Full wwPDB X-ray Structure Validation Report (i)

Aug 5, 2026 – 12:29 PM EDT

PDB ID	:	4KNW / pdb_00004knw
Title	:	The crystal structure of human HDHD4 IN COMPLEX WITH MAGNESIUM AND THE PHOSPHATE MIMETIC VANADATE
Authors	:	Klei, H.E.
Deposited on	:	2013-05-10
Resolution	:	2.70 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:

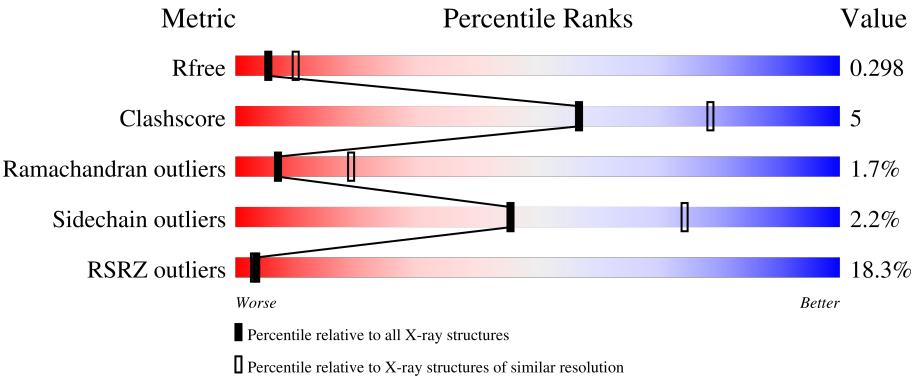
MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.015 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.50

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 2.70 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}	180053	3538 (2.70-2.70)
Clashscore	190562	3843 (2.70-2.70)
Ramachandran outliers	187476	3778 (2.70-2.70)
Sidechain outliers	187428	3778 (2.70-2.70)
RSRZ outliers	180081	3538 (2.70-2.70)

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	257	6% 87% 6% 7%
1	B	257	17% 82% 11% • 7%
1	C	257	28% 75% 16% • 7%

2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 5245 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 N-acylneuraminate-9-phosphatase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	239	Total	C	N	O	S	0	0	0
			1816	1149	308	345	14			
1	B	240	Total	C	N	O	S	0	0	0
			1750	1109	290	338	13			
1	C	238	Total	C	N	O	S	0	0	0
			1657	1047	274	323	13			

There are 30 discrepancies between the modelled and reference sequences:

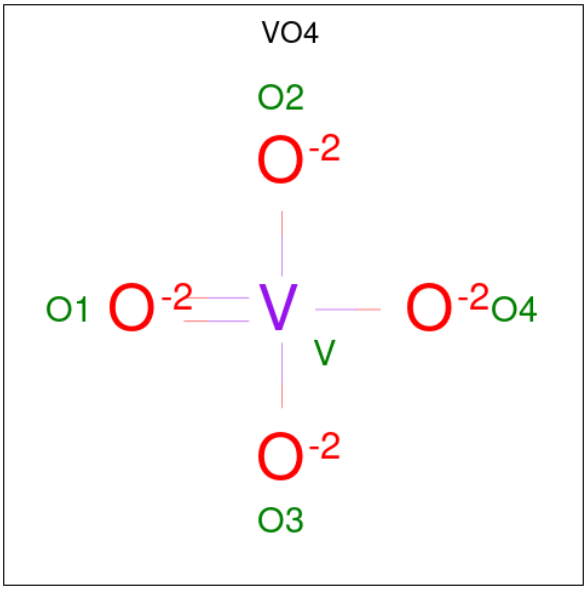
Chain	Residue	Modelled	Actual	Comment	Reference
A	1	MET	-	expression tag	UNP Q8TBE9
A	2	GLY	-	expression tag	UNP Q8TBE9
A	3	SER	-	expression tag	UNP Q8TBE9
A	251	GLU	-	expression tag	UNP Q8TBE9
A	252	PHE	-	expression tag	UNP Q8TBE9
A	253	GLY	-	expression tag	UNP Q8TBE9
A	254	LEU	-	expression tag	UNP Q8TBE9
A	255	VAL	-	expression tag	UNP Q8TBE9
A	256	PRO	-	expression tag	UNP Q8TBE9
A	257	ARG	-	expression tag	UNP Q8TBE9
B	1	MET	-	expression tag	UNP Q8TBE9
B	2	GLY	-	expression tag	UNP Q8TBE9
B	3	SER	-	expression tag	UNP Q8TBE9
B	251	GLU	-	expression tag	UNP Q8TBE9
B	252	PHE	-	expression tag	UNP Q8TBE9
B	253	GLY	-	expression tag	UNP Q8TBE9
B	254	LEU	-	expression tag	UNP Q8TBE9
B	255	VAL	-	expression tag	UNP Q8TBE9
B	256	PRO	-	expression tag	UNP Q8TBE9
B	257	ARG	-	expression tag	UNP Q8TBE9
C	1	MET	-	expression tag	UNP Q8TBE9
C	2	GLY	-	expression tag	UNP Q8TBE9
C	3	SER	-	expression tag	UNP Q8TBE9

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Chain	Residue	Modelled	Actual	Comment	Reference
C	251	GLU	-	expression tag	UNP Q8TBE9
C	252	PHE	-	expression tag	UNP Q8TBE9
C	253	GLY	-	expression tag	UNP Q8TBE9
C	254	LEU	-	expression tag	UNP Q8TBE9
C	255	VAL	-	expression tag	UNP Q8TBE9
C	256	PRO	-	expression tag	UNP Q8TBE9
C	257	ARG	-	expression tag	UNP Q8TBE9

- Molecule 2 is VANADATE ION (CCD ID: VO4) (formula: O_4V).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total O V 5 4 1	0	0
2	B	1	Total O V 5 4 1	0	0
2	C	1	Total O V 5 4 1	0	0

- Molecule 3 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

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

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	C	1	Total Mg 1 1	0	0

- Molecule 4 is water.

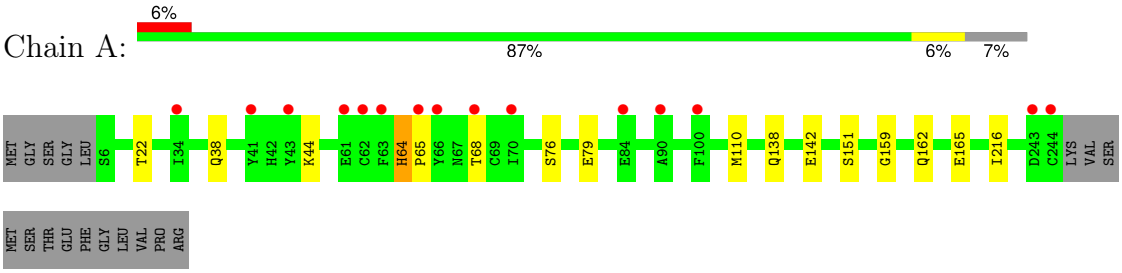
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	2	Total O 2 2	0	0
4	B	2	Total O 2 2	0	0

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.

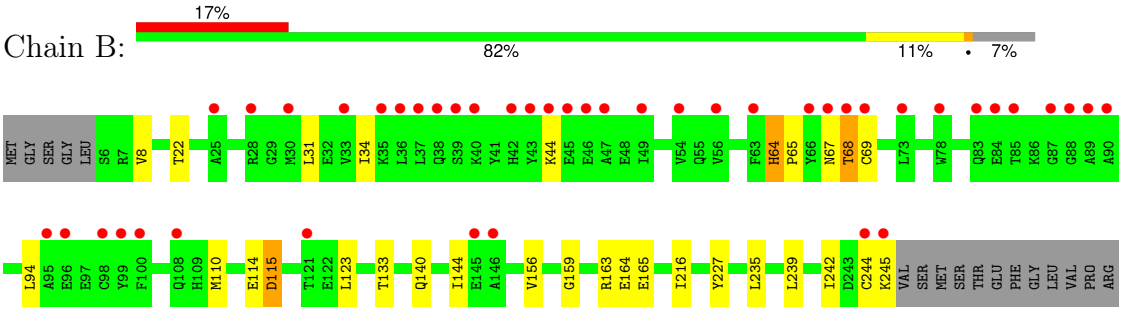
• Molecule 1: N-acylneuraminate-9-phosphatase

Chain A:



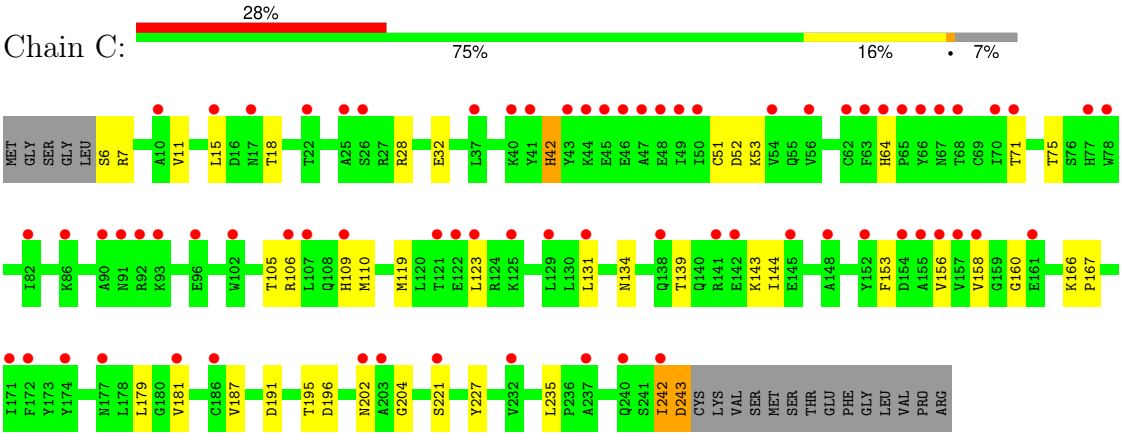
• Molecule 1: N-acylneuraminate-9-phosphatase

Chain B:



• Molecule 1: N-acylneuraminate-9-phosphatase

Chain C:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	46.78Å 102.56Å 186.66Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	35.13 – 2.70 35.13 – 2.70	Depositor EDS
% Data completeness (in resolution range)	98.8 (35.13-2.70) 98.8 (35.13-2.70)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.02 (at 2.68Å)	Xtriage
Refinement program	PHENIX dev_1396, CNS	Depositor
R, R_{free}	0.254 , 0.296 0.256 , 0.298	Depositor DCC
R_{free} test set	619 reflections (2.45%)	wwPDB-VP
Wilson B-factor (Å^2)	60.7	Xtriage
Anisotropy	0.679	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.30 , 39.2	EDS
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.91	EDS
Total number of atoms	5245	wwPDB-VP
Average B, all atoms (Å^2)	69.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.80% 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, 0.333 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: MG, VO4

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	0.32	0/1847	0.72	0/2509
1	B	0.31	0/1780	0.72	0/2427
1	C	0.30	0/1685	0.75	1/2312 (0.0%)
All	All	0.31	0/5312	0.73	1/7248 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	242	ILE	N-CA-C	6.74	116.89	110.42

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	1816	0	1760	10	0
1	B	1750	0	1626	17	0
1	C	1657	0	1467	23	0
2	A	5	0	0	0	0
2	B	5	0	0	0	0
2	C	5	0	0	0	0
3	A	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	B	1	0	0	0	0
3	C	1	0	0	0	0
4	A	2	0	0	0	0
4	B	2	0	0	0	0
All	All	5245	0	4853	46	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 5.

All (46) 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:244:CYS:SG	1:B:245:LYS:N	2.59	0.74
1:B:115:ASP:OD1	1:B:115:ASP:N	2.28	0.63
1:A:138:GLN:NE2	1:A:142:GLU:OE2	2.32	0.62
1:B:159:GLY:HA3	1:B:165:GLU:HG2	1.82	0.61
1:C:51:CYS:O	1:C:53:LYS:N	2.33	0.60
1:C:167:PRO:O	1:C:202:ASN:ND2	2.37	0.57
1:A:22:THR:HG23	1:A:110:MET:HE2	1.88	0.56
1:A:159:GLY:HA3	1:A:165:GLU:HG2	1.88	0.56
1:B:133:THR:OG1	1:B:140:GLN:NE2	2.40	0.55
1:C:139:THR:HG22	1:C:143:LYS:HE3	1.92	0.52
1:C:18:THR:OG1	1:C:191:ASP:OD1	2.28	0.52
1:C:242:ILE:N	1:C:243:ASP:HA	2.24	0.51
1:C:134:ASN:HD21	1:C:166:LYS:HB2	1.76	0.50
1:C:106:ARG:HG2	1:C:110:MET:HE3	1.94	0.49
1:C:243:ASP:OD2	1:C:243:ASP:N	2.39	0.49
1:B:64:HIS:CG	1:B:65:PRO:HA	2.47	0.48
1:B:144:ILE:HD13	1:B:156:VAL:HG11	1.95	0.48
1:A:76:SER:HA	1:A:79:GLU:HG2	1.94	0.48
1:C:195:THR:OG1	1:C:196:ASP:N	2.47	0.48
1:C:144:ILE:HD13	1:C:156:VAL:HG11	1.97	0.47
1:A:38:GLN:NE2	1:A:44:LYS:O	2.48	0.47
1:C:110:MET:HE1	1:C:143:LYS:HE2	1.97	0.47
1:B:216:ILE:HG12	1:C:227:TYR:CE2	2.50	0.47
1:A:64:HIS:CG	1:A:65:PRO:HA	2.50	0.46
1:C:28:ARG:HD3	1:C:109:HIS:CD2	2.51	0.45
1:B:64:HIS:ND1	1:B:65:PRO:HA	2.32	0.45
1:C:158:VAL:HG12	1:C:160:GLY:H	1.81	0.45
1:B:227:TYR:OH	1:B:242:ILE:HG22	2.17	0.45
1:B:31:LEU:HD23	1:B:34:ILE:HD12	1.98	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:71:THR:O	1:C:75:THR:OG1	2.23	0.44
1:C:15:LEU:HB2	1:C:131:LEU:HD11	2.00	0.44
1:C:131:LEU:HB2	1:C:153:PHE:CD2	2.52	0.44
1:A:216:ILE:HG12	1:B:227:TYR:CE2	2.53	0.43
1:B:163:ARG:HG2	1:B:164:GLU:HG3	2.01	0.43
1:B:22:THR:HG23	1:B:110:MET:HE2	2.01	0.43
1:C:119:MET:HE2	1:C:123:LEU:HD22	2.00	0.43
1:C:6:SER:HA	1:C:7:ARG:HA	1.70	0.43
1:A:216:ILE:HG12	1:B:227:TYR:HE2	1.84	0.42
1:A:64:HIS:CD2	1:A:65:PRO:HA	2.55	0.42
1:C:32:GLU:HG3	1:C:105:THR:HG21	2.01	0.42
1:B:216:ILE:HG12	1:C:227:TYR:HE2	1.84	0.42
1:B:239:LEU:O	1:B:242:ILE:HG12	2.20	0.41
1:A:64:HIS:CD2	1:A:165:GLU:HG3	2.56	0.41
1:B:8:VAL:HB	1:B:244:CYS:SG	2.62	0.41
1:C:11:VAL:HG13	1:C:187:VAL:HG23	2.03	0.40
1:C:179:LEU:HB2	1:C:181:VAL:HG22	2.03	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	237/257 (92%)	223 (94%)	12 (5%)	2 (1%)	16 37
1	B	238/257 (93%)	223 (94%)	10 (4%)	5 (2%)	5 15
1	C	236/257 (92%)	208 (88%)	23 (10%)	5 (2%)	5 15
All	All	711/771 (92%)	654 (92%)	45 (6%)	12 (2%)	7 19

All (12) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	67	ASN
1	C	42	HIS
1	C	204	GLY
1	B	44	LYS
1	C	221	SER
1	A	68	THR
1	C	52	ASP
1	C	64	HIS
1	B	68	THR
1	B	69	CYS
1	A	64	HIS
1	B	64	HIS

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	187/223 (84%)	185 (99%)	2 (1%)	65 85
1	B	169/223 (76%)	163 (96%)	6 (4%)	31 60
1	C	150/223 (67%)	147 (98%)	3 (2%)	48 76
All	All	506/669 (76%)	495 (98%)	11 (2%)	45 74

All (11) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	151	SER
1	A	162	GLN
1	B	68	THR
1	B	94	LEU
1	B	114	GLU
1	B	115	ASP
1	B	123	LEU
1	B	235	LEU
1	C	42	HIS
1	C	235	LEU
1	C	243	ASP

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

Mol	Chain	Res	Type
1	A	64	HIS
1	A	138	GLN
1	C	162	GLN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no oligosaccharides in this entry.

5.6 Ligand geometry (i)

Of 6 ligands modelled in this entry, 3 are monoatomic - leaving 3 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
2	VO4	A	301	3,1	0,4,4	-	-	-		
2	VO4	B	301	3,1	0,4,4	-	-	-		
2	VO4	C	301	3,1	0,4,4	-	-	-		

There are no bond length outliers.

There are no bond angle outliers.

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 (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	239/257 (92%)	0.38	15 (6%) 26 23	32, 47, 85, 96	0
1	B	240/257 (93%)	0.88	44 (18%) 3 3	35, 59, 121, 129	0
1	C	238/257 (92%)	1.70	72 (30%) 1 1	44, 91, 125, 148	0
All	All	717/771 (92%)	0.99	131 (18%) 3 3	32, 67, 118, 148	0

All (131) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	66	TYR	7.9
1	C	62	CYS	6.1
1	B	39	SER	6.0
1	C	46	GLU	5.4
1	C	47	ALA	5.3
1	B	47	ALA	5.1
1	C	67	ASN	4.9
1	B	245	LYS	4.8
1	C	157	VAL	4.5
1	C	45	GLU	4.4
1	C	50	ILE	4.4
1	A	63	PHE	4.3
1	A	66	TYR	4.3
1	C	63	PHE	4.0
1	C	240	GLN	4.0
1	B	96	GLU	3.9
1	B	89	ALA	3.9
1	B	33	VAL	3.9
1	C	26	SER	3.8
1	A	34	ILE	3.8
1	C	156	VAL	3.8
1	C	25	ALA	3.7
1	C	65	PRO	3.7

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Mol	Chain	Res	Type	RSRZ
1	C	49	ILE	3.7
1	C	171	ILE	3.7
1	B	244	CYS	3.7
1	C	68	THR	3.7
1	C	22	THR	3.6
1	B	66	TYR	3.6
1	A	65	PRO	3.6
1	B	83	GLN	3.6
1	B	95	ALA	3.6
1	C	43	TYR	3.6
1	B	45	GLU	3.6
1	C	141	ARG	3.5
1	B	54	VAL	3.5
1	C	82	ILE	3.4
1	B	67	ASN	3.4
1	A	100	PHE	3.4
1	C	90	ALA	3.3
1	C	131	LEU	3.3
1	B	145	GLU	3.3
1	C	64	HIS	3.3
1	C	102	TRP	3.3
1	C	109	HIS	3.2
1	B	88	GLY	3.2
1	C	71	THR	3.1
1	C	123	LEU	3.1
1	C	161	GLU	3.0
1	B	38	GLN	3.0
1	B	35	LYS	3.0
1	C	70	ILE	3.0
1	C	148	ALA	3.0
1	C	17	ASN	3.0
1	C	78	TRP	2.9
1	A	244	CYS	2.9
1	C	186	CYS	2.9
1	C	15	LEU	2.9
1	C	92	ARG	2.9
1	C	177	ASN	2.9
1	C	107	LEU	2.8
1	B	69	CYS	2.8
1	C	203	ALA	2.8
1	A	90	ALA	2.8
1	A	62	CYS	2.7

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Mol	Chain	Res	Type	RSRZ
1	B	28	ARG	2.7
1	C	172	PHE	2.7
1	C	181	VAL	2.7
1	B	63	PHE	2.7
1	B	36	LEU	2.6
1	C	48	GLU	2.6
1	C	96	GLU	2.6
1	B	100	PHE	2.6
1	B	49	ILE	2.6
1	C	221	SER	2.5
1	C	37	LEU	2.5
1	B	46	GLU	2.5
1	B	121	THR	2.4
1	B	68	THR	2.4
1	C	56	VAL	2.4
1	B	37	LEU	2.4
1	C	77	HIS	2.4
1	B	44	LYS	2.4
1	C	93	LYS	2.4
1	A	68	THR	2.3
1	C	155	ALA	2.3
1	C	158	VAL	2.3
1	C	154	ASP	2.3
1	B	98	CYS	2.3
1	C	40	LYS	2.3
1	A	43	TYR	2.3
1	C	174	TYR	2.3
1	B	78	TRP	2.3
1	B	42	HIS	2.2
1	A	61	GLU	2.2
1	B	87	GLY	2.2
1	C	232	VAL	2.2
1	C	44	LYS	2.2
1	B	30	MET	2.2
1	A	84	GLU	2.2
1	B	85	THR	2.2
1	C	142	GLU	2.2
1	B	43	TYR	2.2
1	B	84	GLU	2.2
1	B	108	GLN	2.2
1	B	25	ALA	2.2
1	B	90	ALA	2.2

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Mol	Chain	Res	Type	RSRZ
1	A	70	ILE	2.2
1	C	10	ALA	2.1
1	C	121	THR	2.1
1	B	56	VAL	2.1
1	C	237	ALA	2.1
1	B	40	LYS	2.1
1	C	91	ASN	2.1
1	B	146	ALA	2.1
1	B	73	LEU	2.1
1	C	129	LEU	2.1
1	B	99	TYR	2.1
1	C	41	TYR	2.1
1	C	152	TYR	2.1
1	C	242	ILE	2.1
1	A	243	ASP	2.1
1	C	145	GLU	2.1
1	C	125	LYS	2.1
1	C	202	ASN	2.1
1	C	138	GLN	2.0
1	C	106	ARG	2.0
1	C	122	GLU	2.0
1	C	86	LYS	2.0
1	C	54	VAL	2.0
1	A	41	TYR	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 oligosaccharides 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	MG	C	302	1/1	0.80	0.16	68,68,68,68	0
3	MG	B	302	1/1	0.81	0.15	49,49,49,49	0
3	MG	A	302	1/1	0.87	0.17	39,39,39,39	0
2	VO4	C	301	5/5	0.88	0.12	75,76,78,84	0
2	VO4	B	301	5/5	0.98	0.07	42,44,47,49	0
2	VO4	A	301	5/5	0.99	0.07	33,34,38,39	0

6.5 Other polymers (i)

There are no such residues in this entry.