



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 01:44 PM GMT

PDB ID : 3URA
Title : Crystal Structure of PTE mutant H254G/H257W/L303T/K185R/I274N/A80V/S61T
Authors : Tsai, P.; Fox, N.G.; Li, Y.; Barondeau, D.P.; Raushel, F.M.
Deposited on : 2011-11-21
Resolution : 1.88 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 ⓘ symbol.

The following versions of software and data (see [references ⓘ](#)) 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

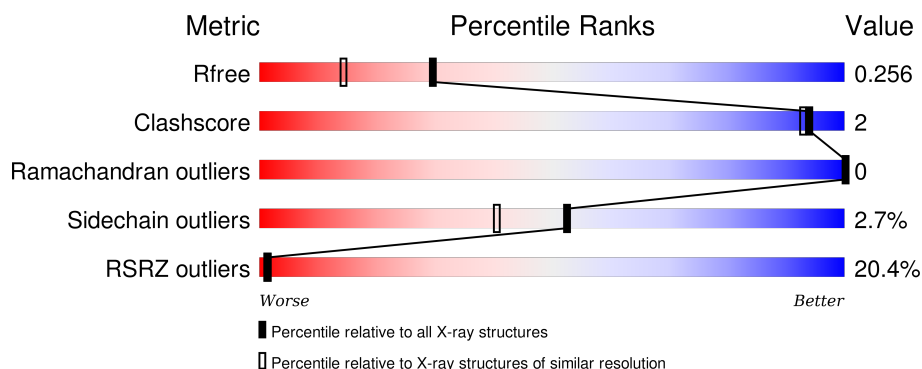
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.88 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	6965 (1.90-1.86)
Clashscore	102246	7778 (1.90-1.86)
Ramachandran outliers	100387	7691 (1.90-1.86)
Sidechain outliers	100360	7692 (1.90-1.86)
RSRZ outliers	91569	6979 (1.90-1.86)

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 $\leq 5\%$. 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	<div> <div>2%</div> <div>96%</div> <div>.</div> </div>
1	B	327	<div> <div>38%</div> <div>89%</div> <div>9%</div> <div>..</div> </div>

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
2	IMD	A	1372	-	-	-	X

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 5351 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.

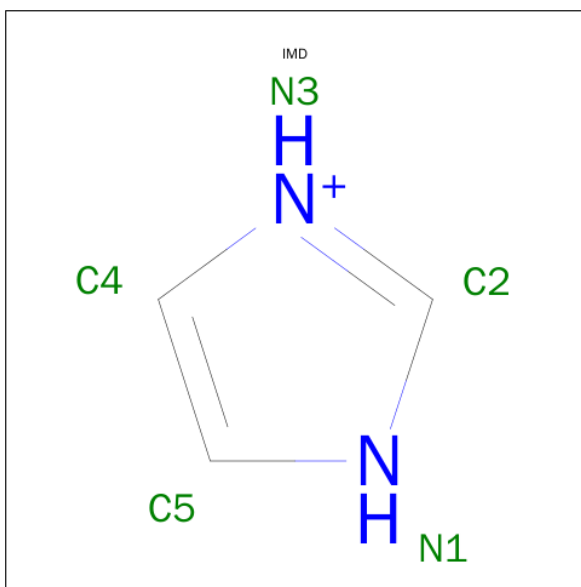
- Molecule 1 is a protein called Parathion hydrolase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	327	Total	C	N	O	S	0	0	0
			2504	1582	444	471	7			
1	B	322	Total	C	N	O	S	0	0	0
			2467	1561	439	460	7			

There are 14 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	61	THR	SER	ENGINEERED MUTATION	UNP P0A434
A	80	VAL	ALA	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	274	ASN	ILE	ENGINEERED MUTATION	UNP P0A434
A	303	THR	LEU	ENGINEERED MUTATION	UNP P0A434
B	61	THR	SER	ENGINEERED MUTATION	UNP P0A434
B	80	VAL	ALA	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	274	ASN	ILE	ENGINEERED MUTATION	UNP P0A434
B	303	THR	LEU	ENGINEERED MUTATION	UNP P0A434

- Molecule 2 is IMIDAZOLE (three-letter code: IMD) (formula: C₃H₅N₂).



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

- Molecule 3 is COBALT (II) ION (three-letter code: CO) (formula: Co).

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

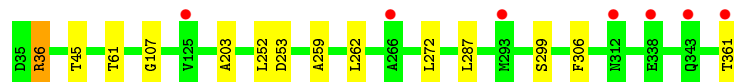
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	279	Total	O	0	0
			279	279		
4	B	92	Total	O	0	0
			92	92		

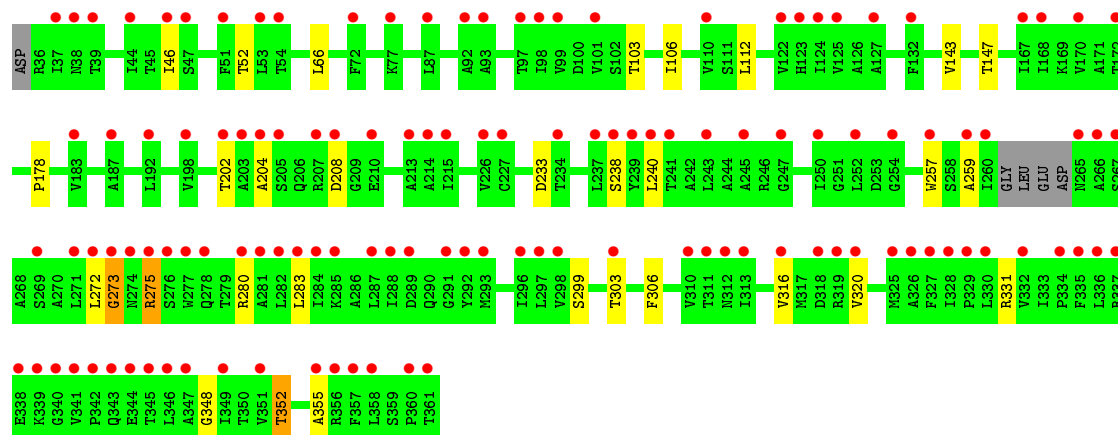
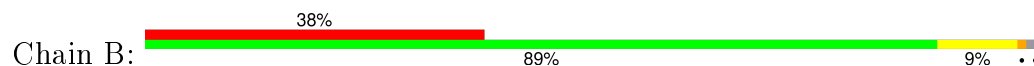
3 Residue-property plots [i](#)

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: Parathion hydrolase



- Molecule 1: Parathion hydrolase



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, α , β , γ	85.21Å 85.52Å 88.14Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	50.00 – 1.88 39.17 – 1.89	Depositor EDS
% Data completeness (in resolution range)	98.2 (50.00-1.88) 99.3 (39.17-1.89)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.11	Depositor
$\langle I/\sigma(I) \rangle$ ¹	9.26 (at 1.88Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.232 , 0.253 0.235 , 0.256	Depositor DCC
R_{free} test set	2662 reflections (5.11%)	DCC
Wilson B-factor (Å ²)	28.5	Xtriage
Anisotropy	0.413	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 35.6	EDS
Estimated twinning fraction	0.025 for -h,l,k 0.023 for -l,-k,-h 0.023 for k,h,-l 0.012 for k,l,h 0.012 for l,h,k	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.46$, $\langle L^2 \rangle = 0.29$	Xtriage
Outliers	0 of 52140 reflections	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	5351	wwPDB-VP
Average B, all atoms (Å ²)	42.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.09% of the height of the origin peak. No significant pseudotranslation is detected.*

¹ Intensities estimated from amplitudes.

² Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 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: CO, IMD, KCX

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	0.63	0/2539	0.76	2/3449 (0.1%)
1	B	0.62	0/2501	0.76	1/3396 (0.0%)
All	All	0.62	0/5040	0.76	3/6845 (0.0%)

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	203	ALA	N-CA-C	-6.55	93.32	111.00
1	B	273	GLY	N-CA-C	5.49	126.83	113.10
1	A	253	ASP	N-CA-C	5.04	124.62	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	2504	0	2512	4	0
1	B	2467	0	2483	14	0
2	A	5	0	5	0	0
3	A	2	0	0	0	0
3	B	2	0	0	0	0
4	A	279	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	B	92	0	0	3	0
All	All	5351	0	5000	18	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 2.

All (18) 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:B:202:THR:HG23	1:B:208:ASP:HB2	1.79	0.64
1:B:275:ARG:HH12	1:B:280:ARG:HE	1.56	0.54
1:B:143:VAL:O	1:B:147:THR:HG23	2.08	0.53
1:B:283:LEU:HD13	4:B:1247:HOH:O	2.12	0.50
1:A:36:ARG:HH21	1:A:45:THR:HG23	1.76	0.49
1:B:46:ILE:HG23	1:B:355:ALA:HB1	1.95	0.48
1:B:259:ALA:HB3	1:B:273:GLY:O	2.15	0.46
1:B:257:TRP:O	1:B:280:ARG:NH1	2.49	0.46
1:B:348:GLY:HA2	1:B:352:THR:HG23	1.97	0.45
1:A:252:LEU:HD11	1:A:287:LEU:HD12	2.00	0.44
1:B:316:VAL:O	1:B:320:VAL:HG23	2.17	0.44
1:B:66:LEU:HD21	1:B:112:LEU:HD22	1.99	0.43
1:B:240:LEU:HD11	4:B:1247:HOH:O	2.18	0.42
1:A:259:ALA:HB2	1:A:272:LEU:HB2	2.02	0.41
1:B:204:ALA:HB3	1:B:233:ASP:HB2	2.03	0.41
1:A:61:THR:HG23	1:A:107:GLY:HA3	2.02	0.41
1:B:103:THR:H	1:B:106:ILE:HD12	1.85	0.40
1:B:238:SER:HB2	4:B:1282:HOH:O	2.21	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	324/327 (99%)	312 (96%)	12 (4%)	0	100	100
1	B	317/327 (97%)	297 (94%)	20 (6%)	0	100	100
All	All	641/654 (98%)	609 (95%)	32 (5%)	0	100	100

There are no Ramachandran outliers to report.

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	262/262 (100%)	257 (98%)	5 (2%)	65	56
1	B	258/262 (98%)	249 (96%)	9 (4%)	43	29
All	All	520/524 (99%)	506 (97%)	14 (3%)	52	40

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

Mol	Chain	Res	Type
1	A	36	ARG
1	A	262	LEU
1	A	299	SER
1	A	306	PHE
1	A	361	THR
1	B	52	THR
1	B	178	PRO
1	B	272	LEU
1	B	275	ARG
1	B	299	SER
1	B	303	THR
1	B	306	PHE
1	B	331	ARG
1	B	352	THR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	155	GLN
1	B	290	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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	A	169	1,3	7,11,12	0.46	0	7,12,14	0.81	0
1	KCX	B	169	1,3	7,11,12	0.48	0	7,12,14	0.94	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
1	KCX	A	169	1,3	-	0/6/10/12	0/0/0/0
1	KCX	B	169	1,3	-	0/6/10/12	0/0/0/0

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates

There are no carbohydrates in this entry.

5.6 Ligand geometry

Of 5 ligands modelled in this entry, 4 are monoatomic - leaving 1 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	$\# Z > 2$
2	IMD	A	1372	-	3,5,5	0.20	0	4,5,5	0.88	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
2	IMD	A	1372	-	-	0/0/0/0	0/1/1/1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

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, 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%)	0.17	7 (2%) 67 69	17, 26, 44, 63	0
1	B	321/327 (98%)	1.84	125 (38%) 0 0	26, 58, 76, 82	0
All	All	647/654 (98%)	1.00	132 (20%) 1 1	17, 39, 74, 82	0

All (132) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	245	ALA	7.2
1	B	282	LEU	6.7
1	B	259	ALA	6.1
1	B	241	THR	5.8
1	B	288	ILE	5.8
1	B	335	PHE	5.7
1	B	347	ALA	5.4
1	B	272	LEU	5.3
1	B	298	VAL	5.2
1	B	293	MET	5.1
1	B	346	LEU	5.1
1	B	274	ASN	5.0
1	B	330	LEU	5.0
1	B	341	VAL	4.9
1	A	361	THR	4.7
1	B	292	TYR	4.5
1	B	254	GLY	4.5
1	B	271	LEU	4.5
1	B	269	SER	4.2
1	B	342	PRO	4.2
1	B	281	ALA	4.2
1	B	337	ARG	4.2
1	B	260	ILE	4.1
1	B	277	TRP	4.0

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Mol	Chain	Res	Type	RSRZ
1	B	198	VAL	3.8
1	B	339	LYS	3.7
1	B	239	TYR	3.7
1	B	240	LEU	3.6
1	B	51	PHE	3.6
1	B	338	GLU	3.6
1	B	98	ILE	3.6
1	B	204	ALA	3.6
1	B	297	LEU	3.5
1	B	213	ALA	3.5
1	B	296	ILE	3.4
1	B	287	LEU	3.4
1	B	289	ASP	3.4
1	B	266	ALA	3.4
1	B	328	ILE	3.4
1	B	326	ALA	3.3
1	B	334	PRO	3.3
1	B	312	ASN	3.3
1	B	125	VAL	3.2
1	B	77	LYS	3.2
1	B	205	SER	3.2
1	B	252	LEU	3.2
1	B	257	TRP	3.2
1	B	340	GLY	3.1
1	B	237	LEU	3.1
1	B	336	LEU	3.1
1	B	203	ALA	3.1
1	B	127	ALA	3.1
1	B	319	ARG	3.1
1	B	283	LEU	3.0
1	B	327	PHE	3.0
1	B	192	LEU	3.0
1	B	167	ILE	3.0
1	B	99	VAL	2.9
1	B	329	PRO	2.9
1	B	238	SER	2.9
1	B	320	VAL	2.9
1	B	332	VAL	2.9
1	B	356	ARG	2.8
1	B	276	SER	2.8
1	B	227	CYS	2.8
1	B	355	ALA	2.8

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Mol	Chain	Res	Type	RSRZ
1	B	122	VAL	2.8
1	B	318	ASP	2.8
1	B	214	ALA	2.7
1	B	343	GLN	2.7
1	B	54	THR	2.7
1	A	125	VAL	2.7
1	B	273	GLY	2.6
1	B	37	ILE	2.6
1	A	312	ASN	2.6
1	B	291	GLY	2.6
1	B	349	ILE	2.6
1	B	357	PHE	2.6
1	B	226	VAL	2.5
1	B	285	LYS	2.5
1	B	303	THR	2.5
1	B	44	ILE	2.5
1	B	97	THR	2.5
1	B	325	MET	2.5
1	B	38	ASN	2.5
1	B	243	LEU	2.5
1	B	168	ILE	2.5
1	B	46	ILE	2.5
1	B	344	GLU	2.4
1	B	208	ASP	2.4
1	B	132	PHE	2.4
1	B	202	THR	2.4
1	B	275	ARG	2.4
1	B	124	ILE	2.4
1	B	361	THR	2.4
1	B	207	ARG	2.4
1	B	351	VAL	2.4
1	A	266	ALA	2.3
1	B	93	ALA	2.3
1	B	110	VAL	2.3
1	B	313	ILE	2.3
1	B	87	LEU	2.3
1	B	265	ASN	2.3
1	B	280	ARG	2.3
1	B	215	ILE	2.3
1	B	47	SER	2.3
1	B	345	THR	2.3
1	B	358	LEU	2.3

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Mol	Chain	Res	Type	RSRZ
1	B	210	GLU	2.2
1	B	360	PRO	2.2
1	B	187	ALA	2.2
1	B	101	VAL	2.2
1	B	234	THR	2.2
1	B	250	ILE	2.2
1	B	284	ILE	2.2
1	B	267	SER	2.2
1	A	338	GLU	2.2
1	B	123	HIS	2.2
1	B	310	VAL	2.2
1	B	39	THR	2.2
1	B	92	ALA	2.2
1	B	170	VAL	2.2
1	B	183	VAL	2.2
1	B	278	GLN	2.1
1	B	316	VAL	2.1
1	B	72	PHE	2.1
1	B	311	THR	2.1
1	B	53	LEU	2.1
1	B	247	GLY	2.1
1	A	343	GLN	2.1
1	B	172	THR	2.1
1	A	293	MET	2.1

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. 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
1	KCX	A	169	12/13	0.95	0.11	-	14,17,22,23	0
1	KCX	B	169	12/13	0.86	0.23	-	45,46,48,51	0

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
2	IMD	A	1372	5/5	0.85	0.22	7.54	33,33,35,36	0
3	CO	A	801	1/1	1.00	0.03	-	22,22,22,22	0
3	CO	B	803	1/1	0.96	0.05	-	48,48,48,48	0
3	CO	B	804	1/1	0.93	0.05	-	57,57,57,57	0
3	CO	A	802	1/1	0.99	0.08	-	21,21,21,21	0

6.5 Other polymers [i](#)

There are no such residues in this entry.