Full wwPDB X-ray Structure Validation Report (i)

Dec 12, 2023 – 08:16 pm GMT

PDB ID	:	4PBW
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	:	3.05 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

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

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

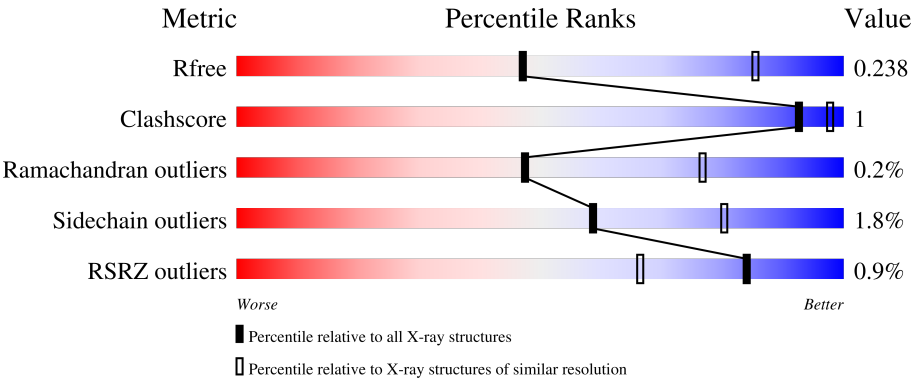
MolProbity	:	4.02b-467
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

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 3.05 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.



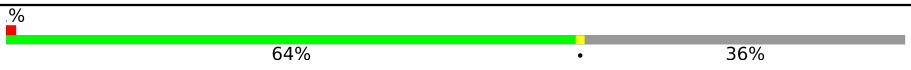
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	1754 (3.10-3.02)
Clashscore	141614	1864 (3.10-3.02)
Ramachandran outliers	138981	1794 (3.10-3.02)
Sidechain outliers	138945	1793 (3.10-3.02)
RSRZ outliers	127900	1713 (3.10-3.02)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5% The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	283	86% 6% • 7%
1	B	283	87% 5% 7%
1	C	283	2% 83% 7% • 10%
2	D	299	63% • 35%
2	E	299	% 64% • 35%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
2	F	299	

2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 10644 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	B	262	Total	C	N	O	S	0	0	0
			2073	1294	369	396	14			
1	A	263	Total	C	N	O	S	0	0	0
			2080	1298	370	398	14			
1	C	255	Total	C	N	O	S	0	0	0
			2018	1259	361	384	14			

There are 57 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	29	GLU	-	expression tag	UNP Q91044
B	30	THR	-	expression tag	UNP Q91044
B	31	GLY	-	expression tag	UNP Q91044
B	68	GLN	ASN	engineered mutation	UNP Q91044
B	72	GLN	ASN	engineered mutation	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
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
A	29	GLU	-	expression tag	UNP Q91044
A	30	THR	-	expression tag	UNP Q91044
A	31	GLY	-	expression tag	UNP Q91044
A	68	GLN	ASN	engineered mutation	UNP Q91044

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
A	72	GLN	ASN	engineered mutation	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
C	29	GLU	-	expression tag	UNP Q91044
C	30	THR	-	expression tag	UNP Q91044
C	31	GLY	-	expression tag	UNP Q91044
C	68	GLN	ASN	engineered mutation	UNP Q91044
C	72	GLN	ASN	engineered mutation	UNP Q91044
C	163	GLN	ASN	engineered mutation	UNP Q91044
C	232	GLN	ASN	engineered mutation	UNP Q91044
C	259	GLN	ASN	engineered mutation	UNP Q91044
C	267	GLN	ASN	engineered mutation	UNP Q91044
C	294	GLN	ASN	engineered mutation	UNP Q91044
C	303	GLY	-	expression tag	UNP Q91044
C	304	THR	-	expression tag	UNP Q91044
C	305	LYS	-	expression tag	UNP Q91044
C	306	HIS	-	expression tag	UNP Q91044
C	307	HIS	-	expression tag	UNP Q91044
C	308	HIS	-	expression tag	UNP Q91044
C	309	HIS	-	expression tag	UNP Q91044
C	310	HIS	-	expression tag	UNP Q91044
C	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	D	193	Total	C	N	O	S	0	0	0
			1487	928	262	291	6			
2	E	194	Total	C	N	O	S	0	0	0
			1492	931	263	292	6			

Continued on next page...

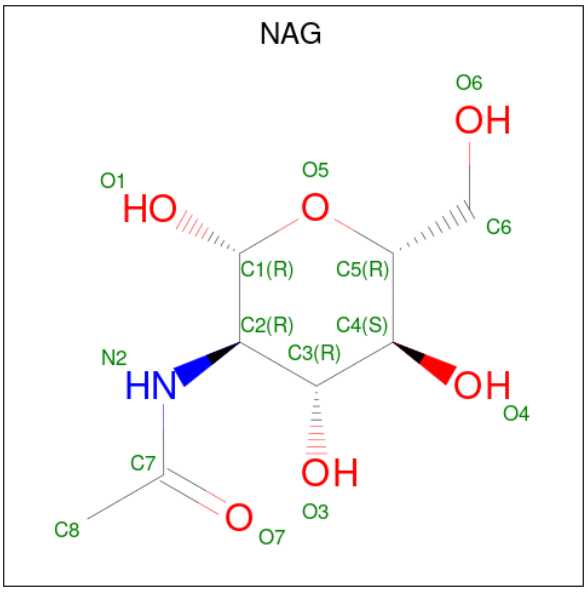
Continued from previous page...

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	F	192	Total	C	N	O	S	0	0	0
			1480	923	261	290	6			

There are 33 discrepancies between the modelled and reference sequences:

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

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



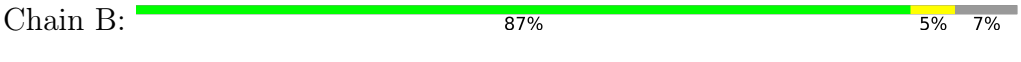
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	B	1	Total C N O 14 8 1 5	0	0

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.

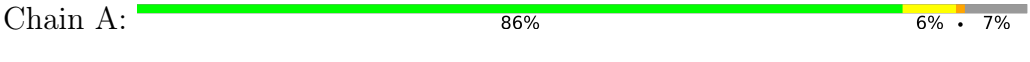
• Molecule 1: NT-3 growth factor receptor

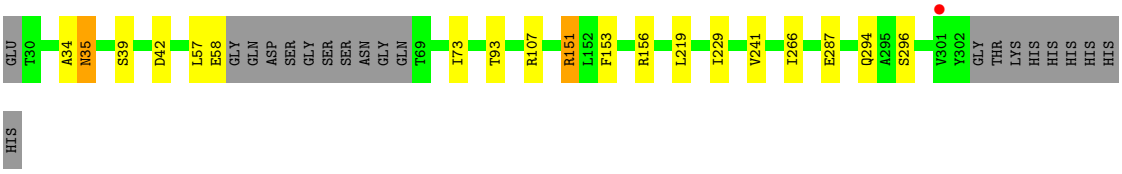
Chain B:



• Molecule 1: NT-3 growth factor receptor

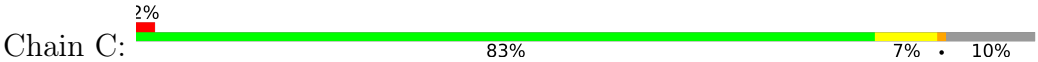
Chain A:

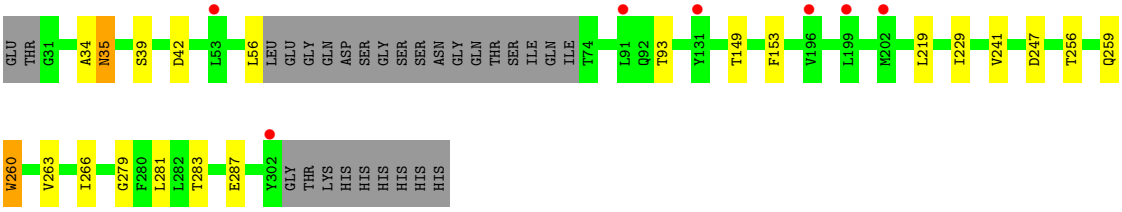




• Molecule 1: NT-3 growth factor receptor

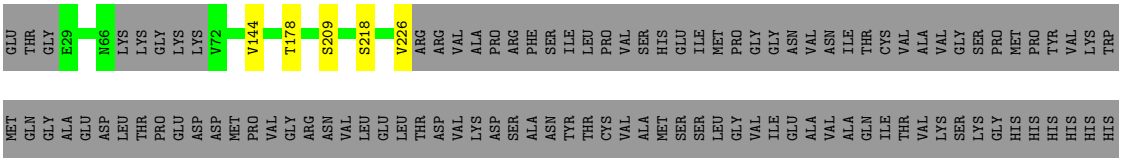
Chain C:





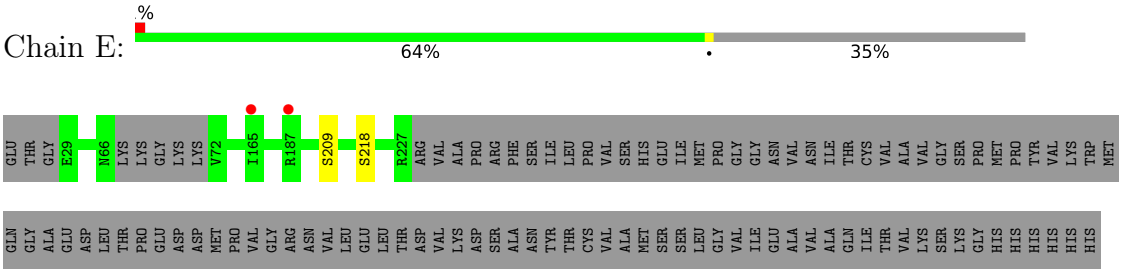
• Molecule 2: Protein-tyrosine phosphatase CRYPalpha1 isoform

Chain D:



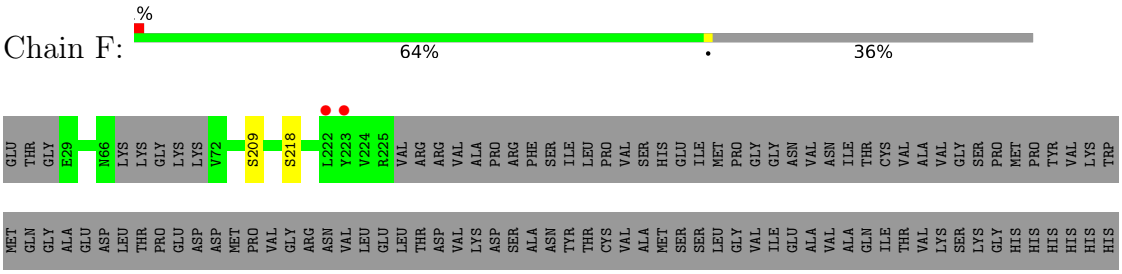
• Molecule 2: Protein-tyrosine phosphatase CRYPalpha1 isoform

Chain E:



• Molecule 2: Protein-tyrosine phosphatase CRYPalpha1 isoform

Chain F:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α, β, γ	84.42Å 93.12Å 99.38Å 73.37° 89.45° 74.23°	Depositor
Resolution (Å)	94.96 – 3.05 81.02 – 3.05	Depositor EDS
% Data completeness (in resolution range)	96.2 (94.96-3.05) 96.2 (81.02-3.05)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.21 (at 3.07Å)	Xtriage
Refinement program	REFMAC 5.8.0073	Depositor
R, R_{free}	0.226 , 0.240 0.225 , 0.238	Depositor DCC
R_{free} test set	2533 reflections (4.96%)	wwPDB-VP
Wilson B-factor (Å^2)	81.1	Xtriage
Anisotropy	0.334	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.29 , 55.0	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.93	EDS
Total number of atoms	10644	wwPDB-VP
Average B, all atoms (Å^2)	116.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.61% 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

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	0.34	0/2115	0.56	0/2882
1	B	0.33	0/2108	0.55	0/2872
1	C	0.31	0/2053	0.55	0/2797
2	D	0.33	0/1519	0.54	0/2067
2	E	0.31	0/1524	0.53	0/2074
2	F	0.30	0/1512	0.53	0/2057
All	All	0.32	0/10831	0.54	0/14749

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

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	2080	0	2058	17	0
1	B	2073	0	2050	8	0
1	C	2018	0	1992	15	0
2	D	1487	0	1454	1	0
2	E	1492	0	1456	0	0
2	F	1480	0	1445	0	0
3	B	14	0	13	2	0
All	All	10644	0	10468	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 1.

All (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:A:294:GLN:HG3	1:C:153:PHE:HE2	1.35	0.92
1:B:76:ILE:HA	3:B:401:NAG:H82	1.58	0.86
1:A:294:GLN:HG3	1:C:153:PHE:CE2	2.17	0.80
1:A:296:SER:HG	1:C:153:PHE:HE1	1.43	0.66
1:A:219:LEU:HD22	1:A:229:ILE:HD11	1.78	0.66
1:A:73:ILE:HG21	2:D:144:VAL:HG21	1.75	0.65
1:A:57:LEU:O	1:A:58:GLU:HB3	1.97	0.65
1:B:57:LEU:HD11	1:B:80:ILE:HD11	1.78	0.64
1:B:219:LEU:HD22	1:B:229:ILE:HD11	1.79	0.64
1:C:219:LEU:HD22	1:C:229:ILE:HD11	1.79	0.63
1:B:76:ILE:CA	3:B:401:NAG:H82	2.30	0.60
1:A:57:LEU:O	1:A:58:GLU:CB	2.49	0.60
1:A:153:PHE:CE1	1:C:283:THR:HG21	2.40	0.57
1:A:151:ARG:NH1	1:C:149:THR:O	2.40	0.55
1:C:260:TRP:HB3	1:C:263:VAL:O	2.09	0.51
1:A:107:ARG:NE	1:C:247:ASP:OD2	2.43	0.51
1:A:156:ARG:HH21	1:C:281:LEU:HB2	1.77	0.50
1:A:153:PHE:HE1	1:C:283:THR:HG21	1.78	0.49
1:A:39:SER:HB3	1:A:42:ASP:HB3	1.94	0.48
1:C:39:SER:HB3	1:C:42:ASP:HB3	1.96	0.48
1:B:39:SER:HB3	1:B:42:ASP:HB3	1.95	0.48
1:A:156:ARG:NH2	1:C:279:GLY:O	2.51	0.44
1:C:34:ALA:O	1:C:35:ASN:CB	2.68	0.42
1:A:34:ALA:O	1:A:35:ASN:CB	2.67	0.42
1:C:241:VAL:HB	1:C:266:ILE:HD13	2.02	0.42
1:B:34:ALA:O	1:B:35:ASN:CB	2.67	0.42
1:B:241:VAL:HB	1:B:266:ILE:HD13	2.02	0.42
1:A:241:VAL:HB	1:A:266:ILE:HD13	2.01	0.41
1:A:34:ALA:O	1:A:35:ASN:HB3	2.21	0.41
1:C:34:ALA:O	1:C:35:ASN:HB3	2.21	0.40
1:B:34:ALA:O	1:B:35:ASN:HB3	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	259/283 (92%)	250 (96%)	8 (3%)	1 (0%)	34	64
1	B	258/283 (91%)	248 (96%)	9 (4%)	1 (0%)	34	64
1	C	251/283 (89%)	240 (96%)	10 (4%)	1 (0%)	34	64
2	D	189/299 (63%)	184 (97%)	5 (3%)	0	100	100
2	E	190/299 (64%)	185 (97%)	5 (3%)	0	100	100
2	F	188/299 (63%)	183 (97%)	5 (3%)	0	100	100
All	All	1335/1746 (76%)	1290 (97%)	42 (3%)	3 (0%)	47	77

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	35	ASN
1	C	35	ASN
1	A	35	ASN

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	241/257 (94%)	238 (99%)	3 (1%)	71	87
1	B	240/257 (93%)	235 (98%)	5 (2%)	53	77
1	C	233/257 (91%)	227 (97%)	6 (3%)	46	72
2	D	167/257 (65%)	163 (98%)	4 (2%)	49	74

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
2	E	167/257 (65%)	165 (99%)	2 (1%)	71 87
2	F	166/257 (65%)	164 (99%)	2 (1%)	71 87
All	All	1214/1542 (79%)	1192 (98%)	22 (2%)	59 80

All (22) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	93	THR
1	B	111	ARG
1	B	256	THR
1	B	260	TRP
1	B	287	GLU
1	A	93	THR
1	A	151	ARG
1	A	287	GLU
1	C	56	LEU
1	C	93	THR
1	C	256	THR
1	C	259	GLN
1	C	260	TRP
1	C	287	GLU
2	D	178	THR
2	D	209	SER
2	D	218	SER
2	D	226	VAL
2	E	209	SER
2	E	218	SER
2	F	209	SER
2	F	218	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	C	255	GLN

5.3.3 RNA

There are no RNA molecules in this entry.

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

1 non-standard protein/DNA/RNA residue is 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	401	1	14,14,15	0.28	0	17,19,21	0.60	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
3	NAG	B	401	1	-	1/6/23/26	0/1/1/1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (1) torsion outliers are listed below:

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

There are no ring outliers.

1 monomer is involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	401	NAG	2	0

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

1 ligand is 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	401	1	14,14,15	0.28	0	17,19,21	0.60	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
3	NAG	B	401	1	-	1/6/23/26	0/1/1/1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (1) torsion outliers are listed below:

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

There are no ring outliers.

1 monomer is involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	401	NAG	2	0

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data

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	263/283 (92%)	0.06	1 (0%) 92 82	65, 92, 129, 162	0
1	B	262/283 (92%)	-0.07	0 100 100	71, 107, 163, 198	0
1	C	255/283 (90%)	0.19	7 (2%) 54 28	107, 146, 192, 211	0
2	D	193/299 (64%)	-0.17	0 100 100	61, 85, 123, 142	0
2	E	194/299 (64%)	-0.18	2 (1%) 82 63	70, 111, 168, 218	0
2	F	192/299 (64%)	-0.05	2 (1%) 82 63	91, 125, 181, 200	0
All	All	1359/1746 (77%)	-0.02	12 (0%) 84 66	61, 111, 176, 218	0

All (12) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	F	223	TYR	3.4
1	C	131	TYR	3.2
1	C	196	VAL	3.1
1	C	91	LEU	2.9
2	E	187	ARG	2.5
1	C	202	MET	2.3
2	E	165	ILE	2.2
1	C	199	LEU	2.2
1	C	302	TYR	2.1
1	C	53	LEU	2.1
2	F	222	LEU	2.1
1	A	301	VAL	2.0

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	B	401	14/15	0.92	0.25	165,174,182,187	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	B	401	14/15	0.92	0.25	165,174,182,187	0

6.5 Other polymers (i)

There are no such residues in this entry.