



wwPDB X-ray Structure Validation Summary Report ⓘ

Jan 22, 2018 – 02:06 PM EST

PDB ID : 5M8S
Title : Crystal structure of human tyrosinase related protein 1 mutant (T391V-R374S-Y362F) in complex with phenylthiourea (PTU)
Authors : Lai, X.; Soler-Lopez, M.; Wichers, H.J.; Dijkstra, B.W.
Deposited on : 2016-10-29
Resolution : 2.20 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

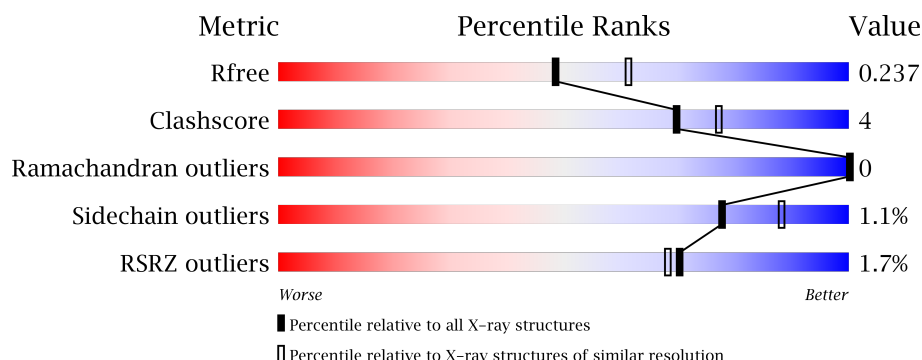
1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.20 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	4002 (2.20-2.20)
Clashscore	112137	4730 (2.20-2.20)
Ramachandran outliers	110173	4656 (2.20-2.20)
Sidechain outliers	110143	4657 (2.20-2.20)
RSRZ outliers	101464	4033 (2.20-2.20)

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	446	<div> <div>91%</div> <div>9%</div> </div>
1	B	446	<div> <div>3%</div> <div>89%</div> <div>10%</div> </div>
1	C	446	<div> <div>2%</div> <div>90%</div> <div>10%</div> </div>
1	D	446	<div> <div>88%</div> <div>12%</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.

ria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
4	URS	B	516	-	X	-	-
4	URS	C	510	-	X	-	-
6	MAN	B	512	-	-	-	X
6	MAN	D	513	-	-	-	X
6	MAN	D	515	-	-	-	X

2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 15622 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 5,6-dihydroxyindole-2-carboxylic acid oxidase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	446	Total	C	N	O	S	0	0	0
			3554	2231	629	671	23			
1	B	446	Total	C	N	O	S	0	0	0
			3554	2231	629	671	23			
1	C	446	Total	C	N	O	S	0	0	0
			3554	2231	629	671	23			
1	D	446	Total	C	N	O	S	0	0	0
			3554	2231	629	671	23			

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	362	PHE	TYR	engineered mutation	UNP P17643
A	374	SER	ARG	engineered mutation	UNP P17643
A	391	VAL	THR	engineered mutation	UNP P17643
B	362	PHE	TYR	engineered mutation	UNP P17643
B	374	SER	ARG	engineered mutation	UNP P17643
B	391	VAL	THR	engineered mutation	UNP P17643
C	362	PHE	TYR	engineered mutation	UNP P17643
C	374	SER	ARG	engineered mutation	UNP P17643
C	391	VAL	THR	engineered mutation	UNP P17643
D	362	PHE	TYR	engineered mutation	UNP P17643
D	374	SER	ARG	engineered mutation	UNP P17643
D	391	VAL	THR	engineered mutation	UNP P17643

- Molecule 2 is N-ACETYL-D-GLUCOSAMINE (three-letter code: NAG) (formula: C₈H₁₅NO₆).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	N	O	0	0
			14	8	1	5		
2	A	1	Total	C	N	O	0	0
			14	8	1	5		
2	A	1	Total	C	N	O	0	0
			14	8	1	5		
2	A	1	Total	C	N	O	0	0
			14	8	1	5		
2	A	1	Total	C	N	O	0	0
			14	8	1	5		
2	A	1	Total	C	N	O	0	0
			14	8	1	5		
2	B	1	Total	C	N	O	0	0
			14	8	1	5		
2	B	1	Total	C	N	O	0	0
			14	8	1	5		
2	B	1	Total	C	N	O	0	0
			14	8	1	5		
2	B	1	Total	C	N	O	0	0
			14	8	1	5		
2	B	1	Total	C	N	O	0	0
			14	8	1	5		

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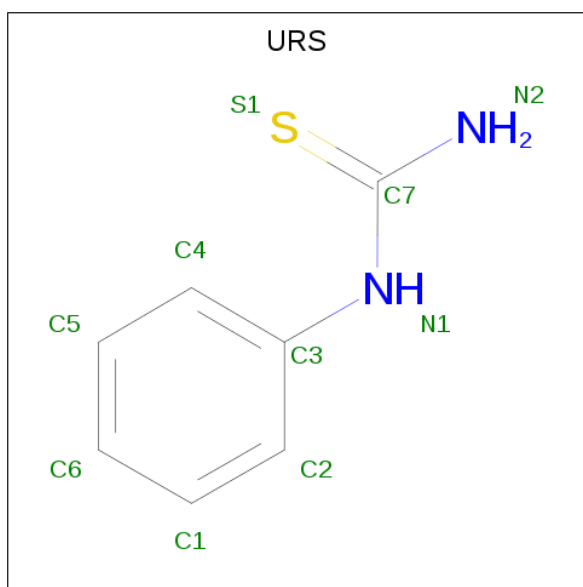
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	B	1	Total	C	N	O	0	0
			14	8	1	5		
2	B	1	Total	C	N	O	0	0
			14	8	1	5		
2	C	1	Total	C	N	O	0	0
			14	8	1	5		
2	C	1	Total	C	N	O	0	0
			14	8	1	5		
2	C	1	Total	C	N	O	0	0
			14	8	1	5		
2	C	1	Total	C	N	O	0	0
			14	8	1	5		
2	C	1	Total	C	N	O	0	0
			14	8	1	5		
2	C	1	Total	C	N	O	0	0
			14	8	1	5		
2	D	1	Total	C	N	O	0	0
			14	8	1	5		
2	D	1	Total	C	N	O	0	0
			14	8	1	5		
2	D	1	Total	C	N	O	0	0
			14	8	1	5		
2	D	1	Total	C	N	O	0	0
			14	8	1	5		
2	D	1	Total	C	N	O	0	0
			14	8	1	5		
2	D	1	Total	C	N	O	0	0
			14	8	1	5		
2	D	1	Total	C	N	O	0	0
			14	8	1	5		

- Molecule 3 is ALPHA-L-FUCOSE (three-letter code: FUC) (formula: C₆H₁₂O₅).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			10	6	4		
3	B	1	Total	C	O	0	0
			10	6	4		
3	B	1	Total	C	O	0	0
			10	6	4		
3	C	1	Total	C	O	0	0
			10	6	4		
3	D	1	Total	C	O	0	0
			10	6	4		
3	D	1	Total	C	O	0	0
			10	6	4		

- Molecule 4 is N-PHENYLTHIOUREA (three-letter code: URS) (formula: C₇H₈N₂S).

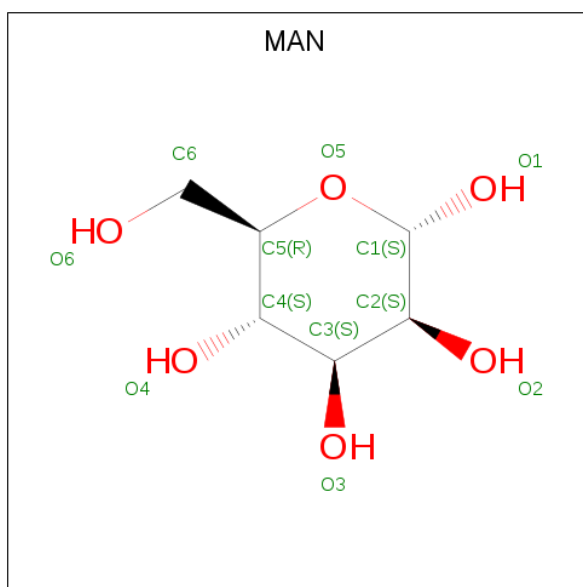


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	1	Total	C	N	S	0	0
			10	7	2	1		
4	B	1	Total	C	N	S	0	0
			10	7	2	1		
4	C	1	Total	C	N	S	0	0
			10	7	2	1		
4	D	1	Total	C	N	S	0	0
			10	7	2	1		

- Molecule 5 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	B	2	Total	Zn	0	0
			2	2		
5	A	3	Total	Zn	0	0
			3	3		
5	D	2	Total	Zn	0	0
			2	2		
5	C	2	Total	Zn	0	0
			2	2		

- Molecule 6 is ALPHA-D-MANNOSE (three-letter code: MAN) (formula: C₆H₁₂O₆).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	B	1	Total	C	O	0	0
			11	6	5		
6	B	1	Total	C	O	0	0
			11	6	5		
6	B	1	Total	C	O	0	0
			11	6	5		
6	B	1	Total	C	O	0	0
			11	6	5		
6	D	1	Total	C	O	0	0
			11	6	5		
6	D	1	Total	C	O	0	0
			11	6	5		
6	D	1	Total	C	O	0	0
			11	6	5		
6	D	1	Total	C	O	0	0
			11	6	5		

- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	205	Total	O	0	0
			205	205		
7	B	168	Total	O	0	0
			168	168		
7	C	159	Total	O	0	0
			159	159		

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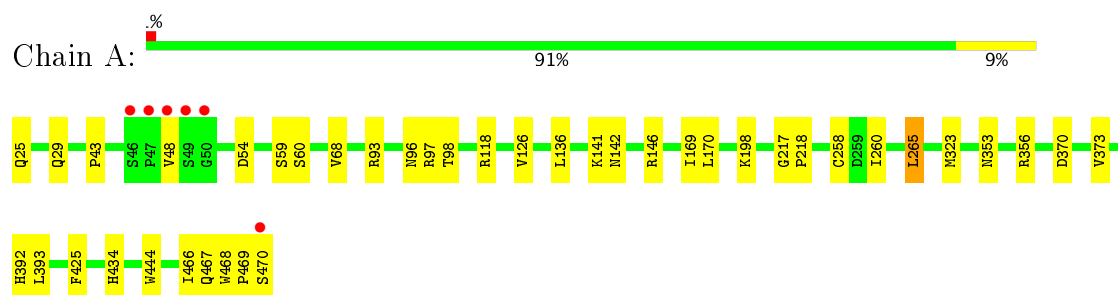
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	D	190	Total 190	O 190	0	0

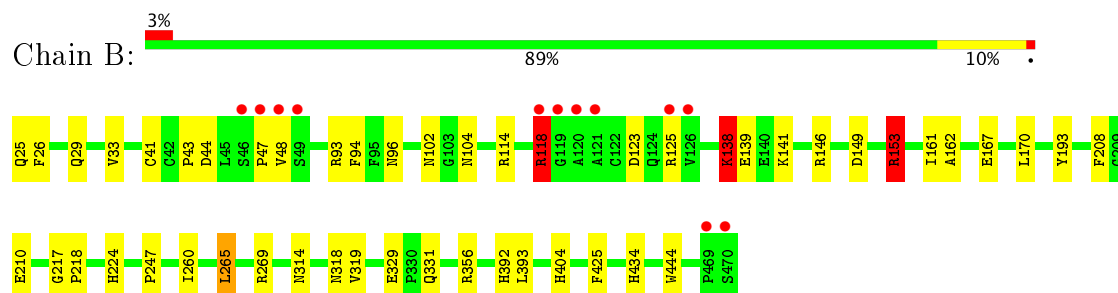
3 Residue-property plots [i](#)

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.

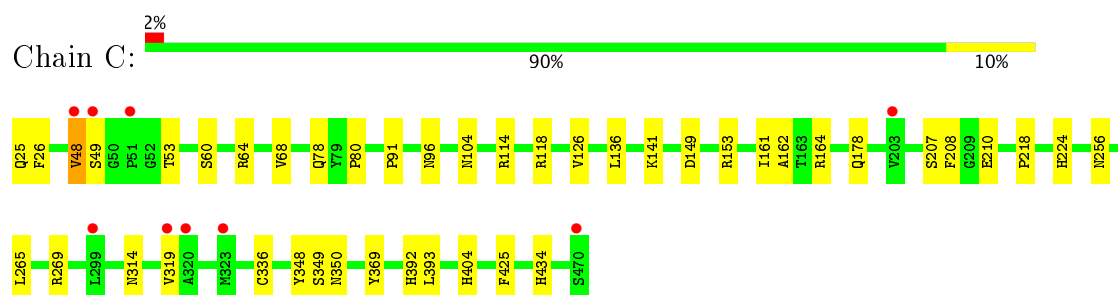
- Molecule 1: 5,6-dihydroxyindole-2-carboxylic acid oxidase



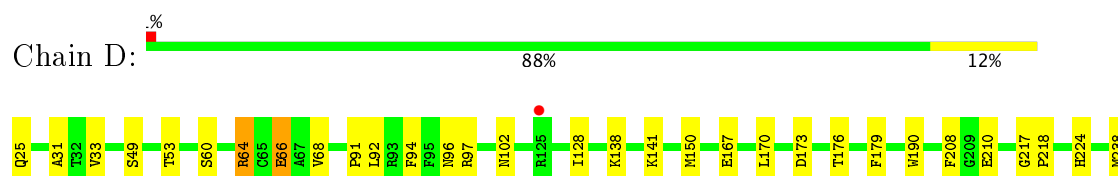
- Molecule 1: 5,6-dihydroxyindole-2-carboxylic acid oxidase

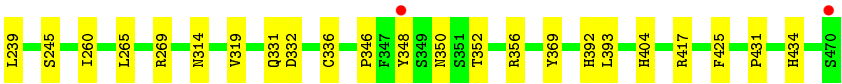


- Molecule 1: 5,6-dihydroxyindole-2-carboxylic acid oxidase



- Molecule 1: 5,6-dihydroxyindole-2-carboxylic acid oxidase





4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	90.08Å 141.77Å 191.73Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	45.88 – 2.20 45.88 – 2.20	Depositor EDS
% Data completeness (in resolution range)	99.2 (45.88-2.20) 92.3 (45.88-2.20)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.14 (at 2.20Å)	Xtriage
Refinement program	REFMAC, PHENIX 1.10.1 _2155	Depositor
R, R_{free}	0.194 , 0.235 0.199 , 0.237	Depositor DCC
R_{free} test set	6287 reflections (5.74%)	DCC
Wilson B-factor (Å ²)	34.8	Xtriage
Anisotropy	0.430	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 40.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	15622	wwPDB-VP
Average B, all atoms (Å ²)	44.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.15% 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: MAN, ZN, URS, NAG, FUC

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	0.47	2/3661 (0.1%)	0.64	3/4990 (0.1%)
1	B	0.55	3/3661 (0.1%)	0.76	10/4990 (0.2%)
1	C	0.42	0/3661	0.62	2/4990 (0.0%)
1	D	0.49	3/3661 (0.1%)	0.63	0/4990
All	All	0.49	8/14644 (0.1%)	0.67	15/19960 (0.1%)

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	B	0	1

The worst 5 of 8 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	66	GLU	CG-CD	-8.53	1.39	1.51
1	A	48	VAL	CB-CG1	6.96	1.67	1.52
1	B	118	ARG	CZ-NH1	-6.73	1.24	1.33
1	D	64	ARG	NE-CZ	-6.18	1.25	1.33
1	A	48	VAL	CB-CG2	5.51	1.64	1.52

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

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	146	ARG	CG-CD-NE	14.06	141.32	111.80
1	B	118	ARG	NE-CZ-NH1	12.62	126.61	120.30
1	B	48	VAL	CG1-CB-CG2	-8.31	97.61	110.90
1	A	48	VAL	CG1-CB-CG2	7.73	123.27	110.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	48	VAL	CG1-CB-CG2	-7.43	99.01	110.90

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	125	ARG	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	3554	0	3321	27	0
1	B	3554	0	3320	29	0
1	C	3554	0	3319	26	0
1	D	3554	0	3319	37	0
2	A	98	0	87	1	0
2	B	126	0	109	4	0
2	C	112	0	101	4	0
2	D	140	0	121	2	0
3	A	10	0	10	0	0
3	B	20	0	20	1	0
3	C	10	0	10	0	0
3	D	20	0	20	1	0
4	A	10	0	8	0	0
4	B	10	0	8	0	0
4	C	10	0	8	0	0
4	D	10	0	8	0	0
5	A	3	0	0	0	0
5	B	2	0	0	0	0
5	C	2	0	0	0	0
5	D	2	0	0	0	0
6	B	44	0	38	1	0
6	D	55	0	47	1	0
7	A	205	0	0	2	0
7	B	168	0	0	0	1
7	C	159	0	0	3	1

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
7	D	190	0	0	4	0
All	All	15622	0	13874	121	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 4.

The worst 5 of 121 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:104:ASN:OD1	1:B:114:ARG:NH1	2.02	0.93
1:C:25:GLN:HG3	1:C:26:PHE:H	1.39	0.86
1:B:25:GLN:HG3	1:B:26:PHE:H	1.41	0.85
1:A:25:GLN:OE1	1:A:25:GLN:N	2.17	0.77
1:C:256:ASN:ND2	7:C:603:HOH:O	2.18	0.76

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)
7:B:649:HOH:O	7:C:750:HOH:O[3_856]	2.18	0.02

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	444/446 (100%)	431 (97%)	13 (3%)	0	100	100
1	B	444/446 (100%)	430 (97%)	14 (3%)	0	100	100
1	C	444/446 (100%)	429 (97%)	15 (3%)	0	100	100
1	D	444/446 (100%)	431 (97%)	13 (3%)	0	100	100
All	All	1776/1784 (100%)	1721 (97%)	55 (3%)	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	395/395 (100%)	392 (99%)	3 (1%)	85	92
1	B	395/395 (100%)	388 (98%)	7 (2%)	64	77
1	C	395/395 (100%)	392 (99%)	3 (1%)	85	92
1	D	395/395 (100%)	391 (99%)	4 (1%)	80	89
All	All	1580/1580 (100%)	1563 (99%)	17 (1%)	78	88

5 of 17 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	193	TYR
1	B	247	PRO
1	D	60	SER
1	B	153	ARG
1	D	138	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 6 such sidechains are listed below:

Mol	Chain	Res	Type
1	A	331	GLN
1	C	142	ASN
1	A	467	GLN
1	A	108	HIS
1	B	142	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](#)

Of 62 ligands modelled in this entry, 9 are monoatomic - leaving 53 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	NAG	A	501	1,3,2	14,14,15	0.55	0	15,19,21	0.78	1 (6%)
2	NAG	A	502	2	14,14,15	0.47	0	15,19,21	0.38	0
3	FUC	A	503	2	9,10,11	0.93	0	13,14,16	1.49	2 (15%)
2	NAG	A	504	1	14,14,15	1.65	2 (14%)	15,19,21	1.13	1 (6%)
2	NAG	A	505	1,2	14,14,15	0.27	0	15,19,21	0.51	0
2	NAG	A	506	2	14,14,15	0.44	0	15,19,21	0.47	0
2	NAG	A	507	1,2	14,14,15	0.46	0	15,19,21	0.86	1 (6%)
2	NAG	A	508	2	14,14,15	0.41	0	15,19,21	0.50	0
4	URS	A	509	-	10,10,10	5.25	9 (90%)	11,12,12	1.00	0
2	NAG	B	501	1,3,2	14,14,15	0.22	0	15,19,21	0.81	1 (6%)
2	NAG	B	502	2	14,14,15	0.40	0	15,19,21	0.57	0
3	FUC	B	503	2	9,10,11	0.79	0	13,14,16	1.68	3 (23%)
2	NAG	B	504	1,6	14,14,15	2.09	1 (7%)	15,19,21	0.95	1 (6%)
6	MAN	B	505	2	11,11,12	1.54	3 (27%)	13,15,17	1.59	2 (15%)
2	NAG	B	506	1,2	14,14,15	0.38	0	15,19,21	0.52	0
2	NAG	B	507	2	14,14,15	0.55	0	15,19,21	0.51	0
2	NAG	B	508	1,3,2	14,14,15	0.49	0	15,19,21	1.00	0
2	NAG	B	509	2,6	14,14,15	0.83	1 (7%)	15,19,21	0.88	1 (6%)
6	MAN	B	510	2,6	11,11,12	0.89	0	13,15,17	0.73	0
6	MAN	B	511	6	11,11,12	1.34	2 (18%)	13,15,17	1.51	1 (7%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
6	MAN	B	512	6	11,11,12	0.82	0	13,15,17	1.35	2 (15%)
3	FUC	B	513	2	9,10,11	1.35	1 (11%)	13,14,16	1.81	4 (30%)
2	NAG	B	514	1,2	14,14,15	0.45	0	15,19,21	0.94	1 (6%)
2	NAG	B	515	2	14,14,15	0.33	0	15,19,21	0.55	0
4	URS	B	516	-	10,10,10	5.48	9 (90%)	11,12,12	1.23	2 (18%)
2	NAG	C	501	1,3	14,14,15	0.42	0	15,19,21	0.61	0
3	FUC	C	502	2	9,10,11	0.68	0	13,14,16	1.36	2 (15%)
2	NAG	C	503	1	14,14,15	0.30	0	15,19,21	0.55	0
2	NAG	C	504	1	14,14,15	1.35	3 (21%)	15,19,21	1.20	1 (6%)
2	NAG	C	505	1,2	14,14,15	0.18	0	15,19,21	0.46	0
2	NAG	C	506	2	14,14,15	0.37	0	15,19,21	0.58	0
2	NAG	C	507	1,2	14,14,15	0.39	0	15,19,21	1.00	1 (6%)
2	NAG	C	508	2	14,14,15	1.29	1 (7%)	15,19,21	1.12	3 (20%)
2	NAG	C	509	1	14,14,15	0.91	1 (7%)	15,19,21	1.13	1 (6%)
4	URS	C	510	-	10,10,10	5.49	10 (100%)	11,12,12	1.15	1 (9%)
2	NAG	D	501	1,3,2	14,14,15	0.36	0	15,19,21	0.75	1 (6%)
2	NAG	D	502	2	14,14,15	0.65	1 (7%)	15,19,21	0.42	0
3	FUC	D	503	2	9,10,11	0.74	0	13,14,16	2.22	6 (46%)
2	NAG	D	504	1,3,2	14,14,15	0.72	1 (7%)	15,19,21	0.68	0
3	FUC	D	505	2	9,10,11	0.98	0	13,14,16	1.19	1 (7%)
2	NAG	D	506	2,6	14,14,15	0.60	0	15,19,21	0.78	1 (6%)
6	MAN	D	507	2,6	11,11,12	1.48	1 (9%)	13,15,17	1.15	1 (7%)
6	MAN	D	508	6	11,11,12	0.85	1 (9%)	13,15,17	1.20	2 (15%)
2	NAG	D	509	1,2	14,14,15	0.21	0	15,19,21	0.66	0
2	NAG	D	510	2	14,14,15	0.48	0	15,19,21	0.59	0
2	NAG	D	511	1,2	14,14,15	0.41	0	15,19,21	0.71	0
2	NAG	D	512	2,6	14,14,15	0.60	0	15,19,21	0.78	1 (6%)
6	MAN	D	513	2,6	11,11,12	0.83	0	13,15,17	1.33	1 (7%)
6	MAN	D	514	6	11,11,12	1.20	1 (9%)	13,15,17	1.64	2 (15%)
6	MAN	D	515	6	11,11,12	1.30	1 (9%)	13,15,17	2.21	3 (23%)
2	NAG	D	516	1,2	14,14,15	0.52	0	15,19,21	0.81	1 (6%)
2	NAG	D	517	2	14,14,15	0.27	0	15,19,21	0.48	0
4	URS	D	518	-	10,10,10	5.20	10 (100%)	11,12,12	0.87	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	NAG	A	501	1,3,2	-	0/6/23/26	0/1/1/1
2	NAG	A	502	2	-	0/6/23/26	0/1/1/1
3	FUC	A	503	2	-	0/0/17/20	0/1/1/1
2	NAG	A	504	1	-	0/6/23/26	0/1/1/1
2	NAG	A	505	1,2	-	0/6/23/26	0/1/1/1
2	NAG	A	506	2	-	0/6/23/26	0/1/1/1
2	NAG	A	507	1,2	-	0/6/23/26	0/1/1/1
2	NAG	A	508	2	-	0/6/23/26	0/1/1/1
4	URS	A	509	-	-	0/4/4/4	0/1/1/1
2	NAG	B	501	1,3,2	-	0/6/23/26	0/1/1/1
2	NAG	B	502	2	-	0/6/23/26	0/1/1/1
3	FUC	B	503	2	-	0/0/17/20	0/1/1/1
2	NAG	B	504	1,6	-	0/6/23/26	0/1/1/1
6	MAN	B	505	2	-	0/2/19/22	0/1/1/1
2	NAG	B	506	1,2	-	0/6/23/26	0/1/1/1
2	NAG	B	507	2	-	0/6/23/26	0/1/1/1
2	NAG	B	508	1,3,2	-	0/6/23/26	0/1/1/1
2	NAG	B	509	2,6	-	0/6/23/26	0/1/1/1
6	MAN	B	510	2,6	-	0/2/19/22	0/1/1/1
6	MAN	B	511	6	-	0/2/19/22	1/1/1/1
6	MAN	B	512	6	-	0/2/19/22	0/1/1/1
3	FUC	B	513	2	-	0/0/17/20	0/1/1/1
2	NAG	B	514	1,2	-	0/6/23/26	0/1/1/1
2	NAG	B	515	2	-	0/6/23/26	0/1/1/1
4	URS	B	516	-	-	0/4/4/4	0/1/1/1
2	NAG	C	501	1,3	-	0/6/23/26	0/1/1/1
3	FUC	C	502	2	-	0/0/17/20	0/1/1/1
2	NAG	C	503	1	-	0/6/23/26	0/1/1/1
2	NAG	C	504	1	-	0/6/23/26	0/1/1/1
2	NAG	C	505	1,2	-	0/6/23/26	0/1/1/1
2	NAG	C	506	2	-	0/6/23/26	0/1/1/1
2	NAG	C	507	1,2	-	0/6/23/26	0/1/1/1
2	NAG	C	508	2	-	0/6/23/26	0/1/1/1
2	NAG	C	509	1	-	0/6/23/26	0/1/1/1
4	URS	C	510	-	-	0/4/4/4	0/1/1/1
2	NAG	D	501	1,3,2	-	0/6/23/26	0/1/1/1
2	NAG	D	502	2	-	0/6/23/26	0/1/1/1
3	FUC	D	503	2	-	0/0/17/20	0/1/1/1
2	NAG	D	504	1,3,2	-	0/6/23/26	0/1/1/1
3	FUC	D	505	2	-	0/0/17/20	0/1/1/1
2	NAG	D	506	2,6	-	0/6/23/26	0/1/1/1
6	MAN	D	507	2,6	-	0/2/19/22	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	MAN	D	508	6	-	0/2/19/22	0/1/1/1
2	NAG	D	509	1,2	-	0/6/23/26	0/1/1/1
2	NAG	D	510	2	-	0/6/23/26	0/1/1/1
2	NAG	D	511	1,2	-	0/6/23/26	0/1/1/1
2	NAG	D	512	2,6	-	0/6/23/26	0/1/1/1
6	MAN	D	513	2,6	-	0/2/19/22	0/1/1/1
6	MAN	D	514	6	-	0/2/19/22	1/1/1/1
6	MAN	D	515	6	-	0/2/19/22	1/1/1/1
2	NAG	D	516	1,2	-	0/6/23/26	0/1/1/1
2	NAG	D	517	2	-	0/6/23/26	0/1/1/1
4	URS	D	518	-	-	0/4/4/4	0/1/1/1

The worst 5 of 59 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	504	NAG	O5-C1	-7.48	1.31	1.43
4	B	516	URS	C7-S1	-7.29	1.59	1.69
4	A	509	URS	C7-S1	-6.37	1.60	1.69
4	C	510	URS	C7-S1	-5.98	1.61	1.69
4	D	518	URS	C7-S1	-5.36	1.62	1.69

The worst 5 of 52 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	B	505	MAN	C1-C2-C3	-4.04	104.53	109.65
6	B	511	MAN	C1-C2-C3	-3.70	104.95	109.65
6	D	514	MAN	C1-C2-C3	-3.17	105.63	109.65
2	C	507	NAG	O4-C4-C3	-3.09	103.64	110.36
4	C	510	URS	S1-C7-N2	-3.05	118.95	123.13

There are no chirality outliers.

There are no torsion outliers.

All (3) ring outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	D	515	MAN	C1-C2-C3-C4-C5-O5
6	B	511	MAN	C1-C2-C3-C4-C5-O5
6	D	514	MAN	C1-C2-C3-C4-C5-O5

14 monomers are involved in 14 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	501	NAG	1	0
2	B	501	NAG	1	0
3	B	503	FUC	1	0
2	B	504	NAG	1	0
6	B	505	MAN	1	0
2	B	514	NAG	2	0
2	C	501	NAG	2	0
2	C	507	NAG	1	0
2	C	508	NAG	1	0
2	C	509	NAG	1	0
2	D	501	NAG	1	0
3	D	503	FUC	1	0
6	D	507	MAN	1	0
2	D	516	NAG	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	446/446 (100%)	-0.18	6 (1%) 77 75	26, 41, 58, 82	0
1	B	446/446 (100%)	-0.10	12 (2%) 55 52	27, 43, 63, 87	0
1	C	446/446 (100%)	-0.19	9 (2%) 65 63	29, 43, 62, 84	0
1	D	446/446 (100%)	-0.20	3 (0%) 87 86	28, 43, 60, 93	0
All	All	1784/1784 (100%)	-0.17	30 (1%) 70 68	26, 42, 61, 93	0

The worst 5 of 30 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	126	VAL	7.3
1	A	48	VAL	5.5
1	B	118	ARG	5.5
1	A	470	SER	4.9
1	B	119	GLY	4.9

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
6	MAN	D	515	11/12	0.80	0.21	7.80	54,63,72,82	0
6	MAN	D	513	11/12	0.92	0.14	4.12	46,50,56,62	0
6	MAN	B	512	11/12	0.89	0.19	2.43	61,67,72,76	0
3	FUC	A	503	10/11	0.83	0.20	1.94	58,68,76,79	0
3	FUC	D	503	10/11	0.89	0.21	1.46	51,60,63,68	0
2	NAG	D	511	14/15	0.87	0.21	1.28	52,62,69,70	0
5	ZN	C	511	1/1	0.99	0.16	1.04	35,35,35,35	0
3	FUC	C	502	10/11	0.87	0.20	0.75	54,64,68,68	0
2	NAG	C	503	14/15	0.87	0.13	0.67	47,52,55,57	0
2	NAG	B	508	14/15	0.94	0.12	0.61	38,43,50,60	0
5	ZN	C	512	1/1	0.98	0.16	0.55	36,36,36,36	0
4	URS	A	509	10/10	0.97	0.14	0.49	35,37,40,40	0
6	MAN	D	507	11/12	0.87	0.12	0.36	47,52,55,57	0
4	URS	C	510	10/10	0.94	0.13	0.33	43,46,49,52	0
2	NAG	C	505	14/15	0.94	0.14	0.16	53,58,64,70	0
2	NAG	D	516	14/15	0.89	0.12	0.16	42,49,60,63	0
2	NAG	D	512	14/15	0.95	0.13	0.13	37,48,58,59	0
2	NAG	A	501	14/15	0.77	0.15	-0.03	55,64,76,81	0
3	FUC	B	503	10/11	0.93	0.11	-0.17	49,56,65,67	0
2	NAG	B	509	14/15	0.95	0.09	-0.18	40,46,48,56	0
5	ZN	D	519	1/1	1.00	0.15	-0.27	30,30,30,30	0
4	URS	D	518	10/10	0.97	0.12	-0.29	34,39,41,43	0
2	NAG	B	506	14/15	0.96	0.10	-0.31	42,49,51,56	0
5	ZN	D	520	1/1	1.00	0.16	-0.52	30,30,30,30	0
2	NAG	D	509	14/15	0.96	0.10	-0.59	41,47,51,52	0
2	NAG	B	514	14/15	0.92	0.11	-0.61	34,46,56,59	0
5	ZN	A	510	1/1	1.00	0.16	-0.69	29,29,29,29	0
2	NAG	C	509	14/15	0.88	0.15	-0.77	49,58,64,66	0
4	URS	B	516	10/10	0.97	0.12	-0.95	32,35,38,38	0
2	NAG	A	507	14/15	0.91	0.10	-0.97	41,48,57,60	0
5	ZN	A	512	1/1	0.99	0.08	-1.04	51,51,51,51	0
2	NAG	A	505	14/15	0.97	0.10	-1.08	44,47,53,57	0
2	NAG	D	504	14/15	0.95	0.08	-1.39	39,46,52,61	0
5	ZN	A	511	1/1	1.00	0.15	-2.03	29,29,29,29	0
5	ZN	B	518	1/1	1.00	0.15	-2.19	30,30,30,30	0
5	ZN	B	517	1/1	0.99	0.14	-2.52	29,29,29,29	0
2	NAG	C	508	14/15	0.67	0.29	-	79,89,97,99	0
2	NAG	C	507	14/15	0.81	0.16	-	60,66,77,86	0
2	NAG	A	508	14/15	0.86	0.22	-	55,62,70,72	0
2	NAG	B	502	14/15	0.84	0.18	-	50,59,68,78	0
2	NAG	D	506	14/15	0.91	0.11	-	48,51,55,55	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
6	MAN	B	510	11/12	0.90	0.12	-	50,56,61,68	0
6	MAN	B	505	11/12	0.83	0.24	-	78,79,81,83	0
6	MAN	D	514	11/12	0.82	0.19	-	58,62,66,69	0
3	FUC	B	513	10/11	0.83	0.26	-	66,73,75,78	0
3	FUC	D	505	10/11	0.86	0.18	-	51,56,62,66	0
2	NAG	C	504	14/15	0.81	0.21	-	61,68,76,82	0
2	NAG	A	502	14/15	0.71	0.27	-	72,82,89,91	0
6	MAN	B	511	11/12	0.82	0.17	-	63,69,75,76	0
2	NAG	D	517	14/15	0.89	0.28	-	60,66,76,80	0
6	MAN	D	508	11/12	0.90	0.15	-	50,53,58,59	0
2	NAG	A	506	14/15	0.92	0.18	-	56,64,67,73	0
2	NAG	D	510	14/15	0.90	0.15	-	51,58,65,68	0
2	NAG	D	502	14/15	0.80	0.29	-	57,74,80,82	0
2	NAG	B	504	14/15	0.82	0.19	-	63,68,70,72	0
2	NAG	B	507	14/15	0.91	0.17	-	56,60,65,67	0
2	NAG	B	515	14/15	0.91	0.16	-	43,57,65,75	0
2	NAG	D	501	14/15	0.83	0.17	-	51,55,62,70	0
2	NAG	A	504	14/15	0.72	0.26	-	58,69,73,73	0
2	NAG	C	501	14/15	0.86	0.19	-	51,58,64,64	0
2	NAG	B	501	14/15	0.90	0.12	-	50,55,63,71	0
2	NAG	C	506	14/15	0.85	0.28	-	59,71,76,77	0

6.5 Other polymers [i](#)

There are no such residues in this entry.