



Full wwPDB X-ray Structure Validation Report ⓘ

Nov 8, 2016 – 01:54 PM EST

PDB ID : 5HEZ
Title : JAK2 kinase (JH1 domain) mutant P1057A in complex with TG101209
Authors : Ultsch, M.; Eigenbrot, C.
Deposited on : 2016-01-06
Resolution : 2.66 Å(reported)

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

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<http://wwpdb.org/validation/2016/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467
Mogul : 1.7.1 (RC1), CSD as537be (2016)
Xtriage (Phenix) : 1.9-1692
EDS : rb-20028320
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac : 5.8.0135
CCP4 : 6.5.0
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : rb-20028320

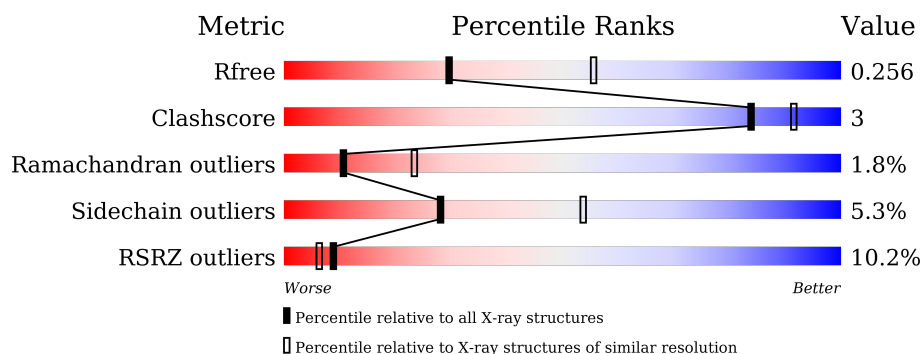
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.66 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	91344	3152 (2.70-2.62)
Clashscore	102246	3524 (2.70-2.62)
Ramachandran outliers	100387	3469 (2.70-2.62)
Sidechain outliers	100360	3469 (2.70-2.62)
RSRZ outliers	91569	3161 (2.70-2.62)

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	302	 9% 81% 13% . .
1	B	302	 9% 80% 15% . .
1	C	302	 11% 86% 9% . .
1	D	302	 11% 83% 12% . .

2 Entry composition [i](#)

There are 5 unique types of molecules in this entry. The entry contains 10024 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 Tyrosine-protein kinase JAK2.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	289	Total	C	N	O	P	S	0	0	0
			2394	1517	414	447	2	14			
1	B	291	Total	C	N	O	P	S	0	0	0
			2409	1525	419	449	2	14			
1	C	291	Total	C	N	O	P	S	0	0	0
			2409	1525	419	449	2	14			
1	D	291	Total	C	N	O	P	S	0	0	0
			2409	1525	419	449	2	14			

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	831	GLY	-	expression tag	UNP O60674
A	832	SER	-	expression tag	UNP O60674
A	1057	ALA	PRO	engineered mutation	UNP O60674
B	831	GLY	-	expression tag	UNP O60674
B	832	SER	-	expression tag	UNP O60674
B	1057	ALA	PRO	engineered mutation	UNP O60674
C	831	GLY	-	expression tag	UNP O60674
C	832	SER	-	expression tag	UNP O60674
C	1057	ALA	PRO	engineered mutation	UNP O60674
D	831	GLY	-	expression tag	UNP O60674
D	832	SER	-	expression tag	UNP O60674
D	1057	ALA	PRO	engineered mutation	UNP O60674

- Molecule 2 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	B	1	Total	Cl	0	0
			1	1		
2	A	1	Total	Cl	0	0
			1	1		

Continued on next page...

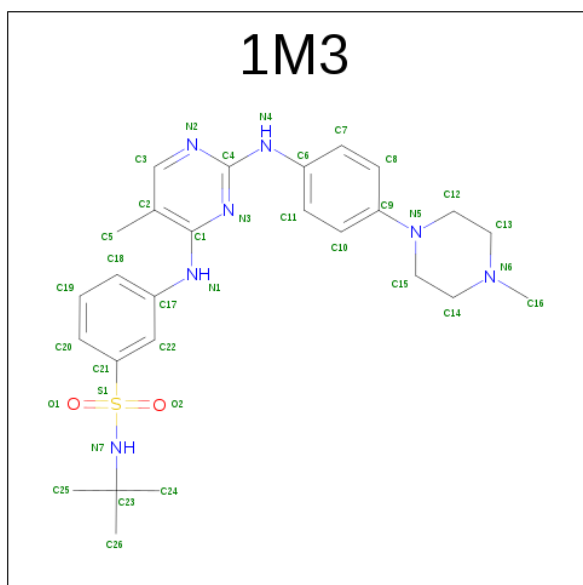
Continued from previous page...

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	D	1	Total	Cl	0	0
			1	1		

- Molecule 3 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	B	1	Total	Zn	0	0
			1	1		
3	A	1	Total	Zn	0	0
			1	1		

- Molecule 4 is N-tert-butyl-3-[(5-methyl-2-{[4-(4-methylpiperazin-1-yl)phenyl]amino}pyrimidin-4-yl)amino]benzenesulfonamide (three-letter code: 1M3) (formula: C₂₆H₃₅N₇O₂S).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	A	1	Total	C	N	O	S	0	0
			36	26	7	2	1		
4	A	1	Total	C	N	O	S	0	0
			36	26	7	2	1		
4	B	1	Total	C	N	O	S	0	0
			36	26	7	2	1		
4	B	1	Total	C	N	O	S	0	0
			36	26	7	2	1		
4	C	1	Total	C	N	O	S	0	0
			36	26	7	2	1		
4	C	1	Total	C	N	O	S	0	0
			36	26	7	2	1		

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	D	1	Total	C	N	O	S	0	0
			36	26	7	2	1		
4	D	1	Total	C	N	O	S	0	0
			36	26	7	2	1		

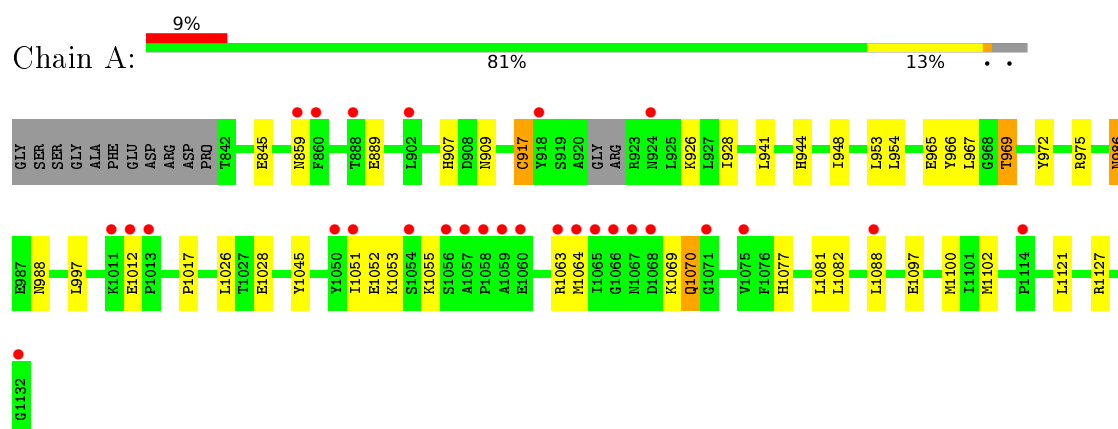
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	34	Total	O	0	0
			34	34		
5	B	37	Total	O	0	0
			37	37		
5	C	22	Total	O	0	0
			22	22		
5	D	17	Total	O	0	0
			17	17		

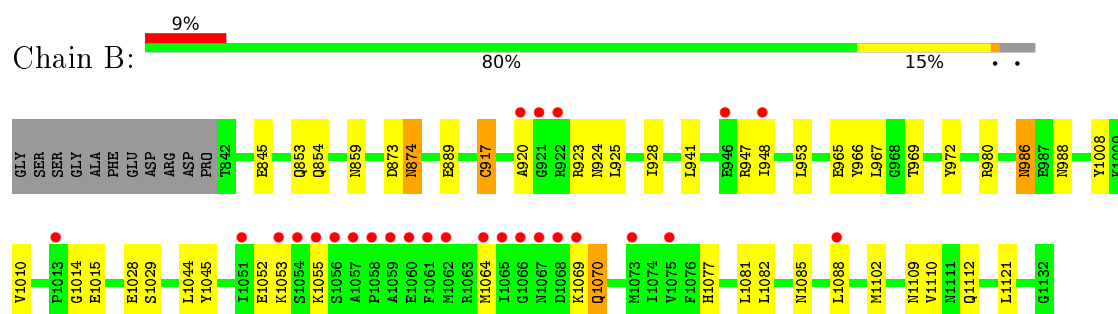
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

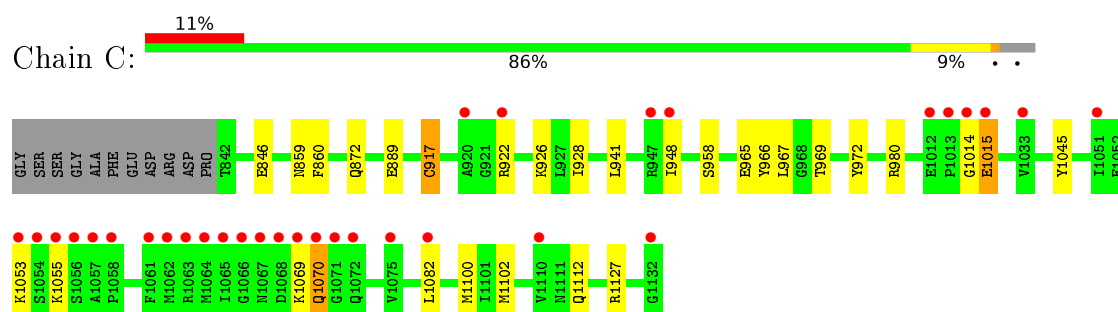
- Molecule 1: Tyrosine-protein kinase JAK2



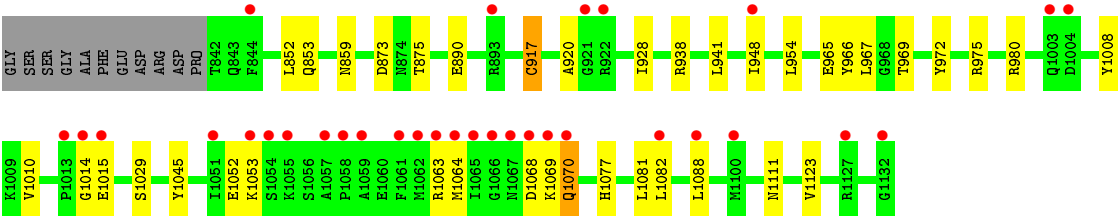
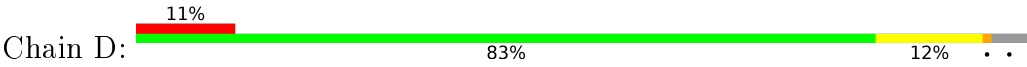
- Molecule 1: Tyrosine-protein kinase JAK2



- Molecule 1: Tyrosine-protein kinase JAK2



- Molecule 1: Tyrosine-protein kinase JAK2



4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 2	Depositor
Cell constants a, b, c, α , β , γ	211.81Å 215.65Å 91.50Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	26.81 – 2.66 26.48 – 2.66	Depositor EDS
% Data completeness (in resolution range)	99.6 (26.81-2.66) 99.7 (26.48-2.66)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.15	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.09 (at 2.68Å)	Xtriage
Refinement program	BUSTER 2.11.5	Depositor
R, R_{free}	0.217 , 0.238 0.230 , 0.256	Depositor DCC
R_{free} test set	2987 reflections (5.22%)	DCC
Wilson B-factor (Å ²)	53.6	Xtriage
Anisotropy	0.565	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 39.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	0.116 for -k,-h,-l	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	10024	wwPDB-VP
Average B, all atoms (Å ²)	67.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.68% 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: 1M3, ZN, PTR, CL

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	0.43	0/2409	0.65	0/3237
1	B	0.44	0/2425	0.66	0/3259
1	C	0.42	0/2425	0.64	0/3259
1	D	0.42	0/2425	0.64	0/3259
All	All	0.43	0/9684	0.65	0/13014

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	2394	0	2366	19	0
1	B	2409	0	2383	17	0
1	C	2409	0	2383	12	0
1	D	2409	0	2383	14	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
2	D	1	0	0	0	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	A	72	0	70	3	0
4	B	72	0	70	1	0
4	C	72	0	70	2	0
4	D	72	0	70	2	0
5	A	34	0	0	0	0
5	B	37	0	0	0	0
5	C	22	0	0	0	0
5	D	17	0	0	0	0
All	All	10024	0	9795	59	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 3.

All (59) 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:1014:GLY:HA2	1:D:1064:MET:HA	1.57	0.85
1:A:986:ASN:HD22	1:A:988:ASN:H	1.29	0.81
1:B:986:ASN:HD22	1:B:988:ASN:H	1.30	0.79
1:A:1082:LEU:HD23	4:C:1202:1M3:H23	1.76	0.67
1:A:1064:MET:HA	1:C:1014:GLY:HA2	1.77	0.65
4:B:1202:1M3:H23	1:D:1082:LEU:HD23	1.79	0.64
1:B:1082:LEU:HD23	4:D:1202:1M3:H23	1.81	0.63
1:C:958:SER:HB2	1:C:1127:ARG:HH12	1.64	0.62
1:C:1045:TYR:HB2	1:C:1102:MET:HE3	1.85	0.59
1:A:907:HIS:HE1	1:A:909:ASN:HD22	1.51	0.59
1:D:941:LEU:HD23	1:D:948:ILE:HD13	1.87	0.55
1:A:941:LEU:HD23	1:A:948:ILE:HD13	1.88	0.55
1:C:860:PHE:CZ	1:C:1015:GLU:HG3	2.42	0.55
1:B:941:LEU:HD23	1:B:948:ILE:HD13	1.88	0.54
1:D:917:CYS:HB2	1:D:928:ILE:HD11	1.91	0.52
1:D:1008:PTR:HE1	1:D:1010:VAL:HG22	1.91	0.51
1:B:1008:PTR:HE1	1:B:1010:VAL:HG22	1.91	0.51
1:B:1109:ASN:HB3	1:B:1112:GLN:HB2	1.91	0.51
1:C:941:LEU:HD23	1:C:948:ILE:HD13	1.94	0.50
4:A:1203:1M3:H23	1:C:1082:LEU:HD23	1.94	0.49
1:A:966:TYR:O	1:A:969:THR:HB	2.12	0.49
1:C:966:TYR:O	1:C:969:THR:HB	2.13	0.49
1:C:917:CYS:HB2	1:C:928:ILE:HD11	1.94	0.49
1:B:966:TYR:O	1:B:969:THR:HB	2.13	0.49
1:A:907:HIS:CE1	1:A:909:ASN:HD22	2.30	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:966:TYR:O	1:D:969:THR:HB	2.13	0.48
1:A:1045:TYR:HD1	1:A:1102:MET:HE3	1.80	0.47
1:A:917:CYS:HB2	1:A:928:ILE:HD11	1.97	0.46
1:B:1044:LEU:HD23	1:B:1102:MET:HG3	1.97	0.46
1:A:997:LEU:HD11	1:A:1017:PRO:HD2	1.97	0.46
1:C:917:CYS:HB3	1:C:926:LYS:HB2	1.98	0.46
1:A:954:LEU:HB3	1:A:1127:ARG:HG2	1.98	0.45
1:B:1064:MET:HA	1:D:1014:GLY:HA2	1.97	0.45
1:D:873:ASP:OD1	1:D:875:THR:HG22	2.17	0.45
1:A:944:HIS:HE1	1:B:845:GLU:OE1	1.99	0.45
4:A:1204:1M3:H21	4:A:1204:1M3:N3	2.32	0.45
1:B:917:CYS:HB2	1:B:928:ILE:HD11	1.98	0.44
1:B:873:ASP:O	1:B:874:ASN:HB2	2.17	0.44
1:D:954:LEU:HD22	1:D:1123:VAL:HG13	1.98	0.44
1:D:1045:TYR:HE2	1:D:1077:HIS:CD2	2.37	0.43
1:A:917:CYS:HB3	1:A:926:LYS:HB2	2.00	0.43
1:B:1045:TYR:HE2	1:B:1077:HIS:CD2	2.36	0.42
4:D:1202:1M3:H5	4:D:1202:1M3:H25	2.01	0.42
1:B:953:LEU:HA	1:B:953:LEU:HD23	1.88	0.42
1:A:1081:LEU:HD13	1:A:1088:LEU:HG	2.00	0.42
1:B:1081:LEU:HD13	1:B:1088:LEU:HG	2.01	0.42
1:A:953:LEU:HG	1:A:1051:ILE:HD12	2.00	0.42
4:C:1201:1M3:H21	4:C:1201:1M3:N3	2.34	0.42
1:D:1010:VAL:O	1:D:1029:SER:HB3	2.20	0.42
1:A:967:LEU:HG	1:A:972:TYR:HB2	2.02	0.42
1:A:1045:TYR:HE2	1:A:1077:HIS:CD2	2.38	0.42
1:C:967:LEU:HG	1:C:972:TYR:HB2	2.02	0.42
1:D:1081:LEU:HD13	1:D:1088:LEU:HG	2.02	0.41
1:A:1026:LEU:HD22	4:A:1203:1M3:H8	2.02	0.41
1:D:967:LEU:HG	1:D:972:TYR:HB2	2.02	0.41
1:B:967:LEU:HG	1:B:972:TYR:HB2	2.02	0.41
1:B:1010:VAL:O	1:B:1029:SER:HB3	2.21	0.40
1:A:1063:ARG:O	1:C:1014:GLY:O	2.39	0.40
1:C:872:GLN:HG2	1:D:852:LEU:HB3	2.03	0.40

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	283/302 (94%)	265 (94%)	14 (5%)	4 (1%)	14	31
1	B	287/302 (95%)	266 (93%)	13 (4%)	8 (3%)	6	13
1	C	287/302 (95%)	270 (94%)	14 (5%)	3 (1%)	19	41
1	D	287/302 (95%)	270 (94%)	11 (4%)	6 (2%)	9	20
All	All	1144/1208 (95%)	1071 (94%)	52 (4%)	21 (2%)	11	23

All (21) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	1053	LYS
1	B	920	ALA
1	B	1053	LYS
1	C	1053	LYS
1	D	1053	LYS
1	B	1015	GLU
1	D	1015	GLU
1	D	1068	ASP
1	B	874	ASN
1	B	1070	GLN
1	D	1052	GLU
1	A	1055	LYS
1	A	1070	GLN
1	B	925	LEU
1	B	1052	GLU
1	B	1055	LYS
1	C	1055	LYS
1	C	1070	GLN
1	D	1070	GLN
1	D	920	ALA
1	A	1052	GLU

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	261/270 (97%)	246 (94%)	15 (6%)	25	49
1	B	262/270 (97%)	245 (94%)	17 (6%)	21	43
1	C	262/270 (97%)	250 (95%)	12 (5%)	33	61
1	D	262/270 (97%)	250 (95%)	12 (5%)	33	61
All	All	1047/1080 (97%)	991 (95%)	56 (5%)	28	54

All (56) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	845	GLU
1	A	859	ASN
1	A	889	GLU
1	A	917	CYS
1	A	965	GLU
1	A	969	THR
1	A	975	ARG
1	A	986	ASN
1	A	1012	GLU
1	A	1028	GLU
1	A	1069	LYS
1	A	1070	GLN
1	A	1097	GLU
1	A	1100	MET
1	A	1121	LEU
1	B	853	GLN
1	B	854	GLN
1	B	859	ASN
1	B	889	GLU
1	B	917	CYS
1	B	923	ARG
1	B	924	ASN
1	B	947	ARG
1	B	965	GLU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	980	ARG
1	B	986	ASN
1	B	1028	GLU
1	B	1069	LYS
1	B	1070	GLN
1	B	1085	ASN
1	B	1110	VAL
1	B	1121	LEU
1	C	846	GLU
1	C	859	ASN
1	C	889	GLU
1	C	917	CYS
1	C	922	ARG
1	C	965	GLU
1	C	980	ARG
1	C	1015	GLU
1	C	1069	LYS
1	C	1070	GLN
1	C	1100	MET
1	C	1112	GLN
1	D	853	GLN
1	D	859	ASN
1	D	890	GLU
1	D	917	CYS
1	D	938	ARG
1	D	965	GLU
1	D	975	ARG
1	D	980	ARG
1	D	1063	ARG
1	D	1069	LYS
1	D	1070	GLN
1	D	1111	ASN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (16) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	909	ASN
1	A	944	HIS
1	A	955	GLN
1	A	986	ASN
1	A	1077	HIS
1	B	955	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	986	ASN
1	B	1077	HIS
1	C	854	GLN
1	C	874	ASN
1	C	1077	HIS
1	D	924	ASN
1	D	955	GLN
1	D	1077	HIS
1	D	1109	ASN
1	D	1111	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

8 non-standard protein/DNA/RNA residues are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the chemical component dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# $ Z > 2$	Counts	RMSZ	# $ Z > 2$
1	PTR	A	1007	1	13,16,17	1.18	1 (7%)	19,22,24	1.38	3 (15%)
1	PTR	A	1008	1	13,16,17	1.54	3 (23%)	19,22,24	1.54	4 (21%)
1	PTR	B	1007	1	13,16,17	1.11	1 (7%)	19,22,24	1.42	3 (15%)
1	PTR	B	1008	1	13,16,17	1.38	3 (23%)	19,22,24	1.62	5 (26%)
1	PTR	C	1007	1	13,16,17	1.20	1 (7%)	19,22,24	1.31	2 (10%)
1	PTR	C	1008	1	13,16,17	1.29	2 (15%)	19,22,24	1.02	2 (10%)
1	PTR	D	1007	1	13,16,17	1.29	2 (15%)	19,22,24	1.25	2 (10%)
1	PTR	D	1008	1	13,16,17	1.22	1 (7%)	19,22,24	1.92	4 (21%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the chemical

component dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	PTR	A	1007	1	-	0/9/11/13	0/1/1/1
1	PTR	A	1008	1	-	0/9/11/13	0/1/1/1
1	PTR	B	1007	1	-	0/9/11/13	0/1/1/1
1	PTR	B	1008	1	-	0/9/11/13	0/1/1/1
1	PTR	C	1007	1	-	0/9/11/13	0/1/1/1
1	PTR	C	1008	1	-	0/9/11/13	0/1/1/1
1	PTR	D	1007	1	-	0/9/11/13	0/1/1/1
1	PTR	D	1008	1	-	0/9/11/13	0/1/1/1

All (14) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	1007	PTR	CD2-CG	2.06	1.43	1.38
1	C	1008	PTR	CE2-CD2	2.22	1.43	1.38
1	A	1008	PTR	CD2-CG	2.29	1.43	1.38
1	B	1008	PTR	CD2-CG	2.37	1.44	1.38
1	B	1007	PTR	CE2-CZ	2.40	1.43	1.38
1	A	1008	PTR	CE2-CD2	2.47	1.43	1.38
1	B	1008	PTR	CE2-CD2	2.57	1.43	1.38
1	C	1008	PTR	CE2-CZ	2.67	1.44	1.38
1	B	1008	PTR	CE2-CZ	2.85	1.44	1.38
1	D	1007	PTR	CE1-CZ	2.87	1.44	1.38
1	A	1007	PTR	CE1-CZ	2.95	1.44	1.38
1	D	1008	PTR	CE2-CZ	2.97	1.44	1.38
1	C	1007	PTR	CE1-CZ	3.00	1.44	1.38
1	A	1008	PTR	CE2-CZ	3.55	1.45	1.38

All (25) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1008	PTR	OH-CZ-CE1	-3.27	109.02	119.22
1	B	1008	PTR	OH-CZ-CE1	-3.10	109.56	119.22
1	D	1008	PTR	OH-CZ-CE1	-2.58	111.20	119.22
1	B	1008	PTR	O-C-CA	-2.31	119.53	125.72
1	C	1008	PTR	O-C-CA	-2.24	119.72	125.72
1	D	1008	PTR	O-C-CA	-2.18	119.88	125.72
1	A	1008	PTR	O-C-CA	-2.12	120.05	125.72
1	A	1007	PTR	O-C-CA	-2.11	120.06	125.72
1	B	1007	PTR	O-C-CA	-2.07	120.16	125.72
1	C	1007	PTR	O-C-CA	-2.03	120.28	125.72

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	1007	PTR	O-C-CA	-2.02	120.29	125.72
1	B	1008	PTR	O3P-P-O2P	2.01	114.83	107.44
1	A	1007	PTR	O3P-P-OH	2.02	111.91	105.47
1	C	1008	PTR	OH-CZ-CE2	2.13	125.83	119.22
1	B	1007	PTR	O3P-P-OH	2.35	112.94	105.47
1	D	1007	PTR	OH-CZ-CE1	2.38	126.64	119.22
1	A	1007	PTR	OH-CZ-CE1	2.56	127.20	119.22
1	C	1007	PTR	OH-CZ-CE1	2.61	127.34	119.22
1	A	1008	PTR	O2P-P-OH	2.72	114.14	105.47
1	B	1008	PTR	O2P-P-OH	3.29	115.94	105.47
1	D	1008	PTR	OH-CZ-CE2	3.34	129.60	119.22
1	B	1008	PTR	OH-CZ-CE2	3.52	130.19	119.22
1	A	1008	PTR	OH-CZ-CE2	3.59	130.40	119.22
1	B	1007	PTR	O2P-P-OH	3.65	117.10	105.47
1	D	1008	PTR	O3P-P-OH	5.94	124.39	105.47

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	B	1008	PTR	1	0
1	D	1008	PTR	1	0

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

Of 13 ligands modelled in this entry, 5 are monoatomic - leaving 8 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
4	1M3	A	1203	-	37,39,39	0.98	2 (5%)	52,57,57	1.81	7 (13%)
4	1M3	A	1204	-	37,39,39	1.26	2 (5%)	52,57,57	2.04	9 (17%)
4	1M3	B	1202	-	37,39,39	1.05	1 (2%)	52,57,57	1.79	8 (15%)
4	1M3	B	1203	-	37,39,39	1.26	3 (8%)	52,57,57	2.18	12 (23%)
4	1M3	C	1201	-	37,39,39	1.19	3 (8%)	52,57,57	2.07	11 (21%)
4	1M3	C	1202	-	37,39,39	1.05	2 (5%)	52,57,57	1.79	6 (11%)
4	1M3	D	1202	-	37,39,39	1.10	2 (5%)	52,57,57	1.73	6 (11%)
4	1M3	D	1203	-	37,39,39	1.42	2 (5%)	52,57,57	1.88	9 (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
4	1M3	A	1203	-	-	0/24/34/34	0/4/4/4
4	1M3	A	1204	-	-	0/24/34/34	0/4/4/4
4	1M3	B	1202	-	-	0/24/34/34	0/4/4/4
4	1M3	B	1203	-	-	0/24/34/34	0/4/4/4
4	1M3	C	1201	-	-	0/24/34/34	0/4/4/4
4	1M3	C	1202	-	-	0/24/34/34	0/4/4/4
4	1M3	D	1202	-	-	0/24/34/34	0/4/4/4
4	1M3	D	1203	-	-	0/24/34/34	0/4/4/4

All (17) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	D	1202	1M3	O1-S1	-2.23	1.41	1.43
4	C	1201	1M3	C1-N1	2.03	1.40	1.36
4	C	1201	1M3	C4-N4	2.20	1.40	1.36
4	A	1203	1M3	C4-N4	2.23	1.40	1.36
4	A	1204	1M3	C1-N1	2.26	1.40	1.36
4	C	1202	1M3	C4-N4	2.33	1.40	1.36
4	B	1203	1M3	C1-N1	2.44	1.40	1.36
4	B	1203	1M3	C4-N4	2.47	1.40	1.36
4	D	1203	1M3	C1-N1	2.50	1.40	1.36
4	A	1203	1M3	S1-N7	3.30	1.66	1.61
4	C	1202	1M3	S1-N7	3.98	1.67	1.61
4	D	1202	1M3	S1-N7	4.07	1.67	1.61
4	B	1202	1M3	S1-N7	4.07	1.67	1.61

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	C	1201	1M3	S1-N7	4.54	1.68	1.61
4	B	1203	1M3	S1-N7	4.63	1.68	1.61
4	A	1204	1M3	S1-N7	5.25	1.69	1.61
4	D	1203	1M3	S1-N7	6.05	1.70	1.61

All (68) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	C	1201	1M3	C2-C3-N2	-7.90	119.18	125.33
4	B	1202	1M3	C2-C3-N2	-7.42	119.55	125.33
4	A	1204	1M3	C2-C3-N2	-7.13	119.78	125.33
4	D	1202	1M3	C2-C3-N2	-7.01	119.87	125.33
4	A	1203	1M3	C2-C3-N2	-6.83	120.01	125.33
4	C	1202	1M3	N2-C4-N3	-6.77	119.45	126.66
4	C	1202	1M3	C2-C3-N2	-6.74	120.08	125.33
4	B	1203	1M3	C2-C3-N2	-6.57	120.21	125.33
4	A	1203	1M3	N2-C4-N3	-6.52	119.71	126.66
4	B	1203	1M3	N2-C4-N3	-6.50	119.74	126.66
4	C	1201	1M3	N2-C4-N3	-6.43	119.81	126.66
4	D	1203	1M3	C2-C3-N2	-6.19	120.51	125.33
4	D	1203	1M3	N2-C4-N3	-6.11	120.15	126.66
4	D	1202	1M3	N2-C4-N3	-5.98	120.29	126.66
4	B	1202	1M3	N2-C4-N3	-5.84	120.44	126.66
4	A	1204	1M3	N2-C4-N3	-5.78	120.51	126.66
4	D	1202	1M3	C17-N1-C1	-3.66	120.49	129.49
4	B	1202	1M3	C17-N1-C1	-3.62	120.58	129.49
4	A	1203	1M3	C17-N1-C1	-3.51	120.84	129.49
4	C	1202	1M3	C17-N1-C1	-3.38	121.17	129.49
4	D	1203	1M3	C2-C1-N3	-2.96	117.32	122.23
4	B	1203	1M3	C2-C1-N3	-2.69	117.77	122.23
4	A	1204	1M3	C2-C1-N3	-2.64	117.86	122.23
4	A	1204	1M3	O1-S1-C21	-2.54	104.70	107.94
4	C	1202	1M3	C2-C1-N3	-2.46	118.16	122.23
4	B	1203	1M3	O2-S1-C21	-2.46	104.81	107.94
4	C	1201	1M3	C2-C1-N3	-2.35	118.35	122.23
4	C	1201	1M3	C12-N5-C9	-2.18	112.17	118.05
4	B	1203	1M3	C20-C21-S1	-2.17	117.31	119.79
4	D	1202	1M3	C15-C14-N6	-2.14	108.43	110.76
4	B	1202	1M3	C2-C1-N3	-2.14	118.69	122.23
4	B	1202	1M3	C15-C14-N6	-2.05	108.53	110.76
4	B	1203	1M3	O1-S1-O2	2.04	122.25	119.54
4	C	1201	1M3	C16-N6-C14	2.08	114.00	110.68

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	C	1201	1M3	C22-C21-S1	2.17	121.43	119.00
4	B	1202	1M3	C13-N6-C14	2.20	112.50	109.50
4	D	1203	1M3	N1-C1-N3	2.22	122.21	119.65
4	D	1203	1M3	C19-C20-C21	2.24	121.33	118.94
4	C	1201	1M3	C19-C20-C21	2.29	121.38	118.94
4	A	1204	1M3	C25-C23-N7	2.41	115.55	109.00
4	D	1203	1M3	C3-N2-C4	2.45	120.64	115.95
4	A	1204	1M3	C12-C13-N6	2.45	113.43	110.76
4	C	1201	1M3	C24-C23-N7	2.63	116.14	109.00
4	A	1204	1M3	C15-C14-N6	2.64	113.64	110.76
4	D	1202	1M3	C13-N6-C14	2.64	113.09	109.50
4	B	1203	1M3	C24-C23-N7	2.65	116.20	109.00
4	B	1203	1M3	C22-C21-S1	2.69	122.00	119.00
4	B	1203	1M3	C3-N2-C4	2.70	121.10	115.95
4	D	1203	1M3	C25-C23-N7	2.72	116.39	109.00
4	A	1204	1M3	C3-N2-C4	2.77	121.23	115.95
4	B	1202	1M3	C3-N2-C4	2.77	121.24	115.95
4	A	1203	1M3	C25-C23-N7	2.79	116.57	109.00
4	A	1203	1M3	O1-S1-O2	2.81	123.27	119.54
4	D	1202	1M3	C3-N2-C4	2.82	121.33	115.95
4	B	1203	1M3	C12-C13-N6	2.83	113.84	110.76
4	A	1203	1M3	C3-N2-C4	2.91	121.52	115.95
4	C	1202	1M3	C3-N2-C4	3.03	121.74	115.95
4	C	1201	1M3	C3-N2-C4	3.13	121.93	115.95
4	C	1201	1M3	C15-C14-N6	3.19	114.23	110.76
4	B	1202	1M3	O1-S1-O2	3.25	123.86	119.54
4	A	1203	1M3	C13-N6-C14	3.55	114.33	109.50
4	D	1203	1M3	C15-C14-N6	3.73	114.82	110.76
4	C	1202	1M3	C13-N6-C14	4.32	115.37	109.50
4	B	1203	1M3	C15-C14-N6	4.33	115.47	110.76
4	D	1203	1M3	C13-N6-C14	4.84	116.09	109.50
4	C	1201	1M3	C13-N6-C14	6.05	117.73	109.50
4	A	1204	1M3	C13-N6-C14	7.35	119.50	109.50
4	B	1203	1M3	C13-N6-C14	7.45	119.63	109.50

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

6 monomers are involved in 8 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	1203	1M3	2	0
4	A	1204	1M3	1	0
4	B	1202	1M3	1	0
4	C	1201	1M3	1	0
4	C	1202	1M3	1	0
4	D	1202	1M3	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, 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	287/302 (95%)	0.69	28 (9%) 10 7	36, 57, 140, 167	0
1	B	289/302 (95%)	0.79	26 (8%) 12 9	38, 57, 146, 179	0
1	C	289/302 (95%)	0.74	32 (11%) 7 5	39, 59, 129, 152	0
1	D	289/302 (95%)	0.77	32 (11%) 7 5	40, 63, 141, 173	0
All	All	1154/1208 (95%)	0.75	118 (10%) 9 6	36, 60, 140, 179	0

All (118) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	1066	GLY	13.9
1	C	1057	ALA	12.3
1	A	1057	ALA	10.2
1	D	1014	GLY	9.6
1	C	1066	GLY	9.5
1	B	1056	SER	9.1
1	A	1065	ILE	8.7
1	B	1062	MET	8.6
1	B	1059	ALA	8.0
1	D	1055	LYS	8.0
1	B	920	ALA	7.9
1	B	1058	PRO	7.8
1	B	1066	GLY	7.7
1	A	1071	GLY	7.4
1	D	1057	ALA	6.9
1	C	1014	GLY	6.9
1	D	922	ARG	6.9
1	B	1051	ILE	6.8
1	D	1058	PRO	6.7
1	D	1068	ASP	6.7
1	B	1057	ALA	6.6

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	B	1053	LYS	6.6
1	A	1067	ASN	6.5
1	D	1065	ILE	6.5
1	D	1062	MET	6.4
1	D	1053	LYS	6.1
1	D	1132	GLY	6.0
1	D	1015	GLU	5.9
1	A	1132	GLY	5.8
1	C	1054	SER	5.6
1	C	1067	ASN	5.5
1	B	921	GLY	5.3
1	C	1064	MET	5.3
1	A	1060	GLU	5.2
1	D	1061	PHE	5.0
1	D	1070	GLN	5.0
1	A	1056	SER	4.9
1	D	1064	MET	4.9
1	D	1069	LYS	4.9
1	A	1064	MET	4.9
1	D	1054	SER	4.8
1	B	1061	PHE	4.8
1	A	1058	PRO	4.8
1	C	1068	ASP	4.7
1	C	1013	PRO	4.7
1	A	1051	ILE	4.6
1	B	1060	GLU	4.5
1	B	1068	ASP	4.5
1	C	1069	LYS	4.5
1	C	1015	GLU	4.4
1	B	948	ILE	4.2
1	C	1055	LYS	4.2
1	D	1067	ASN	4.0
1	B	1065	ILE	4.0
1	D	921	GLY	4.0
1	C	1071	GLY	3.9
1	C	1065	ILE	3.9
1	C	1132	GLY	3.8
1	C	1062	MET	3.8
1	D	948	ILE	3.8
1	C	1033	VAL	3.8
1	C	920	ALA	3.7
1	B	1067	ASN	3.7

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	C	1061	PHE	3.6
1	B	1054	SER	3.6
1	B	1055	LYS	3.5
1	D	1051	ILE	3.5
1	C	948	ILE	3.5
1	A	1075	VAL	3.5
1	D	844	PHE	3.5
1	B	1064	MET	3.5
1	B	1069	LYS	3.4
1	A	1054	SER	3.3
1	C	1051	ILE	3.2
1	C	1053	LYS	3.1
1	C	1012	GLU	3.1
1	A	1088	LEU	3.1
1	A	1068	ASP	2.9
1	C	1070	GLN	2.8
1	A	859	ASN	2.8
1	B	922	ARG	2.8
1	D	1082	LEU	2.7
1	D	1100	MET	2.7
1	A	1012	GLU	2.7
1	D	1063	ARG	2.7
1	A	1011	LYS	2.6
1	C	1056	SER	2.6
1	C	922	ARG	2.6
1	A	860	PHE	2.6
1	B	1013	PRO	2.5
1	C	1075	VAL	2.4
1	D	1127	ARG	2.4
1	D	1004	ASP	2.4
1	C	1082	LEU	2.4
1	D	1059	ALA	2.4
1	B	1075	VAL	2.4
1	C	947	ARG	2.4
1	A	1013	PRO	2.4
1	A	1050	TYR	2.3
1	A	1063	ARG	2.3
1	A	924	ASN	2.3
1	C	1063	ARG	2.3
1	D	1013	PRO	2.2
1	C	1110	VAL	2.2
1	D	1088	LEU	2.2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	B	946	GLU	2.2
1	C	1072	GLN	2.2
1	A	888	THR	2.2
1	A	918	TYR	2.1
1	C	1058	PRO	2.1
1	B	1073	MET	2.1
1	B	1088	LEU	2.1
1	A	1114	PRO	2.1
1	A	902	LEU	2.0
1	D	1066	GLY	2.0
1	A	1059	ALA	2.0
1	D	1003	GLN	2.0
1	D	893	ARG	2.0

6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å ²)	Q<0.9
1	PTR	C	1007	16/17	0.91	0.16	-	78,86,102,104	0
1	PTR	A	1008	16/17	0.90	0.16	-	66,74,89,90	0
1	PTR	C	1008	16/17	0.90	0.18	-	79,83,98,99	0
1	PTR	D	1008	16/17	0.93	0.21	-	80,84,96,99	0
1	PTR	D	1007	16/17	0.92	0.21	-	81,91,109,112	0
1	PTR	A	1007	16/17	0.93	0.19	-	63,70,84,87	0
1	PTR	B	1007	16/17	0.96	0.19	-	60,67,82,85	0
1	PTR	B	1008	16/17	0.92	0.16	-	61,68,85,86	0

6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron

density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å ²)	Q<0.9
4	1M3	D	1203	36/36	0.96	0.21	0.66	38,44,52,53	0
4	1M3	D	1202	36/36	0.96	0.25	0.54	48,54,68,69	0
4	1M3	A	1204	36/36	0.97	0.21	-0.03	43,47,58,60	0
4	1M3	C	1201	36/36	0.98	0.20	-0.15	41,47,54,56	0
4	1M3	A	1203	36/36	0.98	0.21	-0.23	43,50,69,69	0
3	ZN	B	1204	1/1	0.99	0.19	-0.24	54,54,54,54	0
4	1M3	B	1202	36/36	0.98	0.22	-0.25	39,48,64,65	0
3	ZN	A	1202	1/1	1.00	0.18	-0.32	54,54,54,54	0
4	1M3	C	1202	36/36	0.96	0.20	-0.32	51,58,69,71	0
4	1M3	B	1203	36/36	0.98	0.18	-0.49	38,44,54,57	0
2	CL	D	1201	1/1	0.84	0.17	-	89,89,89,89	0
2	CL	B	1201	1/1	0.87	0.27	-	98,98,98,98	0
2	CL	A	1201	1/1	0.82	0.20	-	105,105,105,105	0

6.5 Other polymers

There are no such residues in this entry.