



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 06:22 PM UTC

PDB ID : 1ZZ3 / pdb_00001zz3
Title : Crystal structure of a HDAC-like protein with CypX bound
Authors : Nielsen, T.K.; Hildmann, C.; Dickmanns, A.; Schwienhorst, A.; Ficner, R.
Deposited on : 2005-06-13
Resolution : 1.76 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 : 4-5-2 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 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

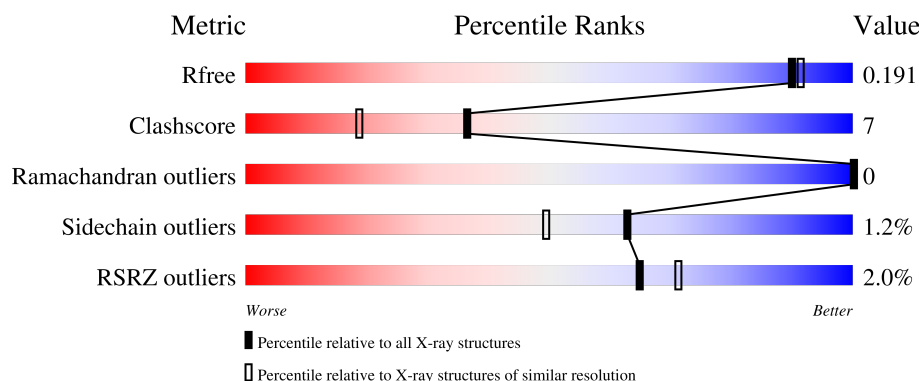
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.76 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	3183 (1.76-1.76)
Clashscore	190562	3299 (1.76-1.76)
Ramachandran outliers	187476	3274 (1.76-1.76)
Sidechain outliers	187428	3274 (1.76-1.76)
RSRZ outliers	180081	3183 (1.76-1.76)

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 $\leq 5\%$. 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	369	3% 87% 11% ..
1	B	369	86% 14% .
1	C	369	2% 88% 11% .
1	D	369	3% 90% 9% ..

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard

residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	3YP	B	1552	-	-	X	-
2	3YP	C	1652	-	-	X	-
2	3YP	D	1752	-	-	X	-

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 12370 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.

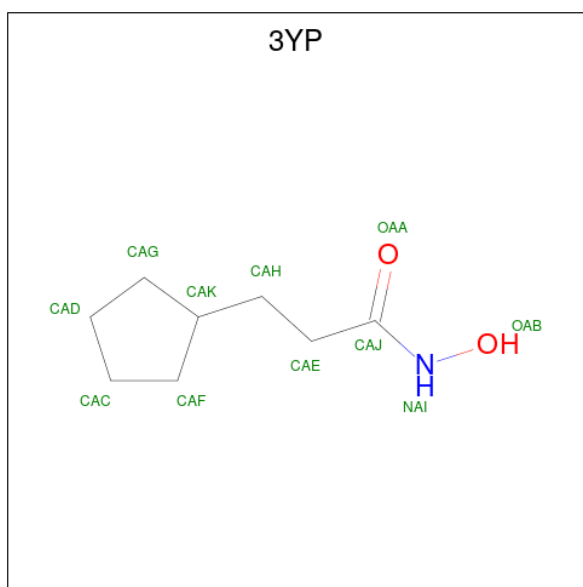
- Molecule 1 is a protein called Histone deacetylase-like amidohydrolase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	367	Total	C	N	O	S	0	4	0
			2761	1734	494	515	18			
1	B	367	Total	C	N	O	S	0	1	0
			2753	1728	496	511	18			
1	C	367	Total	C	N	O	S	0	2	0
			2757	1728	500	511	18			
1	D	367	Total	C	N	O	S	0	3	0
			2755	1730	494	512	19			

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1	MET	-	initiating methionine	UNP Q70I53
A	251	PRO	HIS	SEE REMARK 999	UNP Q70I53
B	1	MET	-	initiating methionine	UNP Q70I53
B	251	PRO	HIS	SEE REMARK 999	UNP Q70I53
C	1	MET	-	initiating methionine	UNP Q70I53
C	251	PRO	HIS	SEE REMARK 999	UNP Q70I53
D	1	MET	-	initiating methionine	UNP Q70I53
D	251	PRO	HIS	SEE REMARK 999	UNP Q70I53

- Molecule 2 is 3-CYCLOPENTYL-N-HYDROXYPROPANAMIDE (CCD ID: 3YP) (formula: C₈H₁₅NO₂).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	N	O	0	0
			11	8	1	2		
2	B	1	Total	C	N	O	0	0
			11	8	1	2		
2	C	1	Total	C	N	O	0	0
			11	8	1	2		
2	D	1	Total	C	N	O	0	0
			11	8	1	2		

- Molecule 3 is ZINC ION (CCD ID: ZN) (formula: Zn).

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

- Molecule 4 is POTASSIUM ION (CCD ID: K) (formula: K).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	2	Total	K	0	0
			2	2		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	B	2	Total 2	K 2	0	0
4	C	2	Total 2	K 2	0	0
4	D	2	Total 2	K 2	0	0

- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	303	Total 303	O 303	0	0
5	B	342	Total 342	O 342	0	0
5	C	321	Total 321	O 321	0	0
5	D	322	Total 322	O 322	0	0

R277	G311	L317	F341 L342	I368	ARG
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4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	68.10Å 94.49Å 122.63Å 90.00° 104.27° 90.00°	Depositor
Resolution (Å)	44.77 – 1.76 44.77 – 1.76	Depositor EDS
% Data completeness (in resolution range)	98.0 (44.77-1.76) 98.1 (44.77-1.76)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.41 (at 1.76Å)	Xtriage
Refinement program	REFMAC 5.2.0005	Depositor
R, R_{free}	0.156 , 0.191 0.155 , 0.191	Depositor DCC
R_{free} test set	7351 reflections (4.90%)	wwPDB-VP
Wilson B-factor (Å ²)	16.9	Xtriage
Anisotropy	0.417	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.38 , 52.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	0.022 for h,-k,-h-l	Xtriage
F_o, F_c correlation	0.97	EDS
Total number of atoms	12370	wwPDB-VP
Average B, all atoms (Å ²)	18.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.40% 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

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: ZN, K, 3YP

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	0.79	0/2845	0.91	2/3881 (0.1%)
1	B	0.87	1/2826 (0.0%)	0.90	0/3855
1	C	0.86	0/2837	0.92	2/3869 (0.1%)
1	D	0.85	0/2837	0.92	1/3869 (0.0%)
All	All	0.84	1/11345 (0.0%)	0.91	5/15474 (0.0%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	233	PRO	CA-C	5.45	1.55	1.52

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	30	MET	CG-SD-CE	-6.59	86.39	100.90
1	D	94	GLY	N-CA-C	5.49	117.94	111.63
1	C	333	SER	N-CA-C	5.24	119.82	113.38
1	A	90	LEU	CA-C-N	5.06	126.17	119.84
1	A	90	LEU	C-N-CA	5.06	126.17	119.84

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	2761	0	2675	41	0
1	B	2753	0	2665	45	1
1	C	2757	0	2672	42	0
1	D	2755	0	2669	30	0
2	A	11	0	13	4	0
2	B	11	0	13	10	0
2	C	11	0	13	12	0
2	D	11	0	13	7	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
3	C	1	0	0	0	0
3	D	1	0	0	0	0
4	A	2	0	0	0	0
4	B	2	0	0	0	0
4	C	2	0	0	0	0
4	D	2	0	0	0	0
5	A	303	0	0	3	0
5	B	342	0	0	3	0
5	C	321	0	0	3	1
5	D	322	0	0	3	0
All	All	12370	0	10733	157	1

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 7.

All (157) 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:C:312:TYR:OH	2:C:1652:3YP:HAE1	1.31	1.25
1:A:100:ILE:HG21	1:A:152:PHE:CE2	1.77	1.17
1:A:36:HIS:HD2	1:A:38:ALA:H	1.10	0.99
1:A:100:ILE:HG21	1:A:152:PHE:HE2	1.26	0.98
1:C:36:HIS:HD2	1:C:38:ALA:H	1.08	0.98
1:B:36:HIS:HD2	1:B:38:ALA:H	1.11	0.96
1:A:204:GLN:HE22	1:A:277:ARG:H	1.10	0.96
1:C:312:TYR:OH	2:C:1652:3YP:CAE	2.13	0.96
1:A:100:ILE:HG21	1:A:152:PHE:CD2	2.04	0.93
1:C:312:TYR:HH	2:C:1652:3YP:HAE1	1.22	0.93
1:D:87:VAL:O	1:D:93:GLY:HA2	1.69	0.92
1:C:76:HIS:HE1	1:C:156:ASN:H	1.18	0.91
1:B:172:GLU:H	1:B:259:GLN:HE22	0.93	0.90
1:C:204:GLN:HE22	1:C:277:ARG:H	1.20	0.88

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:172:GLU:N	1:B:259:GLN:HE22	1.70	0.88
1:D:204:GLN:HE22	1:D:277:ARG:H	1.18	0.86
1:C:152:PHE:CE1	2:C:1652:3YP:HAH2	2.11	0.85
1:A:36:HIS:CD2	1:A:38:ALA:H	1.94	0.85
1:B:36:HIS:CD2	1:B:38:ALA:H	1.94	0.85
1:A:76:HIS:HE1	1:A:156:ASN:H	1.22	0.84
1:B:83:ASN:HD21	1:B:86:ARG:HH21	1.22	0.83
1:C:36:HIS:CD2	1:C:38:ALA:H	1.96	0.83
1:B:172:GLU:H	1:B:259:GLN:NE2	1.74	0.83
1:C:25:ASN:HD22	1:C:28:ALA:H	1.28	0.80
1:B:39:HIS:HD2	1:B:41:ASP:H	1.30	0.79
1:C:76:HIS:CE1	1:C:156:ASN:H	2.00	0.79
1:A:76:HIS:CE1	1:A:156:ASN:H	2.02	0.78
1:B:143:HIS:CD2	2:B:1552:3YP:HAH2	2.19	0.78
1:A:142:HIS:NE2	2:A:1452:3YP:OAB	2.14	0.77
1:A:204:GLN:NE2	1:A:277:ARG:H	1.82	0.76
1:A:100:ILE:CG2	1:A:152:PHE:CE2	2.65	0.76
1:C:188:GLN:HE22	1:C:229:ASN:HD21	1.36	0.74
1:B:243[B]:HIS:CD2	1:B:350:LEU:HD22	2.23	0.73
1:A:100:ILE:CG2	1:A:152:PHE:HE2	1.99	0.73
1:B:173:ARG:H	1:B:259:GLN:HE21	1.38	0.71
1:A:39:HIS:HD2	1:A:41:ASP:H	1.38	0.71
1:A:143:HIS:NE2	2:A:1452:3YP:NAI	2.38	0.70
1:D:143:HIS:CD2	2:D:1752:3YP:HAE2	2.27	0.70
1:B:123:ARG:O	1:B:127:THR:HG23	1.91	0.69
1:B:65:VAL:O	1:B:116:GLY:HA3	1.92	0.69
1:C:123:ARG:O	1:C:127:THR:HG23	1.91	0.69
1:D:105:ASN:HB3	5:D:1881:HOH:O	1.91	0.69
1:D:8:ASN:HD22	1:D:10:LEU:H	1.41	0.68
1:B:124:ARG:HD3	1:B:129:GLU:OE2	1.93	0.68
1:C:129:GLU:OE1	5:C:1972:HOH:O	2.11	0.68
1:D:152:PHE:CD2	2:D:1752:3YP:HAH2	2.29	0.67
1:D:204:GLN:NE2	1:D:277:ARG:H	1.93	0.66
1:A:204:GLN:HE22	1:A:277:ARG:N	1.90	0.65
1:D:65:VAL:O	1:D:116:GLY:HA3	1.96	0.64
1:D:143:HIS:NE2	2:D:1752:3YP:NAI	2.46	0.63
1:C:183:HIS:HD2	1:C:212:SER:OG	1.81	0.63
1:C:204:GLN:NE2	1:C:277:ARG:H	1.95	0.63
1:D:5:TYR:OH	1:D:47:HIS:HD2	1.83	0.62
1:D:80:HIS:HE1	1:D:154:ILE:O	1.84	0.61
1:D:80:HIS:HD2	5:D:1868:HOH:O	1.82	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:39:HIS:CD2	1:A:41:ASP:H	2.19	0.61
1:C:152:PHE:CD1	2:C:1652:3YP:CAE	2.83	0.61
1:B:182:HIS:CE1	2:B:1552:3YP:HAG1	2.37	0.60
1:A:183:HIS:HD2	1:A:212:SER:OG	1.85	0.60
1:B:39:HIS:CD2	1:B:41:ASP:H	2.18	0.60
1:A:100:ILE:CG2	1:A:152:PHE:CD2	2.84	0.59
1:B:173:ARG:H	1:B:259:GLN:NE2	1.99	0.59
1:B:258:PRO:HD2	1:B:299:ILE:HD12	1.84	0.59
1:C:65:VAL:O	1:C:116:GLY:HA3	2.02	0.59
1:B:83:ASN:ND2	1:B:86:ARG:HH21	1.98	0.59
1:D:143:HIS:HD2	2:D:1752:3YP:HAE2	1.68	0.59
1:A:123:ARG:O	1:A:127:THR:HG23	2.03	0.58
1:B:58:HIS:HD2	5:B:1841:HOH:O	1.86	0.58
1:B:152:PHE:CD1	2:B:1552:3YP:HAE1	2.37	0.58
1:A:54:GLY:O	1:A:57[A]:GLU:HG2	2.04	0.58
1:C:201:SER:OG	1:C:203:HIS:HD2	1.87	0.58
1:D:146:HIS:HE1	5:D:1901:HOH:O	1.86	0.57
1:A:65:VAL:O	1:A:116:GLY:HA3	2.04	0.57
1:B:275:LEU:HD22	2:B:1552:3YP:HAD2	1.86	0.57
1:A:36:HIS:HD2	1:A:38:ALA:N	1.93	0.57
1:B:152:PHE:CD1	2:B:1552:3YP:CAE	2.88	0.57
1:A:92:THR:HA	5:A:1668:HOH:O	2.04	0.56
1:B:36:HIS:HD2	1:B:38:ALA:N	1.93	0.56
1:D:77:SER:OG	1:D:147:ASN:ND2	2.36	0.56
1:A:146:HIS:HE1	5:A:1706:HOH:O	1.89	0.55
1:C:25:ASN:ND2	1:C:28:ALA:H	1.99	0.55
1:A:311:GLY:HA3	1:A:317:LEU:HD12	1.89	0.55
1:D:88:SER:O	1:D:105:ASN:HA	2.07	0.55
1:C:152:PHE:CE1	2:C:1652:3YP:CAH	2.89	0.55
1:D:152:PHE:CD2	2:D:1752:3YP:CAH	2.90	0.54
1:D:204:GLN:HE22	1:D:277:ARG:N	1.98	0.54
1:A:21:LEU:O	1:A:36:HIS:HE1	1.91	0.54
1:D:87:VAL:HA	1:D:90:LEU:HD22	1.91	0.53
1:C:36:HIS:HD2	1:C:38:ALA:N	1.92	0.52
1:C:312:TYR:OH	2:C:1652:3YP:CAJ	2.57	0.52
1:C:258:PRO:HD2	1:C:299:ILE:HD12	1.93	0.51
1:B:20:SER:OG	1:C:315:HIS:HD2	1.94	0.51
1:B:152:PHE:CE1	2:B:1552:3YP:HAE1	2.46	0.51
1:B:228:ILE:HD11	1:B:368:ILE:HD11	1.93	0.50
1:D:8:ASN:ND2	1:D:10:LEU:H	2.08	0.50
1:D:35:HIS:HE1	1:D:41:ASP:OD2	1.94	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:165:ALA:HA	1:C:169:LEU:HD12	1.94	0.50
1:B:143:HIS:NE2	2:B:1552:3YP:HAH2	2.25	0.50
1:C:152:PHE:CD1	2:C:1652:3YP:HAE1	2.47	0.49
1:A:348:ASN:ND2	5:A:1675:HOH:O	2.38	0.49
1:D:182:HIS:HB2	2:D:1752:3YP:OAB	2.11	0.49
1:B:172:GLU:N	1:B:259:GLN:NE2	2.45	0.49
1:A:121:LEU:HD23	1:A:305:VAL:HG13	1.94	0.49
1:B:368:ILE:O	5:B:1823:HOH:O	2.20	0.49
1:D:81:LEU:HD22	1:D:85:LYS:HE3	1.95	0.49
1:B:201:SER:OG	1:B:203:HIS:HD2	1.95	0.48
1:A:126:ALA:CB	1:A:169:LEU:HD13	2.43	0.48
1:B:143:HIS:NE2	2:B:1552:3YP:NAI	2.62	0.47
1:A:183:HIS:HE1	1:A:229:ASN:HD21	1.62	0.47
1:B:315:HIS:HD2	1:C:20:SER:OG	1.97	0.47
2:C:1652:3YP:HAK	2:C:1652:3YP:NAI	2.30	0.47
1:B:361:ILE:HA	1:B:364:LEU:HD13	1.97	0.46
1:C:77:SER:OG	1:C:147:ASN:ND2	2.46	0.46
1:C:152:PHE:CD1	2:C:1652:3YP:HAE2	2.51	0.45
1:A:143:HIS:O	1:A:145:PRO:HD3	2.16	0.45
1:A:311:GLY:HA3	1:A:317:LEU:CD1	2.45	0.45
5:B:1724:HOH:O	1:C:315:HIS:HE1	1.99	0.45
1:D:95:ASP:N	1:D:102[A]:MET:HG3	2.32	0.45
1:B:156:ASN:HD22	1:B:159:SER:H	1.64	0.44
1:A:173:ARG:HH11	1:A:173:ARG:HG3	1.82	0.44
1:B:181:VAL:HG12	1:B:268:ASP:CG	2.41	0.44
1:D:311:GLY:HA3	1:D:317:LEU:HD12	2.00	0.43
1:B:21:LEU:O	1:B:36:HIS:HE1	2.01	0.43
1:C:254:ARG:O	1:C:257[A]:ARG:NE	2.48	0.43
1:C:126:ALA:CB	1:C:169:LEU:HD13	2.48	0.43
1:C:291:ARG:HG3	5:C:1857:HOH:O	2.19	0.43
1:C:204:GLN:HE22	1:C:277:ARG:N	2.02	0.43
1:C:257[A]:ARG:NH1	1:C:299:ILE:HG22	2.33	0.43
1:B:355:ARG:O	1:B:359:GLU:HG2	2.19	0.43
1:C:21:LEU:O	1:C:36:HIS:HE1	2.01	0.43
1:C:172:GLU:N	1:C:259:GLN:OE1	2.49	0.43
1:A:143:HIS:CD2	2:A:1452:3YP:HAE2	2.54	0.43
1:C:152:PHE:CE1	2:C:1652:3YP:CAE	3.02	0.43
2:A:1452:3YP:HAD1	1:D:341:PHE:CZ	2.53	0.42
1:B:315:HIS:HE1	5:C:1823:HOH:O	2.01	0.42
1:B:26:LEU:O	1:B:29:ARG:HD3	2.19	0.42
1:D:317:LEU:C	1:D:317:LEU:HD23	2.46	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:65:VAL:HG23	1:B:120:GLU:HG3	2.02	0.41
1:D:34[A]:SER:OG	1:D:35:HIS:HD2	2.03	0.41
1:A:355:ARG:O	1:A:359:GLU:HG2	2.20	0.41
1:D:142:HIS:NE2	2:D:1752:3YP:NAI	2.69	0.41
1:A:183:HIS:CE1	1:A:229:ASN:HD21	2.38	0.41
1:B:208:PHE:CD2	2:B:1552:3YP:HAK	2.55	0.41
1:C:152:PHE:HE1	2:C:1652:3YP:HAH2	1.75	0.41
1:C:183:HIS:CD2	1:C:212:SER:OG	2.66	0.41
1:B:312:TYR:OH	2:B:1552:3YP:HAE1	2.21	0.41
1:A:4:GLY:HA3	1:A:130:LEU:HD13	2.03	0.41
1:B:83:ASN:HD22	1:B:86:ARG:HE	1.69	0.41
1:B:311:GLY:HA3	1:B:317:LEU:HD12	2.03	0.41
1:C:250:LEU:HD11	1:C:291:ARG:HB3	2.03	0.41
1:A:271:MET:HG2	1:A:342:LEU:HD22	2.02	0.41
1:D:271:MET:HG2	1:D:342:LEU:HD22	2.03	0.40
1:A:89:ASN:HD22	1:A:89:ASN:HA	1.61	0.40
1:B:250:LEU:HD22	1:B:295:CYS:HB2	2.03	0.40
1:A:103:MET:HG2	1:A:107:GLY:HA3	2.04	0.40
1:C:188:GLN:NE2	1:C:229:ASN:HD21	2.12	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:243[B]:HIS:NE2	5:C:1820:HOH:O[2_545]	1.71	0.49

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	369/369 (100%)	357 (97%)	12 (3%)	0	100 100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	B	366/369 (99%)	355 (97%)	11 (3%)	0	100	100
1	C	367/369 (100%)	356 (97%)	11 (3%)	0	100	100
1	D	368/369 (100%)	359 (98%)	9 (2%)	0	100	100
All	All	1470/1476 (100%)	1427 (97%)	43 (3%)	0	100	100

There are no Ramachandran outliers to report.

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	284/282 (101%)	280 (99%)	4 (1%)	59	44
1	B	281/282 (100%)	278 (99%)	3 (1%)	65	52
1	C	282/282 (100%)	279 (99%)	3 (1%)	65	52
1	D	283/282 (100%)	280 (99%)	3 (1%)	65	52
All	All	1130/1128 (100%)	1117 (99%)	13 (1%)	63	49

All (13) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	21	LEU
1	A	89	ASN
1	A	100	ILE
1	A	136	LEU
1	B	156	ASN
1	B	202	LEU
1	B	332	ARG
1	C	95	ASP
1	C	102	MET
1	C	202	LEU
1	D	81	LEU
1	D	89	ASN
1	D	90	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (49) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	36	HIS
1	A	39	HIS
1	A	55	GLN
1	A	76	HIS
1	A	89	ASN
1	A	183	HIS
1	A	204	GLN
1	A	227	ASN
1	A	229	ASN
1	A	308	GLN
1	A	348	ASN
1	B	36	HIS
1	B	39	HIS
1	B	58	HIS
1	B	83	ASN
1	B	138	ASN
1	B	156	ASN
1	B	188	GLN
1	B	203	HIS
1	B	222	ASN
1	B	229	ASN
1	B	247	GLN
1	B	259	GLN
1	B	308	GLN
1	B	315	HIS
1	C	25	ASN
1	C	31	GLN
1	C	36	HIS
1	C	76	HIS
1	C	147	ASN
1	C	183	HIS
1	C	188	GLN
1	C	203	HIS
1	C	204	GLN
1	C	227	ASN
1	C	308	GLN
1	C	315	HIS
1	C	348	ASN
1	D	8	ASN
1	D	35	HIS
1	D	47	HIS

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Mol	Chain	Res	Type
1	D	80	HIS
1	D	89	ASN
1	D	138	ASN
1	D	146	HIS
1	D	147	ASN
1	D	204	GLN
1	D	229	ASN
1	D	348	ASN

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 16 ligands modelled in this entry, 12 are monoatomic - leaving 4 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	3YP	A	1452	3	11,11,11	5.04	2 (18%)	12,13,13	1.76	4 (33%)
2	3YP	D	1752	3	11,11,11	3.36	3 (27%)	12,13,13	1.36	1 (8%)
2	3YP	B	1552	3	11,11,11	10.65	1 (9%)	12,13,13	1.20	0
2	3YP	C	1652	3	11,11,11	4.40	2 (18%)	12,13,13	1.65	2 (16%)

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	3YP	A	1452	3	-	1/7/14/14	0/1/1/1
2	3YP	D	1752	3	-	2/7/14/14	0/1/1/1
2	3YP	B	1552	3	-	4/7/14/14	0/1/1/1
2	3YP	C	1652	3	-	2/7/14/14	0/1/1/1

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	1552	3YP	CAJ-NAI	-35.24	0.93	1.32
2	A	1452	3YP	CAJ-NAI	-16.32	1.14	1.32
2	C	1652	3YP	CAJ-NAI	-13.83	1.17	1.32
2	D	1752	3YP	CAJ-NAI	-9.29	1.22	1.32
2	D	1752	3YP	CAE-CAJ	-5.08	1.41	1.51
2	C	1652	3YP	OAB-NAI	-4.25	1.29	1.40
2	A	1452	3YP	OAB-NAI	-3.18	1.32	1.40
2	D	1752	3YP	OAB-NAI	-2.99	1.32	1.40

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	1652	3YP	CAH-CAE-CAJ	-3.38	105.52	113.06
2	A	1452	3YP	CAH-CAE-CAJ	-3.33	105.64	113.06
2	C	1652	3YP	OAA-CAJ-CAE	3.02	127.49	122.02
2	A	1452	3YP	OAA-CAJ-NAI	-2.92	119.68	123.27
2	D	1752	3YP	CAH-CAE-CAJ	-2.86	106.68	113.06
2	A	1452	3YP	CAH-CAK-CAG	-2.16	107.28	115.45
2	A	1452	3YP	OAB-NAI-CAJ	2.16	122.99	119.79

There are no chirality outliers.

All (9) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	B	1552	3YP	CAE-CAH-CAK-CAG
2	C	1652	3YP	CAE-CAH-CAK-CAG
2	D	1752	3YP	CAE-CAH-CAK-CAG
2	B	1552	3YP	CAH-CAE-CAJ-NAI
2	B	1552	3YP	CAE-CAH-CAK-CAF

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Mol	Chain	Res	Type	Atoms
2	C	1652	3YP	CAE-CAH-CAK-CAF
2	D	1752	3YP	CAE-CAH-CAK-CAF
2	A	1452	3YP	CAJ-CAE-CAH-CAK
2	B	1552	3YP	CAH-CAE-CAJ-OAA

There are no ring outliers.

4 monomers are involved in 33 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	1452	3YP	4	0
2	D	1752	3YP	7	0
2	B	1552	3YP	10	0
2	C	1652	3YP	12	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	367/369 (99%)	-0.15	11 (2%)	52	59	11, 17, 29, 36	4 (1%)
1	B	367/369 (99%)	-0.38	1 (0%)	90	92	8, 15, 25, 30	1 (0%)
1	C	367/369 (99%)	-0.30	6 (1%)	70	77	10, 15, 27, 33	2 (0%)
1	D	367/369 (99%)	-0.12	12 (3%)	49	55	11, 17, 29, 37	3 (0%)
All	All	1468/1476 (99%)	-0.23	30 (2%)	65	71	8, 16, 28, 37	10 (0%)

All (30) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	100	ILE	5.6
1	D	90	LEU	5.0
1	D	93	GLY	4.4
1	A	90	LEU	4.1
1	D	104	GLY	3.9
1	A	104	GLY	3.7
1	D	91	PRO	3.5
1	A	94	GLY	3.3
1	D	94	GLY	3.3
1	D	92	THR	3.2
1	D	102[A]	MET	3.2
1	C	92	THR	3.1
1	D	89	ASN	3.1
1	A	93	GLY	3.0
1	A	102	MET	2.8
1	A	95	ASP	2.7
1	C	90	LEU	2.5
1	D	100	ILE	2.5
1	D	105	ASN	2.4
1	D	95	ASP	2.4
1	C	91	PRO	2.4

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Mol	Chain	Res	Type	RSRZ
1	D	99	GLY	2.3
1	A	89	ASN	2.3
1	C	368	ILE	2.3
1	A	92	THR	2.2
1	A	126	ALA	2.2
1	B	298	ASP	2.2
1	C	102	MET	2.2
1	C	89	ASN	2.2
1	A	91	PRO	2.1

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, 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	B-factors($\text{\AA}^2$)	Q<0.9
2	3YP	D	1752	11/11	0.90	0.20	2,27,38,38	0
2	3YP	A	1452	11/11	0.91	0.22	2,25,40,41	0
2	3YP	C	1652	11/11	0.92	0.23	2,32,45,45	0
2	3YP	B	1552	11/11	0.93	0.22	2,24,41,42	0
4	K	B	1549	1/1	0.98	0.06	22,22,22,22	0
4	K	D	1749	1/1	0.98	0.08	23,23,23,23	0
3	ZN	C	1651	1/1	0.99	0.06	19,19,19,19	1
3	ZN	D	1751	1/1	0.99	0.08	20,20,20,20	1
4	K	A	1449	1/1	0.99	0.04	22,22,22,22	0
3	ZN	A	1451	1/1	0.99	0.07	22,22,22,22	1
4	K	C	1649	1/1	0.99	0.06	19,19,19,19	0
3	ZN	B	1551	1/1	0.99	0.07	19,19,19,19	1
4	K	C	1650	1/1	1.00	0.04	18,18,18,18	0
4	K	B	1550	1/1	1.00	0.04	14,14,14,14	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
4	K	D	1750	1/1	1.00	0.04	16,16,16,16	0
4	K	A	1450	1/1	1.00	0.10	20,20,20,20	0

6.5 Other polymers [i](#)

There are no such residues in this entry.