Full wwPDB X-ray Structure Validation Report ⓘ

Feb 15, 2024 – 07:58 AM EST

PDB ID	:	3PNQ
Title	:	Crystal Structure of E.coli Dha kinase DhaK (H56N) complex with Dha
Authors	:	Shi, R.; McDonald, L.; Matte, A.; Cygler, M.; Ekiel, I.; Montreal-Kingston Bacterial Structural Genomics Initiative (BSGI)
Deposited on	:	2010-11-19
Resolution	:	2.20 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 ⓘ 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 ⓘ) were used in the production of this report:

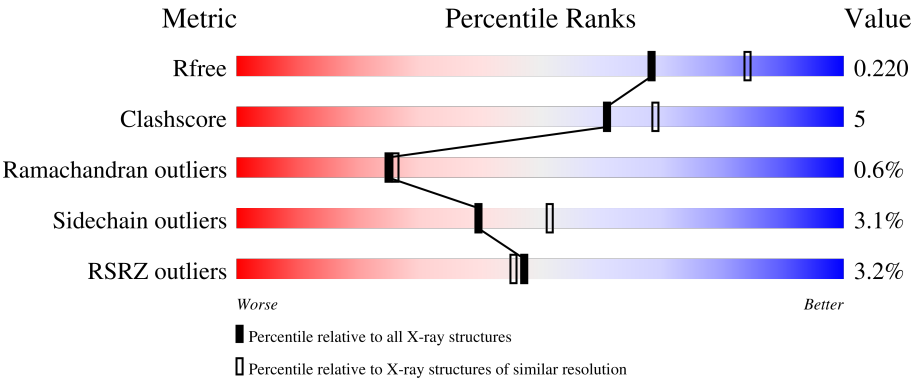
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, 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 2.20 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	4898 (2.20-2.20)
Clashscore	141614	5594 (2.20-2.20)
Ramachandran outliers	138981	5503 (2.20-2.20)
Sidechain outliers	138945	5504 (2.20-2.20)
RSRZ outliers	127900	4800 (2.20-2.20)

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	357	3% 83% 10% 6%
1	B	357	4% 80% 13% • 6%
1	C	357	3% 84% 9% • 6%
1	D	357	2% 81% 12% 6%

2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 10606 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.

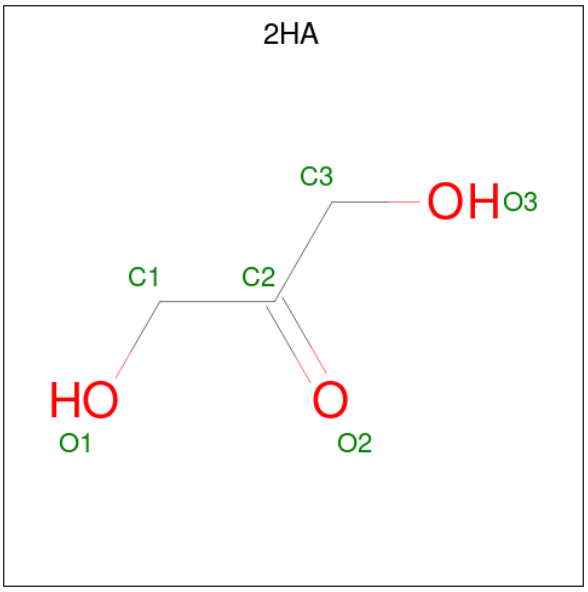
- Molecule 1 is a protein called PTS-dependent dihydroxyacetone kinase, dihydroxyacetone-binding subunit dhaK.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	334	Total	C	N	O	S	0	0	0
			2521	1576	432	501	12			
1	B	336	Total	C	N	O	S	0	2	0
			2544	1594	434	503	13			
1	C	335	Total	C	N	O	S	0	1	0
			2533	1584	435	502	12			
1	D	334	Total	C	N	O	S	0	0	0
			2521	1576	432	501	12			

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	0	GLY	-	expression tag	UNP P76015
A	1	SER	-	expression tag	UNP P76015
A	56	ASN	HIS	engineered mutation	UNP P76015
B	0	GLY	-	expression tag	UNP P76015
B	1	SER	-	expression tag	UNP P76015
B	56	ASN	HIS	engineered mutation	UNP P76015
C	0	GLY	-	expression tag	UNP P76015
C	1	SER	-	expression tag	UNP P76015
C	56	ASN	HIS	engineered mutation	UNP P76015
D	0	GLY	-	expression tag	UNP P76015
D	1	SER	-	expression tag	UNP P76015
D	56	ASN	HIS	engineered mutation	UNP P76015

- Molecule 2 is Dihydroxyacetone (three-letter code: 2HA) (formula: $C_3H_6O_3$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	D	1	Total C O 6 3 3	0	0

- Molecule 3 is water.

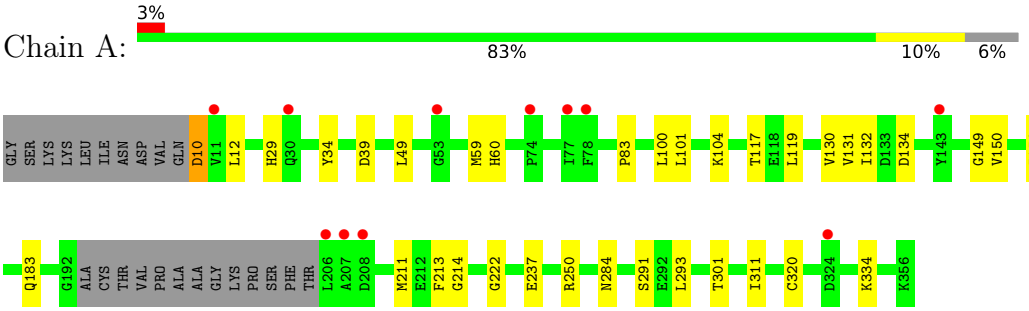
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	124	Total O 124 124	0	0
3	B	115	Total O 115 115	0	0
3	C	116	Total O 116 116	0	0
3	D	126	Total O 126 126	0	0

3 Residue-property plots

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.

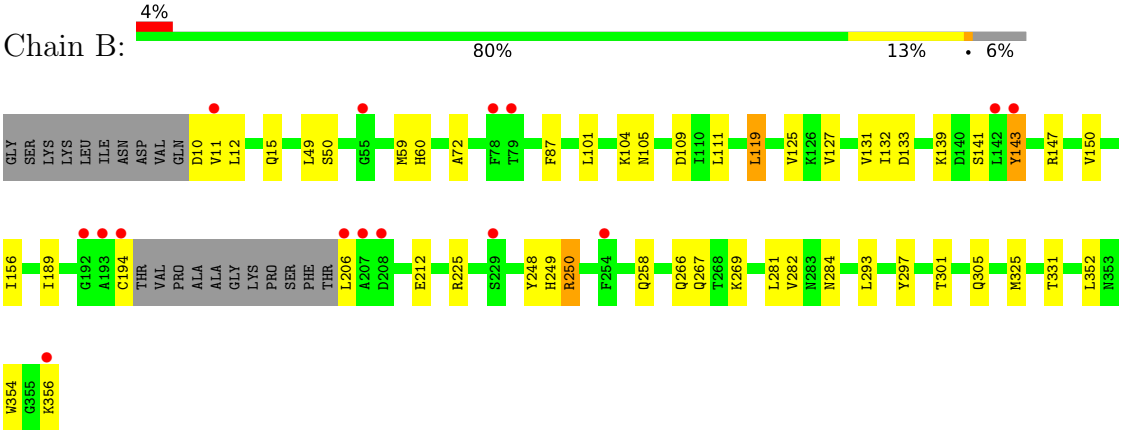
• Molecule 1: PTS-dependent dihydroxyacetone kinase, dihydroxyacetone-binding subunit dhaK

Chain A:



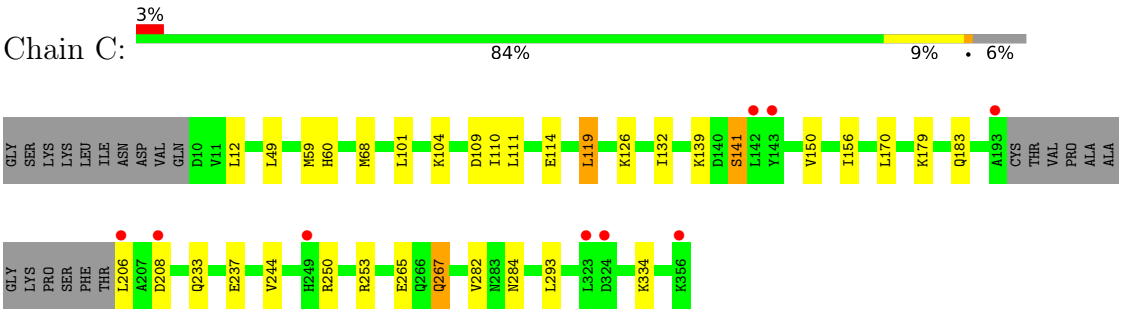
• Molecule 1: PTS-dependent dihydroxyacetone kinase, dihydroxyacetone-binding subunit dhaK

Chain B:



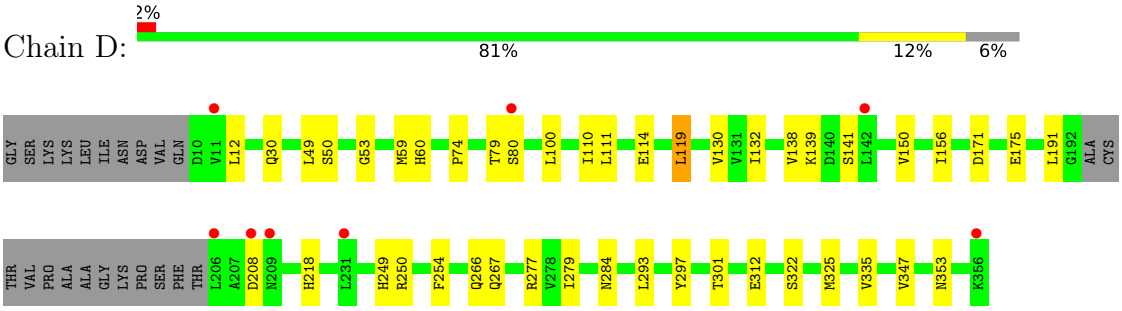
• Molecule 1: PTS-dependent dihydroxyacetone kinase, dihydroxyacetone-binding subunit dhaK

Chain C:



• Molecule 1: PTS-dependent dihydroxyacetone kinase, dihydroxyacetone-binding subunit dhaK

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	82.23Å 101.07Å 99.35Å 90.00° 89.95° 90.00°	Depositor
Resolution (Å)	49.67 – 2.20 49.67 – 2.20	Depositor EDS
% Data completeness (in resolution range)	99.0 (49.67-2.20) 99.1 (49.67-2.20)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	5.27 (at 2.20Å)	Xtriage
Refinement program	REFMAC	Depositor
R, R_{free}	0.200 , 0.220 0.199 , 0.220	Depositor DCC
R_{free} test set	4102 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å^2)	19.1	Xtriage
Anisotropy	1.102	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.34 , 8.3	EDS
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	0.000 for -h,-l,-k 0.000 for -h,l,k 0.384 for h,-k,-l	Xtriage
Reported twinning fraction	0.610 for H, K, L 0.390 for h,-k,-l	Depositor
Outliers	2 of 81898 reflections (0.002%)	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	10606	wwPDB-VP
Average B, all atoms (Å^2)	20.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 34.78 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 6.4678e-04. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

[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: 2HA

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	0.64	0/2565	0.69	1/3484 (0.0%)
1	B	0.61	0/2595	0.68	0/3525
1	C	0.61	0/2581	0.72	0/3506
1	D	0.62	0/2565	0.71	0/3484
All	All	0.62	0/10306	0.70	1/13999 (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	A	49	LEU	CA-CB-CG	5.07	126.96	115.30

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	2521	0	2466	22	0
1	B	2544	0	2494	31	0
1	C	2533	0	2478	18	0
1	D	2521	0	2466	22	0
2	D	6	0	6	3	0
3	A	124	0	0	3	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	B	115	0	0	8	0
3	C	116	0	0	3	0
3	D	126	0	0	3	0
All	All	10606	0	9910	91	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 (91) 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:105:ASN:HB2	3:B:366:HOH:O	1.46	1.13
1:B:111:LEU:HD23	3:B:408:HOH:O	1.60	1.00
1:D:74:PRO:HD2	3:D:457:HOH:O	1.67	0.94
1:D:218:HIS:CE1	2:D:511:2HA:H1C1	2.05	0.91
1:B:131:VAL:HG12	3:B:366:HOH:O	1.79	0.81
1:C:233:GLN:HB3	3:C:525:HOH:O	1.82	0.80
1:A:10:ASP:HA	3:A:448:HOH:O	1.84	0.77
1:B:60:HIS:NE2	1:B:104:LYS:NZ	2.35	0.75
1:D:218:HIS:HE1	2:D:511:2HA:H1C1	1.50	0.74
1:C:60:HIS:NE2	1:C:104:LYS:NZ	2.38	0.72
1:C:265:GLU:HG2	1:C:267:GLN:HE21	1.56	0.70
1:B:249:HIS:CD2	3:B:444:HOH:O	2.47	0.67
1:B:206:LEU:HD23	1:B:225:ARG:HD3	1.78	0.63
1:C:284:ASN:HB2	1:C:293:LEU:HD11	1.82	0.62
1:B:133:ASP:HB3	3:B:366:HOH:O	2.01	0.61
1:B:282:VAL:HG12	1:B:293:LEU:HD22	1.83	0.60
1:A:60:HIS:NE2	1:A:104:LYS:NZ	2.51	0.59
1:A:284:ASN:HB2	1:A:293:LEU:HD11	1.83	0.59
1:C:183:GLN:HG2	3:C:433:HOH:O	2.02	0.58
1:A:131:VAL:HG23	3:A:399:HOH:O	2.02	0.58
1:D:297:TYR:O	1:D:301:THR:HG23	2.03	0.58
1:D:254:PHE:HE2	1:D:267:GLN:HE22	1.50	0.58
1:B:143:TYR:HB3	3:B:496:HOH:O	2.05	0.57
1:B:284:ASN:HB2	1:B:293:LEU:HD11	1.87	0.56
1:B:281:LEU:HB3	1:B:331:THR:HB	1.90	0.54
1:B:11:VAL:O	1:B:15:GLN:HG3	2.08	0.53
1:C:179:LYS:O	1:C:183:GLN:HG3	2.09	0.52
1:D:100:LEU:HD11	1:D:130:VAL:HG23	1.92	0.51
1:A:174:ALA:O	1:A:178:ARG:HG3	2.10	0.51
1:A:134:ASP:HB3	3:A:408:HOH:O	2.09	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:265:GLU:CG	1:C:267:GLN:HE21	2.24	0.51
1:B:132:ILE:HD12	1:B:156:ILE:HD12	1.92	0.51
1:A:214:GLY:O	1:A:222:GLY:HA2	2.11	0.50
1:C:110:ILE:O	1:C:114:GLU:HG3	2.11	0.50
1:D:249:HIS:CD2	3:D:396:HOH:O	2.65	0.49
1:B:87:PHE:CE1	1:B:119:LEU:HD13	2.47	0.49
1:A:59:MET:HE2	1:A:320:CYS:SG	2.52	0.49
1:B:59:MET:HE3	1:B:104:LYS:HE3	1.94	0.48
1:A:104:LYS:HD2	1:A:149:GLY:O	2.13	0.48
1:B:147:ARG:HD2	1:B:248:TYR:CE2	2.48	0.48
1:A:211:MET:HE1	1:A:237:GLU:OE2	2.15	0.47
1:A:291:SER:HB2	1:B:15:GLN:OE1	2.14	0.47
1:D:284:ASN:HB2	1:D:293:LEU:HD11	1.97	0.47
1:A:132:ILE:HD12	1:A:156:ILE:HD12	1.96	0.47
1:A:301:THR:HG22	1:A:311:ILE:HD12	1.97	0.47
1:A:59:MET:CE	1:A:320:CYS:SG	3.03	0.47
1:B:250:ARG:NH1	1:B:269:LYS:HG3	2.30	0.47
1:B:352:LEU:HD22	1:B:354:TRP:CZ3	2.49	0.47
1:D:322:SER:O	1:D:325:MET:HB3	2.15	0.47
1:B:297:TYR:O	1:B:301:THR:HG23	2.15	0.47
1:C:59:MET:HA	1:C:60:HIS:HA	1.68	0.47
1:B:194:CYS:HB3	1:B:325:MET:HB2	1.97	0.46
1:B:212:GLU:HB2	3:B:522:HOH:O	2.14	0.46
1:B:49:LEU:HB3	1:B:101:LEU:CD2	2.46	0.46
1:A:83:PRO:HB2	1:C:244:VAL:HG22	1.97	0.46
1:B:139:LYS:HE3	3:B:429:HOH:O	2.16	0.45
1:C:49:LEU:HD22	1:C:101:LEU:HD22	1.99	0.45
1:A:59:MET:HA	1:A:60:HIS:HA	1.61	0.45
1:D:49:LEU:HD23	1:D:50:SER:O	2.16	0.45
1:D:59:MET:HA	1:D:60:HIS:HA	1.68	0.45
1:D:74:PRO:CD	3:D:457:HOH:O	2.44	0.45
1:D:279:ILE:HG13	1:D:335:VAL:HG11	1.98	0.45
1:D:132:ILE:HD12	1:D:156:ILE:HD12	1.99	0.44
1:D:138:VAL:HG12	1:D:139:LYS:N	2.32	0.44
1:B:59:MET:HA	1:B:60:HIS:HA	1.68	0.44
1:A:39:ASP:OD1	1:A:39:ASP:N	2.48	0.44
1:A:183:GLN:HB3	1:A:334:LYS:HB3	2.00	0.44
1:D:171:ASP:O	1:D:175:GLU:HG2	2.17	0.44
1:D:277:ARG:NE	1:D:312:GLU:OE2	2.45	0.44
1:B:206:LEU:CD2	1:B:225:ARG:HD3	2.47	0.44
1:C:282:VAL:HG12	1:C:293:LEU:HD22	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:59:MET:CE	1:B:104:LYS:HE3	2.48	0.44
1:C:233:GLN:O	1:C:237:GLU:HG2	2.18	0.43
1:B:101:LEU:HA	1:B:101:LEU:HD23	1.74	0.43
1:B:189:ILE:HD12	1:B:189:ILE:C	2.39	0.43
1:D:53:GLY:HA2	1:D:79:THR:O	2.18	0.43
1:A:100:LEU:HD11	1:A:130:VAL:HG23	2.00	0.42
1:D:110:ILE:O	1:D:114:GLU:HG3	2.19	0.42
1:A:29:HIS:CD2	1:A:34:TYR:CE1	3.07	0.42
1:B:125:VAL:HG12	1:B:127[A]:VAL:HG23	2.02	0.42
1:C:126:LYS:HG2	1:C:170:LEU:CD2	2.49	0.42
1:C:139:LYS:HD3	3:C:444:HOH:O	2.20	0.42
1:D:347:VAL:O	1:D:353:ASN:HA	2.19	0.42
1:A:213:PHE:CE1	1:A:237:GLU:HG3	2.55	0.41
1:B:50:SER:O	1:B:72:ALA:HA	2.19	0.41
1:A:101:LEU:HD12	1:A:117:THR:OG1	2.21	0.41
1:D:119:LEU:HD23	1:D:119:LEU:HA	1.93	0.41
1:C:183:GLN:HB3	1:C:334:LYS:HB3	2.04	0.40
1:C:119:LEU:HD22	1:C:119:LEU:HA	1.96	0.40
1:D:218:HIS:NE2	2:D:511:2HA:H1C1	2.36	0.40
1:C:132:ILE:HD12	1:C:156:ILE:HD12	2.04	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	330/357 (92%)	318 (96%)	11 (3%)	1 (0%)	41	46
1	B	334/357 (94%)	320 (96%)	12 (4%)	2 (1%)	25	26
1	C	332/357 (93%)	321 (97%)	8 (2%)	3 (1%)	17	16
1	D	330/357 (92%)	315 (96%)	13 (4%)	2 (1%)	25	26
All	All	1326/1428 (93%)	1274 (96%)	44 (3%)	8 (1%)	25	26

All (8) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	141	SER
1	C	141	SER
1	C	68	MET
1	A	150	VAL
1	B	150	VAL
1	D	141	SER
1	D	150	VAL
1	C	150	VAL

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	270/288 (94%)	266 (98%)	4 (2%)	65	78
1	B	273/288 (95%)	262 (96%)	11 (4%)	31	40
1	C	271/288 (94%)	261 (96%)	10 (4%)	34	43
1	D	270/288 (94%)	261 (97%)	9 (3%)	38	49
All	All	1084/1152 (94%)	1050 (97%)	34 (3%)	40	51

All (34) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	10	ASP
1	A	12	LEU
1	A	119	LEU
1	A	250	ARG
1	B	10	ASP
1	B	12	LEU
1	B	109	ASP
1	B	119	LEU
1	B	143	TYR
1	B	250	ARG
1	B	258	GLN
1	B	266	GLN

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Mol	Chain	Res	Type
1	B	267	GLN
1	B	305	GLN
1	B	356	LYS
1	C	12	LEU
1	C	109	ASP
1	C	111	LEU
1	C	119	LEU
1	C	141	SER
1	C	206	LEU
1	C	208	ASP
1	C	250	ARG
1	C	253	ARG
1	C	267	GLN
1	D	12	LEU
1	D	30	GLN
1	D	80	SER
1	D	111	LEU
1	D	119	LEU
1	D	191	LEU
1	D	208	ASP
1	D	250	ARG
1	D	266	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (10) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	218	HIS
1	A	263	GLN
1	B	218	HIS
1	B	249	HIS
1	C	121	HIS
1	C	249	HIS
1	C	273	GLN
1	D	30	GLN
1	D	218	HIS
1	D	249	HIS

5.3.3 RNA

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 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	$\#\|Z\| > 2$
2	2HA	D	511	-	5,5,5	0.77	0	4,5,5	0.63	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
2	2HA	D	511	-	-	2/2/4/4	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	D	511	2HA	O1-C1-C2-O2
2	D	511	2HA	O2-C2-C3-O3

There are no ring outliers.

1 monomer is involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	D	511	2HA	3	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	334/357 (93%)	0.23	11 (3%) 46 44	11, 19, 32, 48	0
1	B	336/357 (94%)	0.28	15 (4%) 33 32	11, 20, 33, 48	1 (0%)
1	C	335/357 (93%)	0.16	9 (2%) 54 52	10, 18, 31, 45	1 (0%)
1	D	334/357 (93%)	0.18	8 (2%) 59 56	10, 19, 31, 48	0
All	All	1339/1428 (93%)	0.21	43 (3%) 47 45	10, 19, 32, 48	2 (0%)

All (43) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	193	ALA	7.3
1	D	208	ASP	5.1
1	B	207	ALA	4.9
1	B	194	CYS	4.7
1	A	143	TYR	4.5
1	A	206	LEU	4.0
1	B	192	GLY	3.7
1	A	78	PHE	3.1
1	A	208	ASP	2.8
1	B	206	LEU	2.7
1	C	324	ASP	2.7
1	B	254[A]	PHE	2.7
1	D	231	LEU	2.6
1	D	356	LYS	2.6
1	A	11	VAL	2.6
1	B	78	PHE	2.6
1	D	142	LEU	2.5
1	D	209	ASN	2.5
1	A	53	GLY	2.5
1	A	77	ILE	2.5
1	C	208	ASP	2.5

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Mol	Chain	Res	Type	RSRZ
1	B	142	LEU	2.4
1	C	323	LEU	2.4
1	D	80	SER	2.4
1	C	193	ALA	2.3
1	B	356	LYS	2.3
1	B	79	THR	2.3
1	A	207	ALA	2.3
1	C	206	LEU	2.3
1	A	74	PRO	2.3
1	B	55	GLY	2.2
1	B	11	VAL	2.2
1	C	356	LYS	2.2
1	A	324	ASP	2.2
1	C	249	HIS	2.2
1	B	208	ASP	2.1
1	B	143	TYR	2.1
1	C	143	TYR	2.1
1	C	142	LEU	2.1
1	A	30	GLN	2.1
1	D	206	LEU	2.1
1	B	229	SER	2.0
1	D	11	VAL	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 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
2	2HA	D	511	6/6	0.95	0.17	26,29,30,33	0

6.5 Other polymers (i)

There are no such residues in this entry.