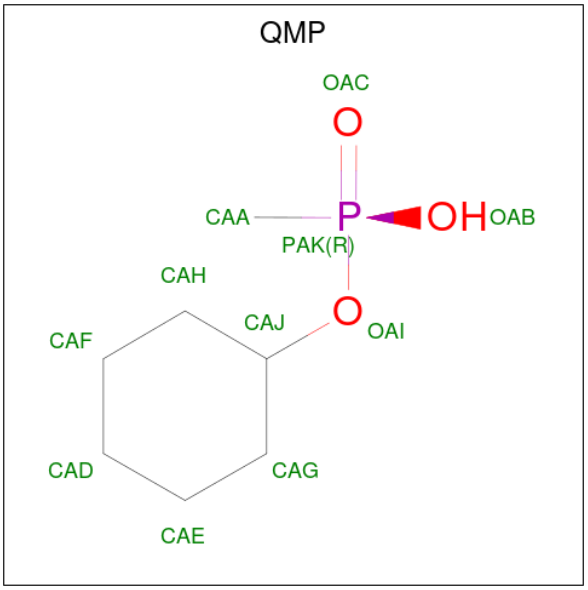
There are 22 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	67	HIS	ARG	engineered mutation	UNP P0A434
A	80	VAL	ALA	engineered mutation	UNP P0A434
A	106	CYS	ILE	engineered mutation	UNP P0A434
A	132	ILE	PHE	engineered mutation	UNP P0A434
A	185	ARG	LYS	engineered mutation	UNP P0A434
A	254	GLY	HIS	engineered mutation	UNP P0A434
A	257	TRP	HIS	engineered mutation	UNP P0A434
A	271	ILE	LEU	engineered mutation	UNP P0A434
A	274	ASN	ILE	engineered mutation	UNP P0A434
A	303	THR	LEU	engineered mutation	UNP P0A434
A	317	LEU	MET	engineered mutation	UNP P0A434
B	67	HIS	ARG	engineered mutation	UNP P0A434
B	80	VAL	ALA	engineered mutation	UNP P0A434
B	106	CYS	ILE	engineered mutation	UNP P0A434
B	132	ILE	PHE	engineered mutation	UNP P0A434
B	185	ARG	LYS	engineered mutation	UNP P0A434
B	254	GLY	HIS	engineered mutation	UNP P0A434
B	257	TRP	HIS	engineered mutation	UNP P0A434
B	271	ILE	LEU	engineered mutation	UNP P0A434
B	274	ASN	ILE	engineered mutation	UNP P0A434
B	303	THR	LEU	engineered mutation	UNP P0A434
B	317	LEU	MET	engineered mutation	UNP P0A434

- Molecule 2 is COBALT (II) ION (three-letter code: CO) (formula: Co).

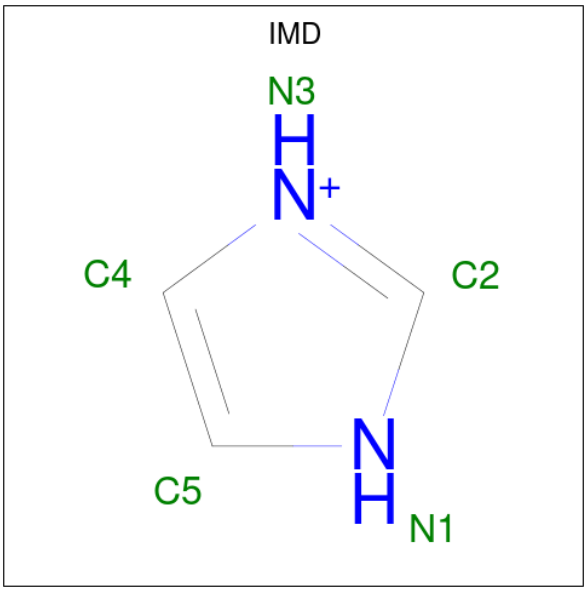
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Co		
2	A	2	2	2	0	0
			Total	Co		
2	B	2	2	2	0	0

- Molecule 3 is cyclohexyl methylphosphonate (three-letter code: QMP) (formula: $C_7H_{15}O_3P$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	O	P		
3	A	1	11	7	3	1	0	0
			Total	C	O	P		
3	B	1	11	7	3	1	0	0

- Molecule 4 is IMIDAZOLE (three-letter code: IMD) (formula: $C_3H_5N_2$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	C	N		
4	A	1	5	3	2	0	0
			Total	C	N		
4	A	1	5	3	2	0	0
			Total	C	N		
4	A	1	5	3	2	0	0
			Total	C	N		
4	B	1	5	3	2	0	0

- Molecule 5 is water.

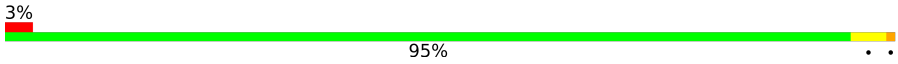
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
5	A	182	182	182	0	0
			Total	O		
5	B	134	134	134	0	0

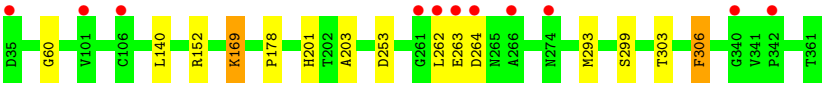
3 Residue-property plots (i)

These plots are drawn for all protein, RNA, DNA and oligosaccharide 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: Parathion hydrolase

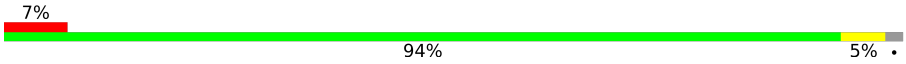
Chain A:

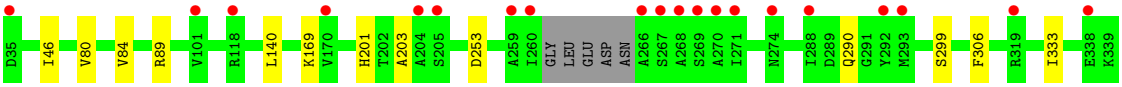


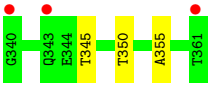


- Molecule 1: Parathion hydrolase

Chain B:







4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, α, β, γ	85.49Å 85.28Å 87.87Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	50.00 – 2.10 35.52 – 2.10	Depositor EDS
% Data completeness (in resolution range)	99.5 (50.00-2.10) 99.7 (35.52-2.10)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.01	Depositor
$< I/\sigma(I) >$ [1]	4.25 (at 2.10Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.203 , 0.235 0.200 , 0.230	Depositor DCC
R_{free} test set	1899 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å^2)	32.0	Xtriage
Anisotropy	0.338	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.31 , 28.7	EDS
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	0.019 for l,-k,h 0.021 for -h,-l,-k 0.019 for k,h,-l 0.006 for l,h,k 0.006 for k,l,h	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	5319	wwPDB-VP
Average B, all atoms (Å^2)	38.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.73% 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, 0.333 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: KCX, CO, IMD, QMP

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	0.62	0/2532	0.76	2/3441 (0.1%)
1	B	0.62	0/2494	0.75	2/3388 (0.1%)
All	All	0.62	0/5026	0.76	4/6829 (0.1%)

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	203	ALA	N-CA-C	-6.53	93.36	111.00
1	B	203	ALA	N-CA-C	-6.12	94.48	111.00
1	A	253	ASP	N-CA-C	5.23	125.12	111.00
1	B	253	ASP	N-CA-C	5.11	124.79	111.00

There are no chirality outliers.

There are no planarity outliers.

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	2497	0	2502	6	0
1	B	2460	0	2471	5	0
2	A	2	0	0	0	0
2	B	2	0	0	0	0
3	A	11	0	14	6	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	B	11	0	14	2	0
4	A	15	0	15	0	0
4	B	5	0	5	0	0
5	A	182	0	0	1	0
5	B	134	0	0	0	0
All	All	5319	0	5021	13	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 1.

All (13) 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)
3:A:902:QMP:H9	3:A:902:QMP:OAC	1.68	0.94
1:A:60:GLY:HA3	3:A:902:QMP:H4	1.49	0.92
1:B:201:HIS:HE1	3:B:901:QMP:H12	1.61	0.65
3:A:902:QMP:OAC	3:A:902:QMP:CAH	2.47	0.60
1:B:201:HIS:CE1	3:B:901:QMP:H12	2.40	0.55
1:A:303:THR:HG21	3:A:902:QMP:H5	1.93	0.50
1:A:306:PHE:CE1	3:A:902:QMP:H3	2.46	0.49
1:B:46:ILE:HG23	1:B:355:ALA:HB1	1.95	0.48
1:B:333:ILE:HD11	1:B:350:THR:HG21	1.98	0.46
1:A:293:MET:HE2	5:A:1169:HOH:O	2.16	0.45
1:A:303:THR:CG2	3:A:902:QMP:H5	2.48	0.43
1:A:169:KCX:OQ1	1:A:201:HIS:HB2	2.20	0.42
1:B:80:VAL:O	1:B:84:VAL:HG23	2.20	0.41

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	324/327 (99%)	312 (96%)	12 (4%)	0	100	100
1	B	317/327 (97%)	305 (96%)	12 (4%)	0	100	100
All	All	641/654 (98%)	617 (96%)	24 (4%)	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	262/262 (100%)	254 (97%)	8 (3%)	40	43
1	B	258/262 (98%)	252 (98%)	6 (2%)	50	55
All	All	520/524 (99%)	506 (97%)	14 (3%)	44	48

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

Mol	Chain	Res	Type
1	A	140	LEU
1	A	152	ARG
1	A	178	PRO
1	A	262	LEU
1	A	263	GLU
1	A	264	ASP
1	A	299	SER
1	A	306	PHE
1	B	89	ARG
1	B	140	LEU
1	B	290	GLN
1	B	299	SER
1	B	306	PHE
1	B	345	THR

Sometimes 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)

2 non-standard protein/DNA/RNA residues 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	$\#\|Z\| > 2$
1	KCX	B	169	1,2	9,11,12	0.85	0	5,12,14	2.11	1 (20%)
1	KCX	A	169	1,2	9,11,12	0.84	1 (11%)	5,12,14	2.07	1 (20%)

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
1	KCX	B	169	1,2	-	0/9/10/12	-
1	KCX	A	169	1,2	-	0/9/10/12	-

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	169	KCX	OQ1-CX	2.01	1.25	1.21

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	169	KCX	OQ1-CX-NZ	-4.48	118.01	124.96
1	A	169	KCX	OQ1-CX-NZ	-4.46	118.05	124.96

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	A	169	KCX	1	0

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 10 ligands modelled in this entry, 4 are monoatomic - leaving 6 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	$\#\|Z\| > 2$
4	IMD	A	906	-	3,5,5	0.19	0	4,5,5	0.87	0
3	QMP	A	902	-	11,11,11	2.51	3 (27%)	10,15,15	0.87	1 (10%)
4	IMD	A	904	-	3,5,5	0.21	0	4,5,5	0.86	0
3	QMP	B	901	2	11,11,11	1.50	2 (18%)	10,15,15	0.50	0
4	IMD	A	903	-	3,5,5	0.22	0	4,5,5	0.85	0
4	IMD	B	905	-	3,5,5	0.21	0	4,5,5	0.83	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
4	IMD	A	906	-	-	-	0/1/1/1
3	QMP	A	902	-	-	2/4/13/13	0/1/1/1
4	IMD	A	904	-	-	-	0/1/1/1
3	QMP	B	901	2	-	0/4/13/13	0/1/1/1
4	IMD	A	903	-	-	-	0/1/1/1
4	IMD	B	905	-	-	-	0/1/1/1

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	902	QMP	PAK-OAC	6.89	1.61	1.50
3	B	901	QMP	PAK-OAB	3.48	1.61	1.54
3	A	902	QMP	PAK-OAB	-3.25	1.48	1.54
3	A	902	QMP	PAK-OAI	2.80	1.61	1.57
3	B	901	QMP	PAK-OAI	2.70	1.61	1.57

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	A	902	QMP	OAC-PAK-CAA	-2.01	105.87	113.74

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	902	QMP	CAH-CAJ-OAI-PAK
3	A	902	QMP	CAJ-OAI-PAK-CAA

There are no ring outliers.

2 monomers are involved in 8 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	902	QMP	6	0
3	B	901	QMP	2	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	326/327 (99%)	0.04	11 (3%)	45	51	23, 32, 58, 76	0
1	B	321/327 (98%)	0.24	23 (7%)	15	19	21, 36, 65, 97	0
All	All	647/654 (98%)	0.14	34 (5%)	26	32	21, 34, 62, 97	0

All (34) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	269	SER	6.6
1	A	261	GLY	5.8
1	A	262	LEU	5.5
1	B	274	ASN	5.0
1	B	270	ALA	4.9
1	A	263	GLU	4.7
1	B	35	ASP	4.6
1	B	266	ALA	4.3
1	A	35	ASP	4.0
1	B	267	SER	4.0
1	B	271	ILE	3.7
1	B	259	ALA	3.7
1	B	268	ALA	3.7
1	B	260	ILE	3.4
1	B	361	THR	3.3
1	A	101	VAL	3.2
1	A	264	ASP	2.8
1	B	340	GLY	2.7
1	A	266	ALA	2.7
1	B	170	VAL	2.6
1	B	118	ARG	2.6
1	B	101	VAL	2.4
1	A	106	CYS	2.4
1	A	274	ASN	2.3

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Mol	Chain	Res	Type	RSRZ
1	A	340	GLY	2.2
1	B	338	GLU	2.2
1	B	343	GLN	2.2
1	B	205	SER	2.2
1	B	319	ARG	2.2
1	B	293	MET	2.1
1	B	204	ALA	2.1
1	A	342	PRO	2.1
1	B	288	ILE	2.0
1	B	292	TYR	2.0

6.2 Non-standard residues in protein, DNA, RNA chains (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. 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	B-factors(Å^2)	Q<0.9
1	KCX	B	169	12/13	0.91	0.20	27,31,40,43	0
1	KCX	A	169	12/13	0.92	0.16	25,28,34,35	0

6.3 Carbohydrates (i)

There are no monosaccharides 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. 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	B-factors(Å^2)	Q<0.9
4	IMD	A	906	5/5	0.79	0.28	52,53,54,54	0
4	IMD	B	905	5/5	0.79	0.23	62,62,62,62	0
3	QMP	B	901	11/11	0.87	0.24	72,72,75,75	0
4	IMD	A	903	5/5	0.88	0.19	45,47,48,48	0
4	IMD	A	904	5/5	0.89	0.20	40,43,44,45	0
3	QMP	A	902	11/11	0.90	0.24	62,64,69,69	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	CO	A	802	1/1	0.97	0.10	33,33,33,33	0
2	CO	B	804	1/1	0.98	0.05	47,47,47,47	0
2	CO	A	801	1/1	0.99	0.03	35,35,35,35	0
2	CO	B	803	1/1	1.00	0.06	37,37,37,37	0

6.5 Other polymers (i)

There are no such residues in this entry.