Full wwPDB X-ray Structure Validation Report (i)

Feb 1, 2016 – 07:46 AM GMT

PDB ID	:	3C4M
Title	:	Structure of human parathyroid hormone in complex with the extracellular domain of its G-protein-coupled receptor (PTH1R)
Authors	:	Pioszak, A.A.; Xu, H.E.
Deposited on	:	2008-01-30
Resolution	:	1.95 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 (i) symbol.

The following versions of software and data (see references (1)) were used in the production of this report:

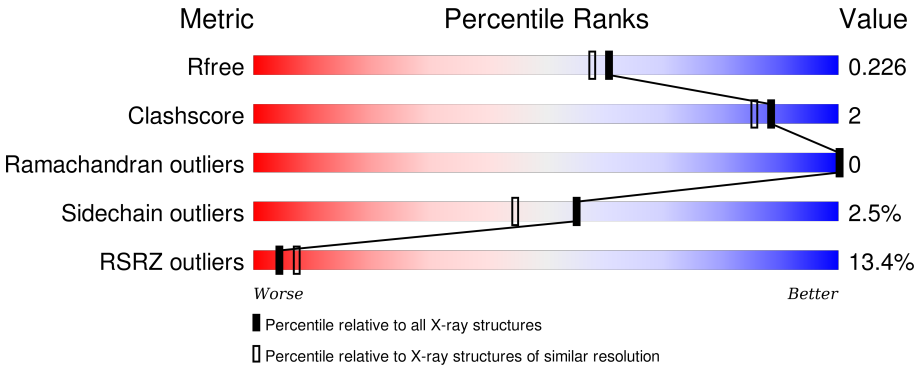
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	trunk26865

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 1.95 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	1833 (1.96-1.96)
Clashscore	102246	1953 (1.96-1.96)
Ramachandran outliers	100387	1936 (1.96-1.96)
Sidechain outliers	100360	1936 (1.96-1.96)
RSRZ outliers	91569	1835 (1.96-1.96)

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 <=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	539	13% 81% 5% • 13%
1	B	539	10% 80% 6% • 13%
2	C	21	24% 86% 14%
2	D	21	14% 95% 5%

2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 8349 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 Fusion protein of Maltose-binding periplasmic protein and Parathyroid hormone/parathyroid hormone-related peptide receptor.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	469	Total	C	N	O	S	0	0	0
			3684	2366	612	693	13			
1	B	469	Total	C	N	O	S	0	0	0
			3681	2363	612	693	13			

There are 26 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-345	MET	-	INITIATING METHIONINE	UNP P0AEX9
A	23	ASN	-	LINKER	UNP P0AEX9
A	24	ALA	-	LINKER	UNP P0AEX9
A	25	ALA	-	LINKER	UNP P0AEX9
A	26	ALA	-	LINKER	UNP P0AEX9
A	27	GLU	-	LINKER	UNP P0AEX9
A	28	PHE	-	LINKER	UNP P0AEX9
A	188	HIS	-	EXPRESSION TAG	UNP P0AEX9
A	189	HIS	-	EXPRESSION TAG	UNP P0AEX9
A	190	HIS	-	EXPRESSION TAG	UNP P0AEX9
A	191	HIS	-	EXPRESSION TAG	UNP P0AEX9
A	192	HIS	-	EXPRESSION TAG	UNP P0AEX9
A	193	HIS	-	EXPRESSION TAG	UNP P0AEX9
B	-345	MET	-	INITIATING METHIONINE	UNP P0AEX9
B	23	ASN	-	LINKER	UNP P0AEX9
B	24	ALA	-	LINKER	UNP P0AEX9
B	25	ALA	-	LINKER	UNP P0AEX9
B	26	ALA	-	LINKER	UNP P0AEX9
B	27	GLU	-	LINKER	UNP P0AEX9
B	28	PHE	-	LINKER	UNP P0AEX9
B	188	HIS	-	EXPRESSION TAG	UNP P0AEX9
B	189	HIS	-	EXPRESSION TAG	UNP P0AEX9
B	190	HIS	-	EXPRESSION TAG	UNP P0AEX9
B	191	HIS	-	EXPRESSION TAG	UNP P0AEX9

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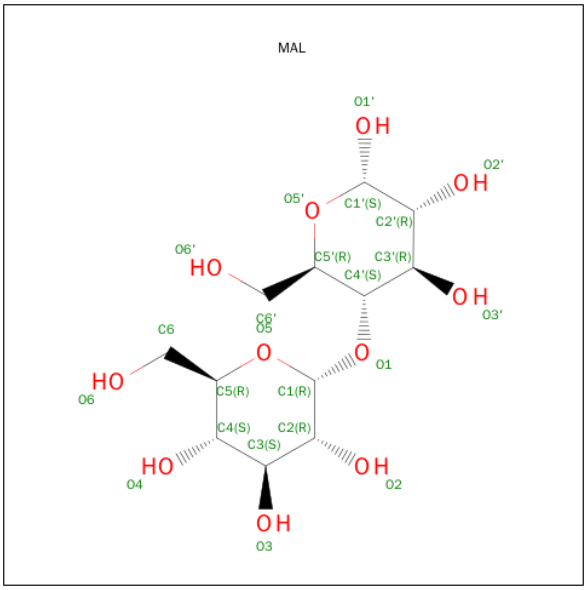
Chain	Residue	Modelled	Actual	Comment	Reference
B	192	HIS	-	EXPRESSION TAG	UNP P0AEX9
B	193	HIS	-	EXPRESSION TAG	UNP P0AEX9

- Molecule 2 is a protein called Parathyroid hormone.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	C	21	Total	C	N	O	S	0	0	1
			179	113	35	30	1			
2	D	21	Total	C	N	O	S	0	0	1
			179	113	35	30	1			

- Molecule 3 is SUGAR (MALTOSE) (three-letter code: MAL) (formula: $C_{12}H_{22}O_{11}$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	O		0	0
			23	12	11			
3	B	1	Total	C	O		0	0
			23	12	11			

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	330	Total	O	0	0
			330	330		
4	B	230	Total	O	0	0
			230	230		

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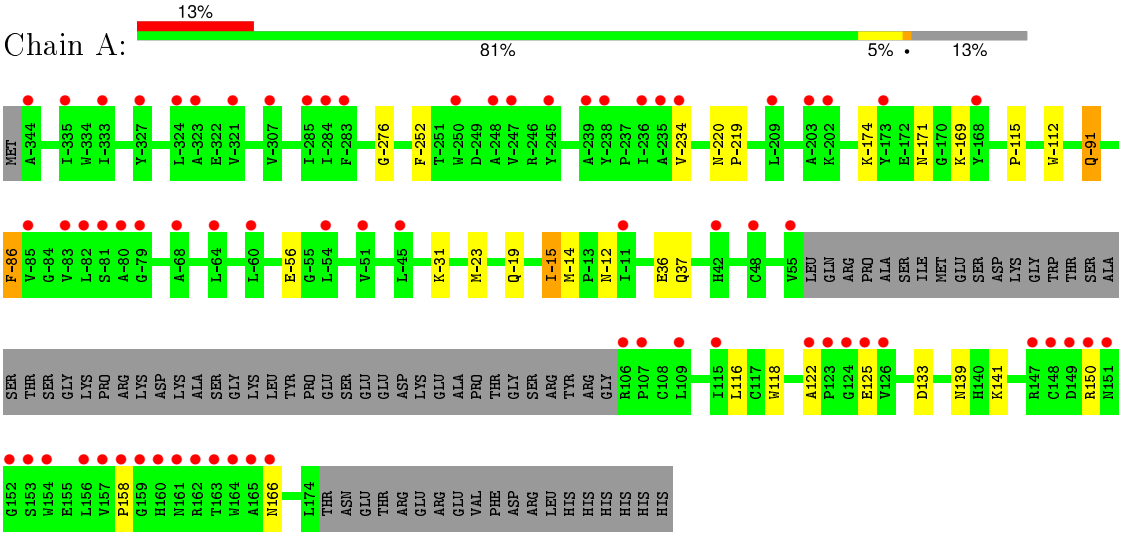
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	C	6	Total O 6 6	0	0
4	D	14	Total O 14 14	0	0

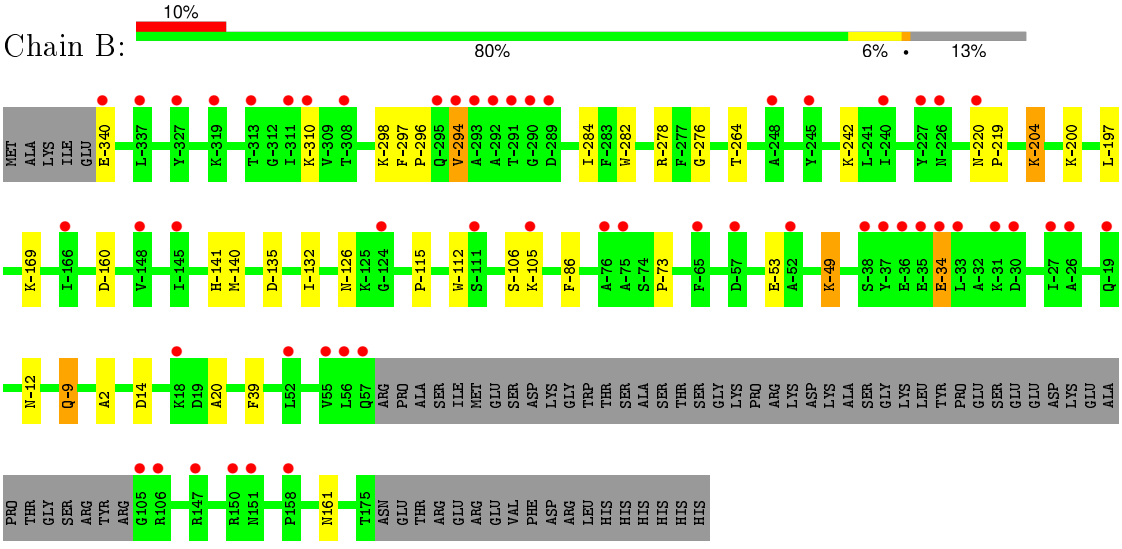
3 Residue-property plots (i)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of 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: Fusion protein of Maltose-binding periplasmic protein and Parathyroid hormone/parathyroid hormone-related peptide receptor

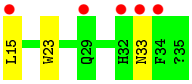


• Molecule 1: Fusion protein of Maltose-binding periplasmic protein and Parathyroid hormone/parathyroid hormone-related peptide receptor



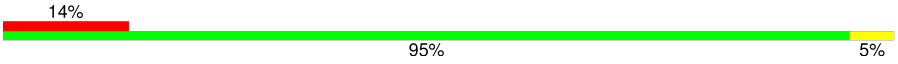
• Molecule 2: Parathyroid hormone

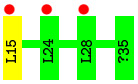
Chain C:



- Molecule 2: Parathyroid hormone

Chain D:





4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	62.92Å 116.79Å 78.42Å 90.00° 108.80° 90.00°	Depositor
Resolution (Å)	50.00 – 1.95 41.70 – 1.95	Depositor EDS
% Data completeness (in resolution range)	97.9 (50.00-1.95) 97.9 (41.70-1.95)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.43 (at 1.95Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.186 , 0.227 0.186 , 0.226	Depositor DCC
R_{free} test set	3847 reflections (5.30%)	DCC
Wilson B-factor (Å^2)	31.0	Xtriage
Anisotropy	0.347	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.33 , 39.8	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.33$	Xtriage
Outliers	0 of 76498 reflections	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	8349	wwPDB-VP
Average B, all atoms (Å^2)	39.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.80% 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, 0.375 respectively for untwinned datasets, and 0.333, 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: MAL, NH2

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	0.58	3/3780 (0.1%)	0.59	1/5134 (0.0%)
1	B	0.47	0/3777	0.57	0/5131
2	C	1.47	2/181 (1.1%)	0.63	0/241
2	D	0.47	0/181	0.59	0/241
All	All	0.57	5/7919 (0.1%)	0.58	1/10747 (0.0%)

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	33	ASN	CG-OD1	15.13	1.57	1.24
2	C	33	ASN	CG-ND2	9.21	1.55	1.32
1	A	150	ARG	C-O	8.27	1.39	1.23
1	A	158	PRO	C-N	7.90	1.47	1.33
1	A	150	ARG	CZ-NH1	5.60	1.40	1.33

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	150	ARG	NE-CZ-NH2	-5.54	117.53	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	3684	0	3604	17	0
1	B	3681	0	3598	22	0
2	C	179	0	178	2	0
2	D	179	0	178	0	0
3	A	23	0	22	0	0
3	B	23	0	22	0	0
4	A	330	0	0	3	0
4	B	230	0	0	1	0
4	C	6	0	0	0	0
4	D	14	0	0	0	0
All	All	8349	0	7602	38	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.

All (38) 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:122:ALA:HB3	1:A:125:GLU:HG3	1.69	0.73
1:A:-23:MET:O	1:A:-19:GLN:HG2	1.90	0.71
1:B:-135:ASP:OD1	1:B:-132:ILE:HG12	1.99	0.63
1:B:-141:HIS:HE1	4:B:263:HOH:O	1.86	0.58
4:A:309:HOH:O	2:C:15:LEU:HB2	2.04	0.56
1:A:-276:GLY:HA3	1:A:-12:ASN:O	2.05	0.56
1:B:-53:GLU:O	1:B:-49:LYS:HG3	2.06	0.55
1:B:-197:LEU:HD23	1:B:-140:MET:CE	2.37	0.54
1:B:-276:GLY:HA3	1:B:-12:ASN:O	2.10	0.51
1:B:-282:TRP:CD1	1:B:-278:ARG:HG3	2.46	0.51
1:A:-115:PRO:HA	1:A:-112:TRP:CE2	2.46	0.49
1:A:-56:GLU:CD	1:A:-56:GLU:H	2.15	0.49
1:B:-106:SER:O	1:B:-105:LYS:HG3	2.13	0.49
1:A:-91:GLN:NE2	4:A:279:HOH:O	2.46	0.48
1:B:-297:PHE:HB3	1:B:-296:PRO:HD3	1.95	0.47
1:B:-204:LYS:HD2	1:B:-200:LYS:O	2.13	0.47
1:A:-23:MET:O	1:A:-19:GLN:CG	2.62	0.47
1:B:-9:GLN:NE2	1:B:-9:GLN:H	2.14	0.46
1:A:-15:ILE:HD13	4:A:272:HOH:O	2.15	0.46
1:B:-298:LYS:O	1:B:-294:VAL:HB	2.16	0.46
1:A:-171:ASN:OD1	1:B:-242:LYS:HE2	2.16	0.45
1:B:-9:GLN:HE21	1:B:-9:GLN:H	1.63	0.45
1:A:36:GLU:HA	1:B:39:PHE:CZ	2.52	0.45
1:B:-126:ASN:N	1:B:-126:ASN:HD22	2.12	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:-106:SER:O	1:B:-105:LYS:CG	2.65	0.44
1:A:37:GLN:HG3	2:C:23:TRP:CZ3	2.52	0.44
1:B:-197:LEU:HG	1:B:-140:MET:HE2	1.99	0.44
1:B:2:ALA:HB2	1:B:20:ALA:HB2	2.00	0.43
1:A:-252:PHE:CZ	1:A:-234:VAL:HG21	2.54	0.43
1:A:-86:PHE:CG	1:A:-14:MET:HG2	2.54	0.43
1:A:139:ASN:OD1	1:A:141:LYS:HG2	2.19	0.42
1:B:-115:PRO:HA	1:B:-112:TRP:CE2	2.55	0.41
1:A:-169:LYS:NZ	1:A:133:ASP:OD1	2.54	0.41
1:A:116:LEU:HD11	1:A:118:TRP:CE2	2.56	0.41
1:B:-220:ASN:HA	1:B:-219:PRO:HD2	1.94	0.41
1:A:-220:ASN:HA	1:A:-219:PRO:HD2	1.91	0.41
1:B:-340:GLU:HG2	1:B:-73:PRO:HG3	2.02	0.41
1:B:-34:GLU:H	1:B:-34:GLU:HG3	1.62	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	465/539 (86%)	454 (98%)	11 (2%)	0	100	100
1	B	465/539 (86%)	458 (98%)	7 (2%)	0	100	100
2	C	19/21 (90%)	19 (100%)	0	0	100	100
2	D	19/21 (90%)	19 (100%)	0	0	100	100
All	All	968/1120 (86%)	950 (98%)	18 (2%)	0	100	100

There are no Ramachandran outliers to report.

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	381/442 (86%)	375 (98%)	6 (2%)	70 66
1	B	381/442 (86%)	368 (97%)	13 (3%)	44 30
2	C	20/20 (100%)	20 (100%)	0	100 100
2	D	20/20 (100%)	19 (95%)	1 (5%)	30 14
All	All	802/924 (87%)	782 (98%)	20 (2%)	55 45

All (20) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	-174	LYS
1	A	-91	GLN
1	A	-86	PHE
1	A	-31	LYS
1	A	-15	ILE
1	A	166	ASN
1	B	-310	LYS
1	B	-294	VAL
1	B	-284	ILE
1	B	-264	THR
1	B	-204	LYS
1	B	-169	LYS
1	B	-160	ASP
1	B	-86	PHE
1	B	-49	LYS
1	B	-34	GLU
1	B	-9	GLN
1	B	14	ASP
1	B	161	ASN
2	D	15	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (12) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	-295	GLN
1	A	-244	ASN
1	A	-126	ASN
1	A	-91	GLN
1	A	-9	GLN
1	A	166	ASN
1	B	-326	ASN
1	B	-141	HIS
1	B	-126	ASN
1	B	-9	GLN
1	B	23	ASN
2	D	33	ASN

5.3.3 RNA

There are no RNA molecules in this entry.

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

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates

There are no carbohydrates in this entry.

5.6 Ligand geometry

2 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	MAL	A	194	-	24,24,24	0.55	0	35,35,35	0.76	0
3	MAL	B	194	-	24,24,24	0.48	0	35,35,35	0.85	1 (2%)

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	MAL	A	194	-	-	0/8/48/48	0/2/2/2
3	MAL	B	194	-	-	0/8/48/48	0/2/2/2

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	B	194	MAL	O5'-C1'-C2'	2.96	114.52	109.80

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

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	469/539 (87%)	1.06	69 (14%) 3 5	33, 38, 45, 60	0
1	B	469/539 (87%)	1.02	54 (11%) 6 11	32, 39, 46, 57	0
2	C	20/21 (95%)	1.53	5 (25%) 1 1	34, 42, 48, 48	0
2	D	20/21 (95%)	0.97	3 (15%) 3 5	36, 40, 43, 45	0
All	All	978/1120 (87%)	1.04	131 (13%) 4 7	32, 38, 46, 60	0

All (131) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	157	VAL	13.3
1	A	159	GLY	7.1
1	A	156	LEU	6.9
1	A	152	GLY	6.5
1	A	161	ASN	6.4
2	C	15	LEU	6.4
1	A	106	ARG	6.2
1	B	-52	ALA	6.2
1	A	123	PRO	6.1
1	B	-34	GLU	6.1
1	B	-292	ALA	5.6
1	B	-35	GLU	5.3
1	A	154	TRP	4.9
1	A	55	VAL	4.8
2	C	33	ASN	4.8
1	A	147	ARG	4.6
1	A	151	ASN	4.6
1	A	124	GLY	4.5
1	A	-344	ALA	4.4
1	A	164	TRP	4.2
1	B	-105	LYS	4.2

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Mol	Chain	Res	Type	RSRZ
1	B	-37	TYR	4.1
1	A	158	PRO	4.1
1	B	-33	LEU	4.1
1	B	-319	LYS	4.0
1	B	-291	THR	4.0
1	B	-295	GLN	3.9
1	B	-289	ASP	3.9
1	A	148	CYS	3.8
1	A	107	PRO	3.7
2	C	29	GLN	3.6
1	A	149	ASP	3.5
1	A	150	ARG	3.5
1	A	-236	ILE	3.5
1	A	160	HIS	3.5
1	A	165	ALA	3.5
1	B	56	LEU	3.5
1	B	-311	ILE	3.4
1	A	153	SER	3.4
1	B	-75	ALA	3.4
1	A	162	ARG	3.4
1	B	57	GLN	3.4
2	C	32	HIS	3.4
1	A	122	ALA	3.3
1	B	55	VAL	3.3
1	B	-31	LYS	3.3
1	A	-283	PHE	3.3
1	B	106	ARG	3.2
1	A	163	THR	3.2
1	B	18	LYS	3.1
1	B	-166	ILE	3.1
1	B	-220	ASN	3.1
1	B	-36	GLU	3.0
1	A	-64	LEU	3.0
1	A	-80	ALA	3.0
1	B	-26	ALA	3.0
1	A	126	VAL	3.0
1	A	-82	LEU	3.0
2	D	15	LEU	2.9
1	A	-203	ALA	2.9
1	B	-290	GLY	2.8
1	A	-333	ILE	2.7
1	B	-327	TYR	2.7

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Mol	Chain	Res	Type	RSRZ
2	C	34	PHE	2.7
1	A	-324	LEU	2.7
1	B	158	PRO	2.7
1	A	-45	LEU	2.7
1	A	-285	ILE	2.6
1	A	42	HIS	2.6
1	A	-323	ALA	2.6
1	B	-111	SER	2.6
1	B	105	GLY	2.6
1	B	-308	THR	2.6
1	A	-51	VAL	2.6
1	A	-284	ILE	2.6
1	A	-11	ILE	2.6
1	B	-65	PHE	2.6
1	B	-27	ILE	2.5
1	A	109	LEU	2.5
1	B	-337	LEU	2.5
1	A	-54	LEU	2.5
1	A	-235	ALA	2.5
1	A	-60	LEU	2.5
1	A	125	GLU	2.5
1	B	-38	SER	2.4
1	A	-209	LEU	2.4
1	B	-294	VAL	2.4
1	B	-148	VAL	2.4
1	B	-19	GLN	2.4
1	A	-83	VAL	2.4
1	B	-227	TYR	2.3
1	B	-310	LYS	2.3
1	A	-234	VAL	2.3
1	A	-168	TYR	2.3
1	B	150	ARG	2.3
1	A	-79	GLY	2.3
1	B	-245	TYR	2.3
1	A	-321	VAL	2.2
1	A	-239	ALA	2.2
1	B	-240	ILE	2.2
1	B	-57	ASP	2.2
1	B	-248	ALA	2.2
1	B	-76	ALA	2.2
1	B	-30	ASP	2.2
1	A	-335	ILE	2.2

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Mol	Chain	Res	Type	RSRZ
1	A	-68	ALA	2.2
2	D	24	LEU	2.2
1	B	-340	GLU	2.2
1	A	-248	ALA	2.2
1	A	-85	VAL	2.2
1	A	48	CYS	2.1
1	A	-245	TYR	2.1
1	A	-173	TYR	2.1
1	B	-124	GLY	2.1
1	A	-307	VAL	2.1
1	A	-247	VAL	2.1
1	B	-313	THR	2.1
1	A	-327	TYR	2.1
1	A	-238	TYR	2.1
1	B	151	ASN	2.1
1	A	-81	SER	2.1
1	A	-250	TRP	2.1
1	B	-293	ALA	2.1
1	A	166	ASN	2.1
1	B	52	LEU	2.1
1	A	115	ILE	2.0
1	B	-145	ILE	2.0
1	A	-202	LYS	2.0
2	D	28	LEU	2.0
1	B	-226	ASN	2.0
1	B	147	ARG	2.0

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, 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	LLDF	B-factors(Å^2)	Q<0.9
3	MAL	A	194	23/23	0.94	0.15	-0.36	35,37,44,47	0
3	MAL	B	194	23/23	0.91	0.12	-0.85	34,36,43,44	0

6.5 Other polymers (i)

There are no such residues in this entry.