wwPDB X-ray Structure Validation Summary Report (i)

Aug 10, 2020 – 10:15 AM BST

PDB ID	:	4PBV
Title	:	Crystal structure of chicken receptor protein tyrosine phosphatase sigma in complex with TrkC
Authors	:	Coles, C.H.; Mitakidis, N.; Zhang, P.; Elegheert, J.; Lu, W.; Stoker, A.W.; Nakagawa, T.; Craig, A.M.; Jones, E.Y.; Aricescu, A.R.
Deposited on	:	2014-04-14
Resolution	:	2.50 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
https://www.wwpdb.org/validation/2017/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:

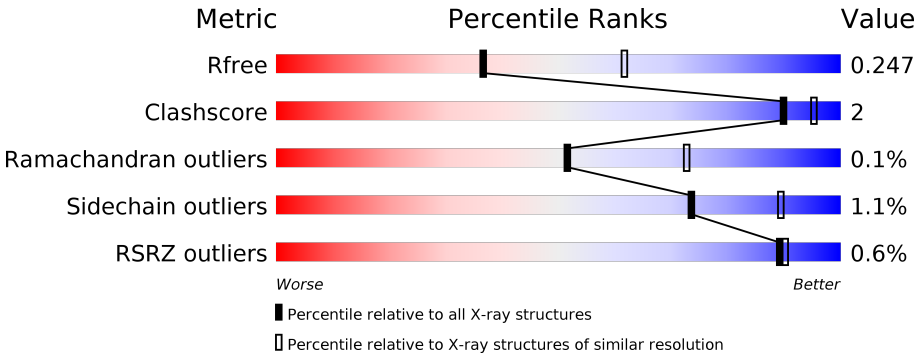
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.13.1
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.13.1

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 2.50 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	4661 (2.50-2.50)
Clashscore	141614	5346 (2.50-2.50)
Ramachandran outliers	138981	5231 (2.50-2.50)
Sidechain outliers	138945	5233 (2.50-2.50)
RSRZ outliers	127900	4559 (2.50-2.50)

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 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	268	90% 6%
1	B	268	% 88% 7% 5%
2	C	299	61% 35%
2	D	299	63% 35%
2	E	299	% 63% 35%

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 8734 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 NT-3 growth factor receptor.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	257	Total	C	N	O	S	0	0	0
			2022	1256	362	390	14			
1	B	254	Total	C	N	O	S	0	0	0
			1999	1243	359	383	14			

There are 34 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	29	GLU	-	expression tag	UNP Q91044
A	30	THR	-	expression tag	UNP Q91044
A	31	GLY	-	expression tag	UNP Q91044
A	163	GLN	ASN	engineered mutation	UNP Q91044
A	232	GLN	ASN	engineered mutation	UNP Q91044
A	259	GLN	ASN	engineered mutation	UNP Q91044
A	267	GLN	ASN	engineered mutation	UNP Q91044
A	294	GLN	ASN	engineered mutation	UNP Q91044
A	303	GLY	-	expression tag	UNP Q91044
A	304	THR	-	expression tag	UNP Q91044
A	305	LYS	-	expression tag	UNP Q91044
A	306	HIS	-	expression tag	UNP Q91044
A	307	HIS	-	expression tag	UNP Q91044
A	308	HIS	-	expression tag	UNP Q91044
A	309	HIS	-	expression tag	UNP Q91044
A	310	HIS	-	expression tag	UNP Q91044
A	311	HIS	-	expression tag	UNP Q91044
B	29	GLU	-	expression tag	UNP Q91044
B	30	THR	-	expression tag	UNP Q91044
B	31	GLY	-	expression tag	UNP Q91044
B	163	GLN	ASN	engineered mutation	UNP Q91044
B	232	GLN	ASN	engineered mutation	UNP Q91044
B	259	GLN	ASN	engineered mutation	UNP Q91044
B	267	GLN	ASN	engineered mutation	UNP Q91044
B	294	GLN	ASN	engineered mutation	UNP Q91044

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Chain	Residue	Modelled	Actual	Comment	Reference
B	303	GLY	-	expression tag	UNP Q91044
B	304	THR	-	expression tag	UNP Q91044
B	305	LYS	-	expression tag	UNP Q91044
B	306	HIS	-	expression tag	UNP Q91044
B	307	HIS	-	expression tag	UNP Q91044
B	308	HIS	-	expression tag	UNP Q91044
B	309	HIS	-	expression tag	UNP Q91044
B	310	HIS	-	expression tag	UNP Q91044
B	311	HIS	-	expression tag	UNP Q91044

- Molecule 2 is a protein called Protein-tyrosine phosphatase CRYPalpha1 isoform.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	C	195	Total	C	N	O	S	0	0	0
			1507	940	268	293	6			
2	D	195	Total	C	N	O	S	0	0	0
			1505	940	266	293	6			
2	E	194	Total	C	N	O	S	0	0	0
			1503	937	269	291	6			

There are 33 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	26	GLU	-	expression tag	UNP Q90815
C	27	THR	-	expression tag	UNP Q90815
C	28	GLY	-	expression tag	UNP Q90815
C	317	LYS	-	expression tag	UNP Q90815
C	318	GLY	-	expression tag	UNP Q90815
C	319	HIS	-	expression tag	UNP Q90815
C	320	HIS	-	expression tag	UNP Q90815
C	321	HIS	-	expression tag	UNP Q90815
C	322	HIS	-	expression tag	UNP Q90815
C	323	HIS	-	expression tag	UNP Q90815
C	324	HIS	-	expression tag	UNP Q90815
D	26	GLU	-	expression tag	UNP Q90815
D	27	THR	-	expression tag	UNP Q90815
D	28	GLY	-	expression tag	UNP Q90815
D	317	LYS	-	expression tag	UNP Q90815
D	318	GLY	-	expression tag	UNP Q90815
D	319	HIS	-	expression tag	UNP Q90815
D	320	HIS	-	expression tag	UNP Q90815
D	321	HIS	-	expression tag	UNP Q90815

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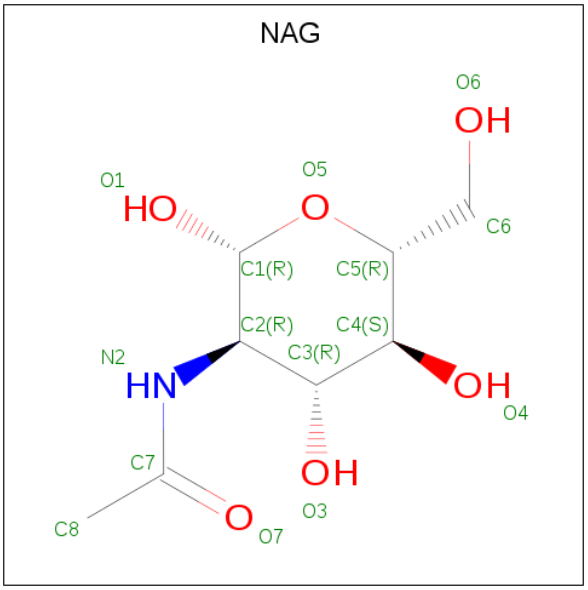
Chain	Residue	Modelled	Actual	Comment	Reference
D	322	HIS	-	expression tag	UNP Q90815
D	323	HIS	-	expression tag	UNP Q90815
D	324	HIS	-	expression tag	UNP Q90815
E	26	GLU	-	expression tag	UNP Q90815
E	27	THR	-	expression tag	UNP Q90815
E	28	GLY	-	expression tag	UNP Q90815
E	317	LYS	-	expression tag	UNP Q90815
E	318	GLY	-	expression tag	UNP Q90815
E	319	HIS	-	expression tag	UNP Q90815
E	320	HIS	-	expression tag	UNP Q90815
E	321	HIS	-	expression tag	UNP Q90815
E	322	HIS	-	expression tag	UNP Q90815
E	323	HIS	-	expression tag	UNP Q90815
E	324	HIS	-	expression tag	UNP Q90815

- Molecule 3 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).



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

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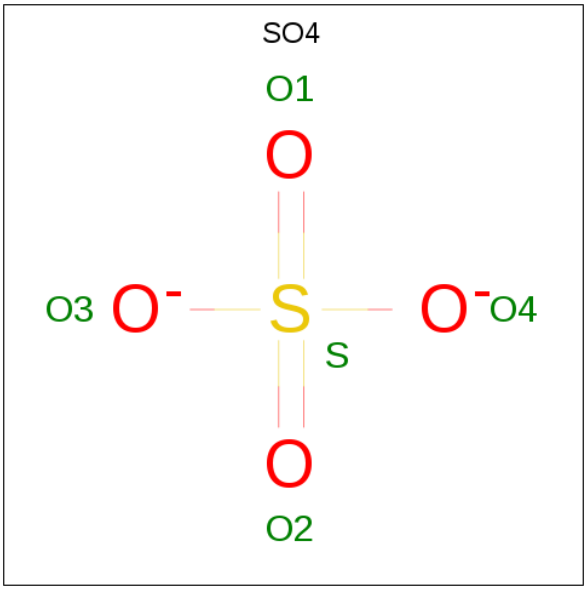
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	B	1	Total C N O 14 8 1 5	0	0

- Molecule 4 is SULFATE ION (three-letter code: SO4) (formula: O_4S).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	D	1	Total O S 5 4 1	0	0
4	E	1	Total O S 5 4 1	0	0

- Molecule 5 is water.

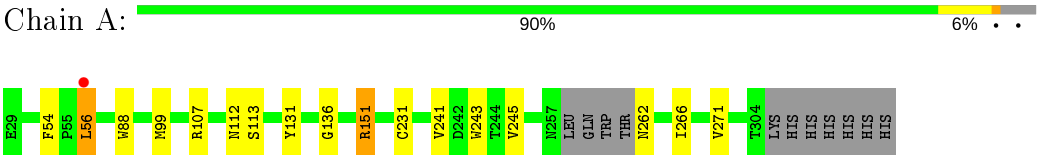
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	24	Total O 24 24	0	0
5	B	24	Total O 24 24	0	0
5	C	17	Total O 17 17	0	0
5	D	42	Total O 42 42	0	0
5	E	11	Total O 11 11	0	0

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.

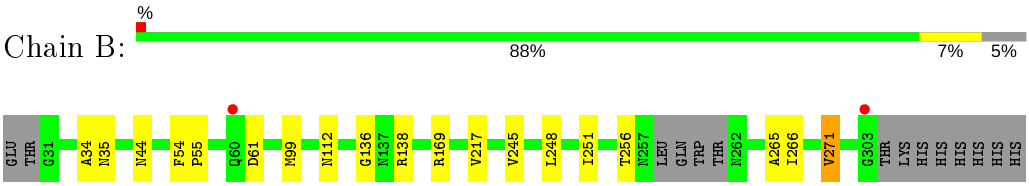
- Molecule 1: NT-3 growth factor receptor

Chain A:



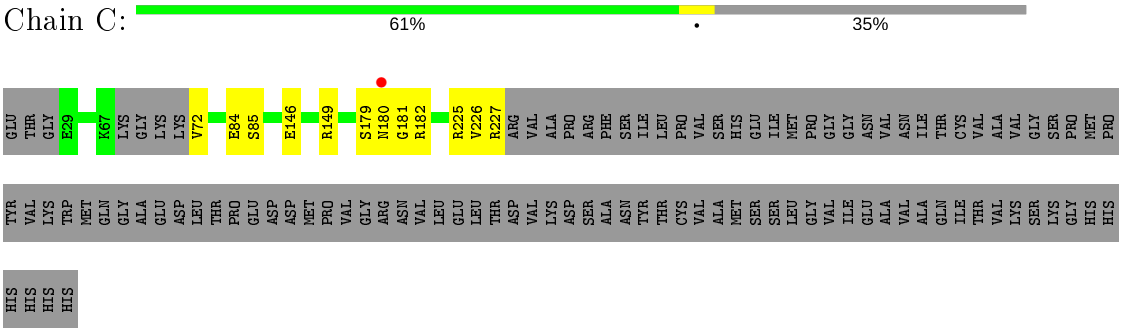
- Molecule 1: NT-3 growth factor receptor

Chain B:



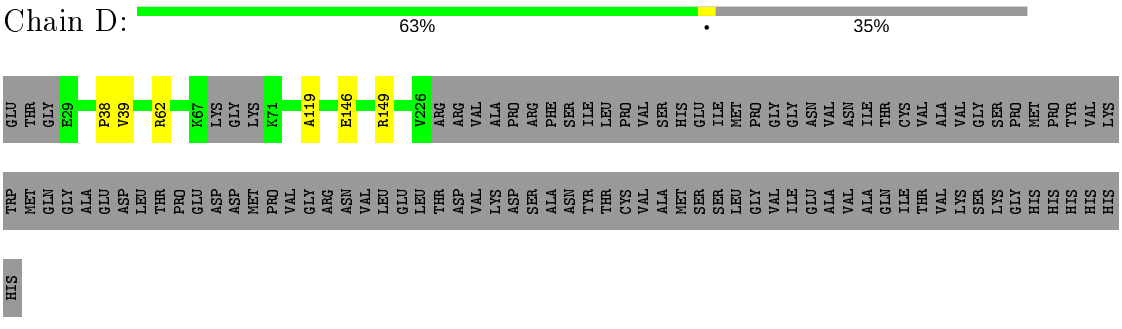
- Molecule 2: Protein-tyrosine phosphatase CRYPalpha1 isoform

Chain C:



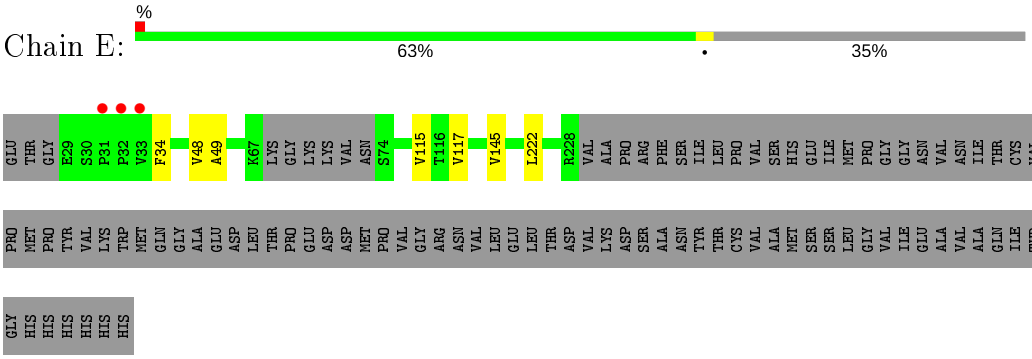
- Molecule 2: Protein-tyrosine phosphatase CRYPalpha1 isoform

Chain D:



• Molecule 2: Protein-tyrosine phosphatase CRYPalpha1 isoform

Chain E:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	68.30Å 122.16Å 98.61Å 90.00° 109.79° 90.00°	Depositor
Resolution (Å)	92.79 – 2.50 92.79 – 2.30	Depositor EDS
% Data completeness (in resolution range)	99.9 (92.79-2.50) 99.6 (92.79-2.30)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.10 (at 2.29Å)	Xtriage
Refinement program	REFMAC 5.7.0032	Depositor
R, R_{free}	0.209 , 0.247 0.211 , 0.247	Depositor DCC
R_{free} test set	3405 reflections (5.06%)	wwPDB-VP
Wilson B-factor (Å^2)	49.3	Xtriage
Anisotropy	0.251	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.32 , 29.2	EDS
L-test for twinning[2]	$< \|L\| > = 0.46$, $< L^2 > = 0.29$	Xtriage
Estimated twinning fraction	0.037 for h,-k,-h-l	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	8734	wwPDB-VP
Average B, all atoms (Å^2)	57.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.28% 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

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: NAG, SO4

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	0.41	0/2055	0.64	1/2797 (0.0%)
1	B	0.41	0/2032	0.66	1/2765 (0.0%)
2	C	0.40	0/1539	0.63	0/2092
2	D	0.42	0/1537	0.61	0/2089
2	E	0.40	0/1535	0.62	0/2085
All	All	0.41	0/8698	0.63	2/11828 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	151	ARG	NE-CZ-NH1	5.23	122.91	120.30
1	B	138	ARG	NE-CZ-NH2	5.09	122.85	120.30

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	2022	0	1986	9	0
1	B	1999	0	1967	10	0
2	C	1507	0	1480	5	0
2	D	1505	0	1480	3	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	E	1503	0	1478	4	0
3	A	42	0	39	0	0
3	B	28	0	26	1	0
4	D	5	0	0	0	0
4	E	5	0	0	0	0
5	A	24	0	0	1	0
5	B	24	0	0	1	0
5	C	17	0	0	0	0
5	D	42	0	0	1	0
5	E	11	0	0	0	0
All	All	8734	0	8456	31	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.

The worst 5 of 31 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:256:THR:HG21	5:B:504:HOH:O	1.92	0.68
1:B:54:PHE:CZ	1:B:99:MET:HE3	2.31	0.66
1:A:54:PHE:CZ	1:A:99:MET:HE3	2.35	0.61
1:B:54:PHE:CE2	1:B:99:MET:CE	2.87	0.57
2:C:180:ASN:C	2:C:182:ARG:H	2.09	0.55

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	253/268 (94%)	247 (98%)	6 (2%)	0	100	100
1	B	250/268 (93%)	243 (97%)	7 (3%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
2	C	191/299 (64%)	186 (97%)	4 (2%)	1 (0%)	29 48
2	D	191/299 (64%)	188 (98%)	3 (2%)	0	100 100
2	E	190/299 (64%)	186 (98%)	4 (2%)	0	100 100
All	All	1075/1433 (75%)	1050 (98%)	24 (2%)	1 (0%)	51 73

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	C	181	GLY

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	233/244 (96%)	230 (99%)	3 (1%)	69 87
1	B	230/244 (94%)	225 (98%)	5 (2%)	52 77
2	C	169/257 (66%)	167 (99%)	2 (1%)	71 88
2	D	169/257 (66%)	168 (99%)	1 (1%)	86 95
2	E	168/257 (65%)	168 (100%)	0	100 100
All	All	969/1259 (77%)	958 (99%)	11 (1%)	73 89

5 of 11 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	55	PRO
1	B	169	ARG
2	C	72	VAL
1	B	44	ASN
1	B	271	VAL

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	106	GLN
1	A	262	ASN
1	B	181	ASN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

5 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	$\#\|Z\| > 2$
3	NAG	A	403	1	14,14,15	0.48	0	17,19,21	1.42	2 (11%)
3	NAG	B	402	1	14,14,15	0.84	0	17,19,21	1.39	2 (11%)
3	NAG	A	401	1	14,14,15	0.46	0	17,19,21	1.10	1 (5%)
3	NAG	B	401	1	14,14,15	0.49	0	17,19,21	1.12	2 (11%)
3	NAG	A	402	1	14,14,15	0.63	0	17,19,21	1.33	3 (17%)

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	NAG	A	403	1	-	0/6/23/26	0/1/1/1
3	NAG	B	402	1	-	0/6/23/26	0/1/1/1
3	NAG	A	401	1	-	2/6/23/26	0/1/1/1
3	NAG	B	401	1	-	0/6/23/26	0/1/1/1
3	NAG	A	402	1	-	0/6/23/26	0/1/1/1

There are no bond length outliers.

The worst 5 of 10 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	A	403	NAG	O5-C1-C2	-3.28	106.11	111.29
3	A	403	NAG	C3-C4-C5	3.17	115.89	110.24
3	B	402	NAG	C4-C3-C2	2.97	115.38	111.02
3	B	402	NAG	O5-C1-C2	2.77	115.67	111.29
3	A	402	NAG	C1-C2-N2	-2.66	105.94	110.49

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	401	NAG	O5-C5-C6-O6
3	A	401	NAG	C4-C5-C6-O6

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	401	NAG	1	0

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

7 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	$\#\|Z\| > 2$
3	NAG	B	402	1	14,14,15	0.84	0	17,19,21	1.39	2 (11%)
3	NAG	A	402	1	14,14,15	0.63	0	17,19,21	1.33	3 (17%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
3	NAG	A	401	1	14,14,15	0.46	0	17,19,21	1.10	1 (5%)
4	SO4	E	401	-	4,4,4	0.34	0	6,6,6	0.17	0
3	NAG	A	403	1	14,14,15	0.48	0	17,19,21	1.42	2 (11%)
4	SO4	D	401	-	4,4,4	0.37	0	6,6,6	0.17	0
3	NAG	B	401	1	14,14,15	0.49	0	17,19,21	1.12	2 (11%)

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	NAG	A	403	1	-	0/6/23/26	0/1/1/1
3	NAG	B	402	1	-	0/6/23/26	0/1/1/1
3	NAG	A	401	1	-	2/6/23/26	0/1/1/1
3	NAG	A	402	1	-	0/6/23/26	0/1/1/1
3	NAG	B	401	1	-	0/6/23/26	0/1/1/1

There are no bond length outliers.

The worst 5 of 10 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	A	403	NAG	O5-C1-C2	-3.28	106.11	111.29
3	A	403	NAG	C3-C4-C5	3.17	115.89	110.24
3	B	402	NAG	C4-C3-C2	2.97	115.38	111.02
3	B	402	NAG	O5-C1-C2	2.77	115.67	111.29
3	A	402	NAG	C1-C2-N2	-2.66	105.94	110.49

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	401	NAG	O5-C5-C6-O6
3	A	401	NAG	C4-C5-C6-O6

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	401	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

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	257/268 (95%)	-0.12	1 (0%) 92 93	35, 56, 77, 94	0
1	B	254/268 (94%)	-0.10	2 (0%) 86 87	36, 52, 78, 96	0
2	C	195/299 (65%)	-0.09	1 (0%) 91 91	42, 59, 83, 98	0
2	D	195/299 (65%)	-0.15	0 100 100	35, 50, 69, 102	0
2	E	194/299 (64%)	-0.07	3 (1%) 73 75	37, 58, 102, 138	0
All	All	1095/1433 (76%)	-0.11	7 (0%) 89 90	35, 55, 83, 138	0

The worst 5 of 7 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	56	LEU	3.1
1	B	303	GLY	2.9
2	E	33	VAL	2.8
2	E	32	PRO	2.7
1	B	60	GLN	2.5

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

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, 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	B-factors(Å^2)	Q<0.9
3	NAG	A	403	14/15	0.79	0.24	89,94,98,103	0
3	NAG	B	402	14/15	0.82	0.20	79,92,94,97	0
3	NAG	A	401	14/15	0.89	0.15	58,67,76,83	0
3	NAG	A	402	14/15	0.90	0.13	72,82,87,89	0
3	NAG	B	401	14/15	0.90	0.13	68,76,83,83	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, 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	B-factors(Å^2)	Q<0.9
3	NAG	A	403	14/15	0.79	0.24	89,94,98,103	0
3	NAG	B	402	14/15	0.82	0.20	79,92,94,97	0
3	NAG	A	401	14/15	0.89	0.15	58,67,76,83	0
4	SO4	E	401	5/5	0.90	0.21	96,96,101,101	0
3	NAG	A	402	14/15	0.90	0.13	72,82,87,89	0
3	NAG	B	401	14/15	0.90	0.13	68,76,83,83	0
4	SO4	D	401	5/5	0.96	0.16	81,82,83,86	0

6.5 Other polymers (i)

There are no such residues in this entry.