



wwPDB X-ray Structure Validation Summary Report ⓘ

Jan 22, 2018 – 03:49 AM EST

PDB ID : 2OBY
Title : Crystal structure of Human P53 inducible oxidoreductase (TP53I3,PIG3)
Authors : Porte, S.; Valencia, E.; Farres, J.; Fita, I.; Pike, A.C.W.; Shafqat, N.; Debreczeni, J.; Johansson, C.; Haroniti, A.; Gileadi, O.; Arrowsmith, C.H.; Edwards, A.; Weigelt, J.; Sundstrom, M.; von Delft, F.; Oppermann, U.; Pares, X.
Deposited on : 2006-12-20
Resolution : 3.00 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 ⓘ symbol.

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

MolProbity	:	4.02b-467
Mogul	:	1.7.2 (RC1), CSD as538be (2017)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20030736
Percentile statistics	:	20161228.v01 (using entries in the PDB archive December 28th 2016)
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)	:	rb-20030736

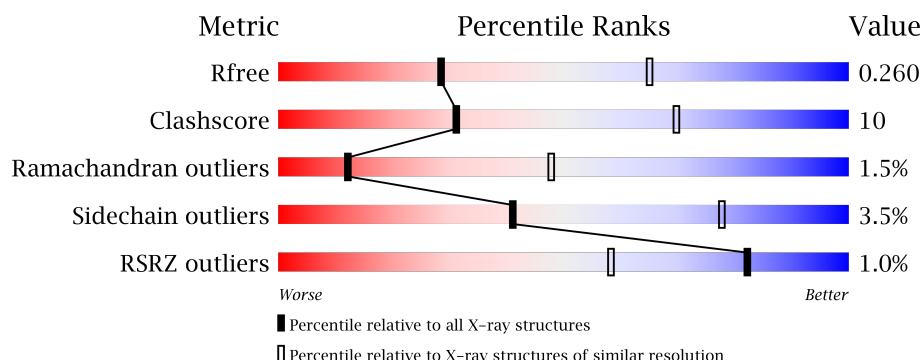
1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.00 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}	100719	1692 (3.00-3.00)
Clashscore	112137	2037 (3.00-3.00)
Ramachandran outliers	110173	1973 (3.00-3.00)
Sidechain outliers	110143	1976 (3.00-3.00)
RSRZ outliers	101464	1716 (3.00-3.00)

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	338	<div> <div></div> <div>75%</div> <div>22%</div> <div>..</div> </div>
1	B	338	<div> <div></div> <div>75%</div> <div>22%</div> <div>..</div> </div>
1	C	338	<div> <div></div> <div>78%</div> <div>21%</div> <div>..</div> </div>
1	D	338	<div> <div></div> <div>78%</div> <div>20%</div> <div>..</div> </div>
1	E	338	<div> <div></div> <div>74%</div> <div>23%</div> <div>..</div> </div>

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 12823 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 Putative quinone oxidoreductase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	334	Total	C	N	O	S	0	0	0
			2516	1613	429	462	12			
1	B	334	Total	C	N	O	S	0	0	0
			2516	1613	429	462	12			
1	C	334	Total	C	N	O	S	0	0	0
			2516	1613	429	462	12			
1	D	334	Total	C	N	O	S	0	0	0
			2516	1613	429	462	12			
1	E	334	Total	C	N	O	S	0	0	0
			2516	1613	429	462	12			

There are 30 discrepancies between the modelled and reference sequences:

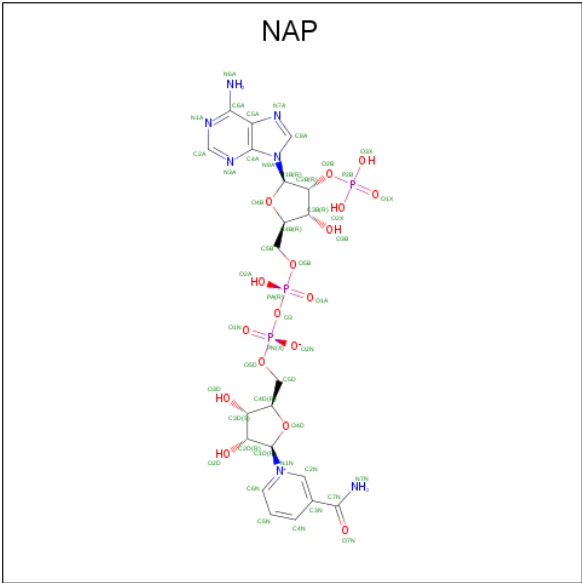
Chain	Residue	Modelled	Actual	Comment	Reference
A	-5	GLY	-	CLONING ARTIFACT	UNP Q53FA7
A	-4	SER	-	CLONING ARTIFACT	UNP Q53FA7
A	-3	PRO	-	CLONING ARTIFACT	UNP Q53FA7
A	-2	GLY	-	CLONING ARTIFACT	UNP Q53FA7
A	-1	ILE	-	CLONING ARTIFACT	UNP Q53FA7
A	0	PRO	-	CLONING ARTIFACT	UNP Q53FA7
B	-5	GLY	-	CLONING ARTIFACT	UNP Q53FA7
B	-4	SER	-	CLONING ARTIFACT	UNP Q53FA7
B	-3	PRO	-	CLONING ARTIFACT	UNP Q53FA7
B	-2	GLY	-	CLONING ARTIFACT	UNP Q53FA7
B	-1	ILE	-	CLONING ARTIFACT	UNP Q53FA7
B	0	PRO	-	CLONING ARTIFACT	UNP Q53FA7
C	-5	GLY	-	CLONING ARTIFACT	UNP Q53FA7
C	-4	SER	-	CLONING ARTIFACT	UNP Q53FA7
C	-3	PRO	-	CLONING ARTIFACT	UNP Q53FA7
C	-2	GLY	-	CLONING ARTIFACT	UNP Q53FA7
C	-1	ILE	-	CLONING ARTIFACT	UNP Q53FA7
C	0	PRO	-	CLONING ARTIFACT	UNP Q53FA7
D	-5	GLY	-	CLONING ARTIFACT	UNP Q53FA7

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Chain	Residue	Modelled	Actual	Comment	Reference
D	-4	SER	-	CLONING ARTIFACT	UNP Q53FA7
D	-3	PRO	-	CLONING ARTIFACT	UNP Q53FA7
D	-2	GLY	-	CLONING ARTIFACT	UNP Q53FA7
D	-1	ILE	-	CLONING ARTIFACT	UNP Q53FA7
D	0	PRO	-	CLONING ARTIFACT	UNP Q53FA7
E	-5	GLY	-	CLONING ARTIFACT	UNP Q53FA7
E	-4	SER	-	CLONING ARTIFACT	UNP Q53FA7
E	-3	PRO	-	CLONING ARTIFACT	UNP Q53FA7
E	-2	GLY	-	CLONING ARTIFACT	UNP Q53FA7
E	-1	ILE	-	CLONING ARTIFACT	UNP Q53FA7
E	0	PRO	-	CLONING ARTIFACT	UNP Q53FA7

- Molecule 2 is NADP NICOTINAMIDE-ADENINE-DINUCLEOTIDE PHOSPHATE (three-letter code: NAP) (formula: C₂₁H₂₈N₇O₁₇P₃).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	0	0
			48	21	7	17	3		
2	B	1	Total	C	N	O	P	0	0
			48	21	7	17	3		
2	C	1	Total	C	N	O	P	0	0
			48	21	7	17	3		
2	D	1	Total	C	N	O	P	0	0
			48	21	7	17	3		
2	E	1	Total	C	N	O	P	0	0
			48	21	7	17	3		

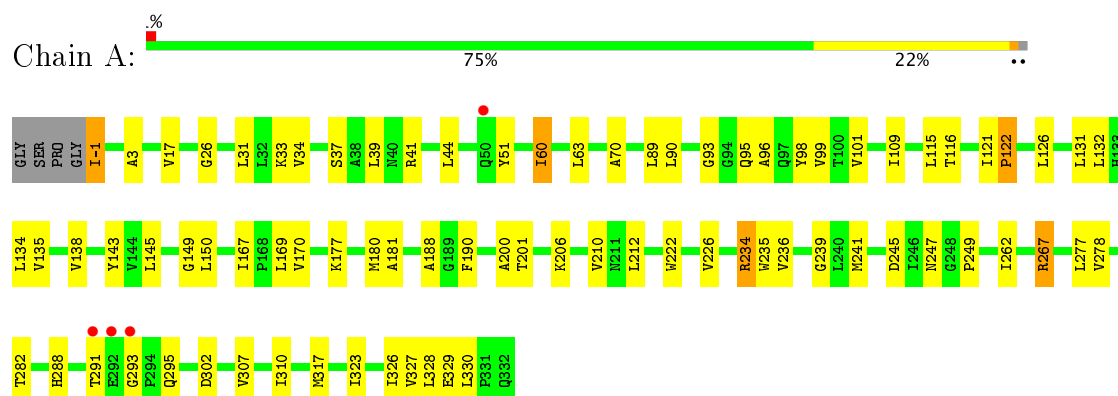
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	1	Total 1	O 1	0	0
3	C	1	Total 1	O 1	0	0
3	E	1	Total 1	O 1	0	0

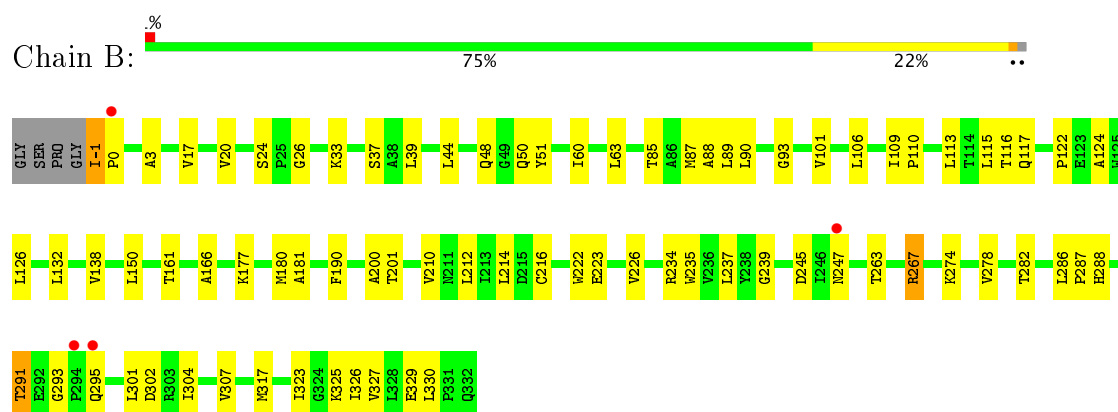
3 Residue-property plots

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.

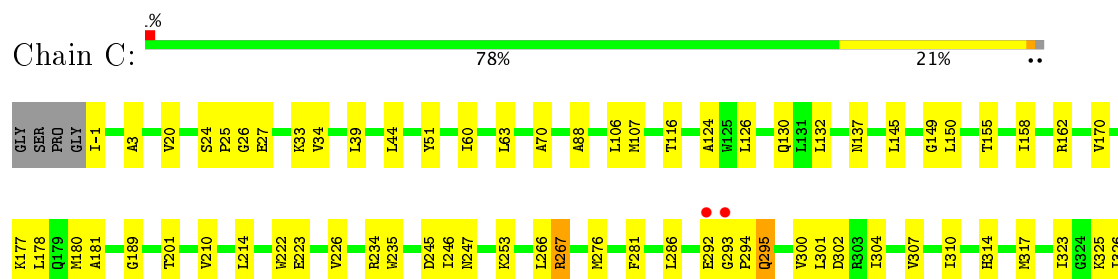
• Molecule 1: Putative quinone oxidoreductase



• Molecule 1: Putative quinone oxidoreductase




• Molecule 1: Putative quinone oxidoreductase



V327
L328
E329
L330
P331
Q332

• Molecule 1: Putative quinone oxidoreductase


Chain D:  78% 20%

GLY SER PRO GLY I-1 A3 V20 A21 K22 E27 K33 L39 L44 Y61 P55 Q56 I60 A70 T85 L89 L90 G93 A96 Q97 Y101 L105 I109 L115 T116 A120 I121 P122 E123 L131 L132 H133 L134 V138

G149 L150 I158 L169 V170 T171 A172 K177 L178 G179 M180 A181 A188 G189 F190 A200 L212 W222 V226 R234 W235 V236 G239 N247 I262 R267 K274 L277 V278 H288 T291 E292 G293 P294 Q295 L301 D302 H303 I304 V307

A313 M317 I323 I326 E329 L330 P331 Q332

• Molecule 1: Putative quinone oxidoreductase

Chain E:  74% 23%

GLY SER PRO GLY I-1 P0 A3 V20 A21 G26 E27 K33 L39 L44 Q50 Y51 P55 I60 L63 A70 Q77 W80 K81 T85 L89 L90 G93 A96 Q97 Y98 V99 L105 L106 I109 P110 E111 T114 L115 Q117

A120 I121 P122 E123 L132 H133 L134 V138 Y143 V144 L145 G149 L150 I167 V170 T171 K177 M180 F190 A200 T201 V210 N211 L212 I217 Y221 W222 V226 R234 W235 G239 N247 R267 K274 Q275 W276 L277 V278 H288

T291 E292 G293 P294 Q295 L301 D302 R303 I304 V307 T308 E309 I310 M317 I323 I326 V327 L328 E329 L330 P331 Q332

4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α , β , γ	68.35Å 184.36Å 318.05Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	19.94 – 3.00 19.94 – 3.00	Depositor EDS
% Data completeness (in resolution range)	88.6 (19.94-3.00) 88.9 (19.94-3.00)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.85 (at 2.98Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.220 , 0.260 0.224 , 0.260	Depositor DCC
R_{free} test set	1792 reflections (5.24%)	DCC
Wilson B-factor (Å ²)	53.7	Xtriage
Anisotropy	0.051	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.29 , 43.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.45$, $\langle L^2 \rangle = 0.27$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.89	EDS
Total number of atoms	12823	wwPDB-VP
Average B, all atoms (Å ²)	48.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.24% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ 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: NAP

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	0.30	0/2570	0.46	0/3485
1	B	0.33	0/2570	0.46	0/3485
1	C	0.31	0/2570	0.48	0/3485
1	D	0.31	0/2570	0.46	0/3485
1	E	0.31	0/2570	0.46	0/3485
All	All	0.31	0/12850	0.47	0/17425

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 [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	2516	0	2566	61	0
1	B	2516	0	2566	55	0
1	C	2516	0	2566	46	0
1	D	2516	0	2566	52	0
1	E	2516	0	2566	56	0
2	A	48	0	25	1	0
2	B	48	0	25	0	0
2	C	48	0	25	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	D	48	0	25	0	0
2	E	48	0	25	0	0
3	A	1	0	0	0	0
3	C	1	0	0	0	0
3	E	1	0	0	0	0
All	All	12823	0	12955	266	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 10.

The worst 5 of 266 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:E:150:LEU:HD13	1:E:177:LYS:HB3	1.56	0.86
1:E:116:THR:HG21	1:E:304:ILE:HD13	1.65	0.78
1:B:150:LEU:HD11	1:B:181:ALA:HB2	1.67	0.77
1:D:150:LEU:HD13	1:D:177:LYS:HB3	1.64	0.77
1:C:310:ILE:HD13	1:C:328:LEU:HD11	1.67	0.76

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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	332/338 (98%)	307 (92%)	21 (6%)	4 (1%)	15	53
1	B	332/338 (98%)	307 (92%)	21 (6%)	4 (1%)	15	53
1	C	332/338 (98%)	309 (93%)	17 (5%)	6 (2%)	10	43
1	D	332/338 (98%)	309 (93%)	18 (5%)	5 (2%)	12	48
1	E	332/338 (98%)	311 (94%)	15 (4%)	6 (2%)	10	43
All	All	1660/1690 (98%)	1543 (93%)	92 (6%)	25 (2%)	12	48

5 of 25 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	293	GLY
1	C	27	GLU
1	C	292	GLU
1	D	27	GLU
1	D	291	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	261/263 (99%)	253 (97%)	8 (3%)	45	80
1	B	261/263 (99%)	252 (97%)	9 (3%)	42	78
1	C	261/263 (99%)	252 (97%)	9 (3%)	42	78
1	D	261/263 (99%)	255 (98%)	6 (2%)	56	85
1	E	261/263 (99%)	247 (95%)	14 (5%)	26	64
All	All	1305/1315 (99%)	1259 (96%)	46 (4%)	41	78

5 of 46 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	162	ARG
1	C	295	GLN
1	E	267	ARG
1	C	234	ARG
1	C	267	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 22 such sidechains are listed below:

Mol	Chain	Res	Type
1	C	95	GLN
1	D	50	GLN
1	E	130	GLN
1	C	247	ASN

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Mol	Chain	Res	Type
1	C	295	GLN

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](#)

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	$\# Z > 2$
2	NAP	A	1400	-	44,52,52	1.69	3 (6%)	51,80,80	1.54	1 (1%)
2	NAP	B	1401	-	44,52,52	1.61	3 (6%)	51,80,80	1.59	1 (1%)
2	NAP	C	1402	-	44,52,52	1.61	3 (6%)	51,80,80	1.53	1 (1%)
2	NAP	D	1403	-	44,52,52	1.61	3 (6%)	51,80,80	1.54	1 (1%)
2	NAP	E	1404	-	44,52,52	1.63	3 (6%)	51,80,80	1.61	2 (3%)

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	NAP	A	1400	-	-	0/27/67/67	0/5/5/5
2	NAP	B	1401	-	-	0/27/67/67	0/5/5/5
2	NAP	C	1402	-	-	0/27/67/67	0/5/5/5
2	NAP	D	1403	-	-	0/27/67/67	0/5/5/5
2	NAP	E	1404	-	-	0/27/67/67	0/5/5/5

The worst 5 of 15 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	1401	NAP	C2A-N1A	2.52	1.38	1.33
2	C	1402	NAP	C2A-N1A	2.55	1.38	1.33
2	D	1403	NAP	C2A-N1A	2.61	1.38	1.33
2	E	1404	NAP	C2A-N1A	2.70	1.39	1.33
2	A	1400	NAP	C2A-N1A	2.74	1.39	1.33

The worst 5 of 6 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	1401	NAP	N3A-C2A-N1A	-10.34	119.85	128.86
2	E	1404	NAP	N3A-C2A-N1A	-10.27	119.92	128.86
2	D	1403	NAP	N3A-C2A-N1A	-10.12	120.04	128.86
2	A	1400	NAP	N3A-C2A-N1A	-10.04	120.11	128.86
2	C	1402	NAP	N3A-C2A-N1A	-9.88	120.25	128.86

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
2	A	1400	NAP	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	334/338 (98%)	-0.36	4 (1%) 79 53	48, 49, 49, 49	0
1	B	334/338 (98%)	-0.19	4 (1%) 79 53	48, 49, 49, 50	0
1	C	334/338 (98%)	-0.43	2 (0%) 89 71	48, 49, 49, 50	0
1	D	334/338 (98%)	-0.31	4 (1%) 79 53	48, 49, 49, 50	0
1	E	334/338 (98%)	-0.33	3 (0%) 84 61	48, 49, 49, 50	0
All	All	1670/1690 (98%)	-0.32	17 (1%) 82 58	48, 49, 49, 50	0

The worst 5 of 17 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	293	GLY	4.0
1	B	295	GLN	2.8
1	E	55	PRO	2.8
1	A	292	GLU	2.7
1	D	294	PRO	2.5

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
2	NAP	D	1403	48/48	0.95	0.18	-0.27	48,48,49,49	0
2	NAP	B	1401	48/48	0.94	0.19	-0.28	48,48,49,49	0
2	NAP	A	1400	48/48	0.94	0.17	-0.34	47,48,49,50	0
2	NAP	E	1404	48/48	0.94	0.16	-0.43	48,48,49,50	0
2	NAP	C	1402	48/48	0.95	0.14	-1.03	48,48,49,50	0

6.5 Other polymers [i](#)

There are no such residues in this entry.