



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 12:21 PM UTC

PDB ID : 4CFS / pdb_00004cfs
Title : CRYSTAL STRUCTURE OF THE COFACTOR-DEVOID 1-H-3-HYDROXY-4- OXOQUINALDINE 2,4-DIOXYGENASE (HOD) CATALYTICALLY INACTIVE H251A VARIANT COMPLEXED WITH ITS NATURAL SUBSTRATE 1-H-3-HYDROXY-4- OXOQUINALDINE
Authors : Bui, S.; Steiner, R.A.
Deposited on : 2013-11-19
Resolution : 1.94 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

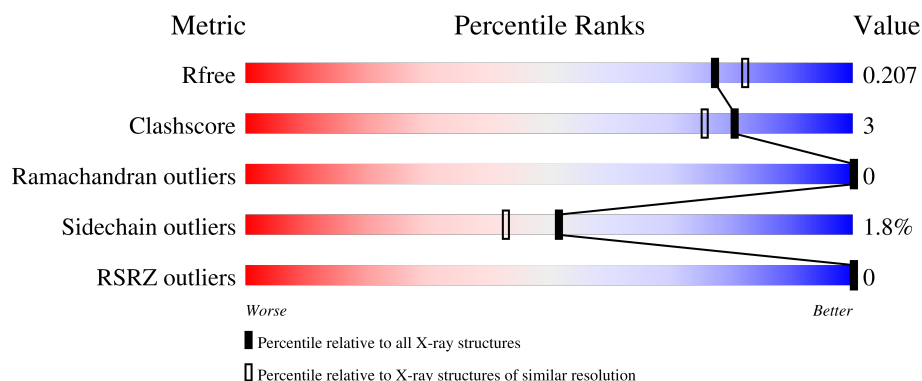
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

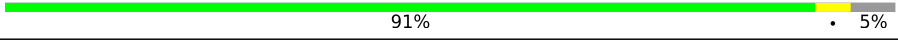
The reported resolution of this entry is 1.94 Å.

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	1452 (1.94-1.94)
Clashscore	190562	1494 (1.94-1.94)
Ramachandran outliers	187476	1479 (1.94-1.94)
Sidechain outliers	187428	1479 (1.94-1.94)
RSRZ outliers	180081	1453 (1.94-1.94)

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	287	 90% 5% 5%
1	B	287	 90% 6% 5%
1	C	287	 91% • 5%
1	D	287	 89% 5% • 5%

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
4	TAR	C	1278	-	X	-	-
4	TAR	C	1279[A]	-	X	-	-

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 9772 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 1-H-3-HYDROXY-4-OXOQUINALDINE 2,4-DIOXYGENASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	273	Total	C	N	O	S	0	4	0
			2240	1434	389	409	8			
1	B	273	Total	C	N	O	S	0	6	0
			2262	1447	395	412	8			
1	C	273	Total	C	N	O	S	0	4	0
			2244	1434	389	412	9			
1	D	272	Total	C	N	O	S	0	6	0
			2252	1442	393	409	8			

There are 64 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-10	MET	-	expression tag	UNP O31266
A	-9	ARG	-	expression tag	UNP O31266
A	-8	GLY	-	expression tag	UNP O31266
A	-7	SER	-	expression tag	UNP O31266
A	-6	HIS	-	expression tag	UNP O31266
A	-5	HIS	-	expression tag	UNP O31266
A	-4	HIS	-	expression tag	UNP O31266
A	-3	HIS	-	expression tag	UNP O31266
A	-2	HIS	-	expression tag	UNP O31266
A	-1	HIS	-	expression tag	UNP O31266
A	0	GLY	-	expression tag	UNP O31266
A	1	SER	-	expression tag	UNP O31266
A	2	MET	-	expression tag	UNP O31266
A	276	ASN	-	expression tag	UNP O31266
A	69	SER	CYS	engineered mutation	UNP O31266
A	251	ALA	HIS	engineered mutation	UNP O31266
B	-10	MET	-	expression tag	UNP O31266
B	-9	ARG	-	expression tag	UNP O31266
B	-8	GLY	-	expression tag	UNP O31266
B	-7	SER	-	expression tag	UNP O31266
B	-6	HIS	-	expression tag	UNP O31266

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Chain	Residue	Modelled	Actual	Comment	Reference
B	-5	HIS	-	expression tag	UNP O31266
B	-4	HIS	-	expression tag	UNP O31266
B	-3	HIS	-	expression tag	UNP O31266
B	-2	HIS	-	expression tag	UNP O31266
B	-1	HIS	-	expression tag	UNP O31266
B	0	GLY	-	expression tag	UNP O31266
B	1	SER	-	expression tag	UNP O31266
B	2	MET	-	expression tag	UNP O31266
B	276	ASN	-	expression tag	UNP O31266
B	69	SER	CYS	engineered mutation	UNP O31266
B	251	ALA	HIS	engineered mutation	UNP O31266
C	-10	MET	-	expression tag	UNP O31266
C	-9	ARG	-	expression tag	UNP O31266
C	-8	GLY	-	expression tag	UNP O31266
C	-7	SER	-	expression tag	UNP O31266
C	-6	HIS	-	expression tag	UNP O31266
C	-5	HIS	-	expression tag	UNP O31266
C	-4	HIS	-	expression tag	UNP O31266
C	-3	HIS	-	expression tag	UNP O31266
C	-2	HIS	-	expression tag	UNP O31266
C	-1	HIS	-	expression tag	UNP O31266
C	0	GLY	-	expression tag	UNP O31266
C	1	SER	-	expression tag	UNP O31266
C	2	MET	-	expression tag	UNP O31266
C	276	ASN	-	expression tag	UNP O31266
C	69	SER	CYS	engineered mutation	UNP O31266
C	251	ALA	HIS	engineered mutation	UNP O31266
D	-10	MET	-	expression tag	UNP O31266
D	-9	ARG	-	expression tag	UNP O31266
D	-8	GLY	-	expression tag	UNP O31266
D	-7	SER	-	expression tag	UNP O31266
D	-6	HIS	-	expression tag	UNP O31266
D	-5	HIS	-	expression tag	UNP O31266
D	-4	HIS	-	expression tag	UNP O31266
D	-3	HIS	-	expression tag	UNP O31266
D	-2	HIS	-	expression tag	UNP O31266
D	-1	HIS	-	expression tag	UNP O31266
D	0	GLY	-	expression tag	UNP O31266
D	1	SER	-	expression tag	UNP O31266
D	2	MET	-	expression tag	UNP O31266
D	276	ASN	-	expression tag	UNP O31266
D	69	SER	CYS	engineered mutation	UNP O31266

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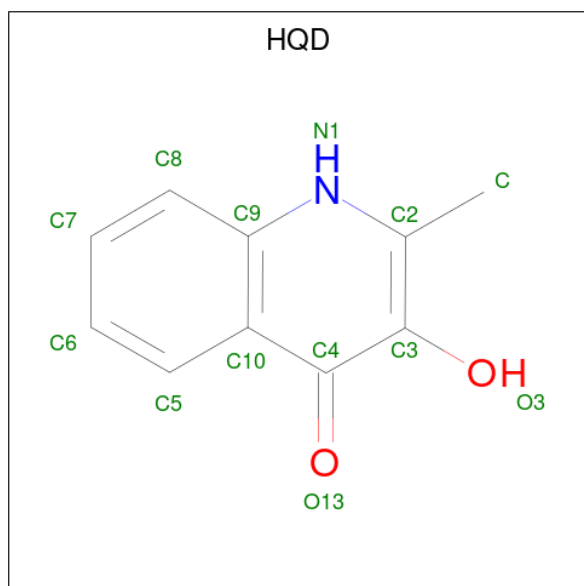
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Chain	Residue	Modelled	Actual	Comment	Reference
D	251	ALA	HIS	engineered mutation	UNP O31266

- Molecule 2 is POTASSIUM ION (CCD ID: K) (formula: K).

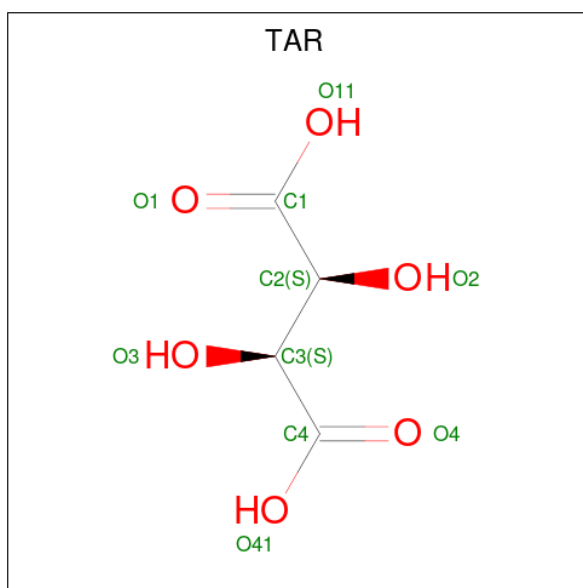
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total K 1 1	0	0
2	B	1	Total K 1 1	0	0
2	C	1	Total K 1 1	0	0
2	D	1	Total K 1 1	0	0

- Molecule 3 is 3-HYDROXY-2-METHYLQUINOLIN-4(1H)-ONE (CCD ID: HQD) (formula: C₁₀H₉NO₂).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total C N O 13 10 1 2	0	0
3	B	1	Total C N O 13 10 1 2	0	0
3	C	1	Total C N O 13 10 1 2	0	0
3	D	1	Total C N O 13 10 1 2	0	0

- Molecule 4 is D(-)-TARTARIC ACID (CCD ID: TAR) (formula: $C_4H_6O_6$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total C O 10 4 6	0	0
4	C	1	Total C O 10 4 6	0	0
4	C	1	Total C O 20 8 12	0	1
4	C	1	Total C O 10 4 6	0	0
4	D	1	Total C O 10 4 6	0	0
4	D	1	Total C O 10 4 6	0	0
4	D	1	Total C O 10 4 6	0	0

- Molecule 5 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	159	Total O 159 159	0	0
5	B	176	Total O 176 176	0	0
5	C	125	Total O 125 125	0	0
5	D	178	Total O 178 178	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: 1-H-3-HYDROXY-4-OXOQUINALDINE 2,4-DIOXYGENASE

Chain A: 



- Molecule 1: 1-H-3-HYDROXY-4-OXOQUINALDINE 2,4-DIOXYGENASE

Chain B: 



- Molecule 1: 1-H-3-HYDROXY-4-OXOQUINALDINE 2,4-DIOXYGENASE

Chain C: 



- Molecule 1: 1-H-3-HYDROXY-4-OXOQUINALDINE 2,4-DIOXYGENASE

Chain D: 



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	44.73Å 166.85Å 167.74Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	46.45 – 1.94 46.45 – 1.95	Depositor EDS
% Data completeness (in resolution range)	98.5 (46.45-1.94) 98.5 (46.45-1.95)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.91 (at 1.95Å)	Xtriage
Refinement program	REFMAC 5.8.0049	Depositor
R, R_{free}	0.163 , 0.198 (Not available) , 0.207	Depositor DCC
R_{free} test set	4709 reflections (5.08%)	wwPDB-VP
Wilson B-factor (Å ²)	28.1	Xtriage
Anisotropy	0.159	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.37 , 30.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.41$, $\langle L^2 \rangle = 0.24$	Xtriage
Estimated twinning fraction	0.449 for -h,l,k	Xtriage
Reported twinning fraction	0.511 for H, K, L 0.489 for -H, L, K	Depositor
Outliers	3 of 92719 reflections (0.003%)	Xtriage
F_o, F_c correlation	0.97	EDS
Total number of atoms	9772	wwPDB-VP
Average B, all atoms (Å ²)	30.0	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 23.58 % 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 4.5321e-03.*

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: TAR, K, HQD

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	0.56	0/2322	0.79	1/3161 (0.0%)
1	B	0.60	0/2347	0.78	1/3192 (0.0%)
1	C	0.57	0/2326	0.79	1/3165 (0.0%)
1	D	0.58	0/2337	0.78	1/3180 (0.0%)
All	All	0.58	0/9332	0.78	4/12698 (0.0%)

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	213	ARG	CB-CA-C	-6.86	101.16	110.22
1	A	213	ARG	CB-CA-C	-6.37	101.81	110.22
1	C	213	ARG	CB-CA-C	-6.21	102.02	110.22
1	B	213	ARG	CB-CA-C	-6.04	102.25	110.22

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	2240	0	2149	14	1
1	B	2262	0	2174	13	0
1	C	2244	0	2143	8	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	D	2252	0	2167	11	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
2	C	1	0	0	0	0
2	D	1	0	0	0	0
3	A	13	0	8	0	0
3	B	13	0	8	0	0
3	C	13	0	8	0	0
3	D	13	0	8	0	0
4	A	10	0	4	0	0
4	C	40	0	16	5	0
4	D	30	0	12	3	0
5	A	159	0	0	6	0
5	B	176	0	0	5	0
5	C	125	0	0	4	0
5	D	178	0	0	7	0
All	All	9772	0	8697	46	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 3.

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:228:GLU:HG3	1:B:245[B]:LYS:HD3	1.45	0.98
1:B:273:ARG:NH1	5:B:2173:HOH:O	2.01	0.89
5:A:2108:HOH:O	4:C:1280:TAR:H3	1.71	0.89
4:D:1279:TAR:H3	5:D:2121:HOH:O	1.81	0.79
1:B:4:THR:HA	5:B:2001:HOH:O	1.80	0.79
1:A:260:ARG:HD3	1:D:165:ASP:OD2	1.84	0.78
1:A:165:ASP:OD2	1:C:260:ARG:HD3	1.91	0.69
1:A:8:GLU:OE1	5:A:2006:HOH:O	2.11	0.67
4:C:1279[B]:TAR:C4	4:C:1279[B]:TAR:O1	2.43	0.67
1:D:94:THR:HG22	5:D:2069:HOH:O	1.96	0.65
4:D:1278:TAR:H2	5:D:2126:HOH:O	1.96	0.65
1:B:245[A]:LYS:HG2	5:B:2146:HOH:O	1.98	0.64
1:A:260:ARG:CD	1:D:165:ASP:OD2	2.52	0.57
1:A:190:ARG:CD	1:B:77:GLN:HB3	2.35	0.56
1:D:164:HIS:HD2	4:D:1279:TAR:O41	1.88	0.56
1:C:164:HIS:HE1	5:C:2084:HOH:O	1.88	0.56
1:B:198:ARG:HB2	1:B:198:ARG:NH1	2.21	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:245:LYS:HE3	5:C:2107:HOH:O	2.06	0.54
1:D:4:THR:OG1	1:D:5:TYR:N	2.31	0.54
1:B:150:ARG:NH1	5:B:2094:HOH:O	2.27	0.52
4:C:1279[B]:TAR:O4	4:C:1279[B]:TAR:C1	2.58	0.51
1:A:165:ASP:OD2	1:C:260:ARG:CD	2.59	0.50
4:C:1279[B]:TAR:O1	4:C:1279[B]:TAR:O4	2.30	0.47
1:B:198:ARG:HB2	1:B:198:ARG:CZ	2.44	0.47
1:D:138:LYS:NZ	5:D:2100:HOH:O	2.38	0.47
1:A:266:ARG:HD3	5:A:2035:HOH:O	2.14	0.47
1:C:81:LYS:HG2	5:C:2042:HOH:O	2.15	0.46
4:C:1279[A]:TAR:O4	4:C:1279[A]:TAR:O2	2.23	0.46
1:B:138:LYS:NZ	5:B:2085:HOH:O	2.36	0.46
1:D:27:GLY:HA3	5:D:2018:HOH:O	2.15	0.46
1:A:4:THR:HG23	1:A:5:TYR:CD1	2.51	0.46
1:A:198:ARG:NH1	5:A:2131:HOH:O	2.50	0.45
1:A:3:ASP:HA	5:A:2001:HOH:O	2.18	0.43
1:A:190:ARG:HD3	1:B:77:GLN:HB3	2.00	0.43
1:A:260:ARG:O	1:A:263[B]:VAL:HG22	2.19	0.43
1:A:164:HIS:HE1	5:A:2105:HOH:O	2.00	0.43
1:B:260:ARG:O	1:B:263:VAL:HG22	2.19	0.43
1:C:221[A]:GLN:CD	1:C:251:ALA:HB2	2.44	0.42
1:D:221[A]:GLN:CD	1:D:251:ALA:HB2	2.45	0.42
1:C:260:ARG:O	1:C:263:VAL:HG22	2.20	0.41
1:A:190:ARG:CZ	1:B:77:GLN:HG2	2.51	0.41
1:C:220:SER:C	5:C:2107:HOH:O	2.63	0.41
1:D:259:ASP:O	1:D:263[B]:VAL:HG23	2.20	0.41
1:D:199:ASN:ND2	5:D:2142:HOH:O	2.53	0.41
1:B:107:LEU:C	1:B:107:LEU:HD23	2.46	0.41
1:D:23:ARG:HD3	5:D:2014:HOH:O	2.21	0.41

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:A:4:THR:OG1	1:A:208:ASN:OD1[1_655]	2.16	0.04

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	275/287 (96%)	268 (98%)	7 (2%)	0	100	100
1	B	277/287 (96%)	270 (98%)	7 (2%)	0	100	100
1	C	275/287 (96%)	267 (97%)	8 (3%)	0	100	100
1	D	276/287 (96%)	267 (97%)	9 (3%)	0	100	100
All	All	1103/1148 (96%)	1072 (97%)	31 (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	238/246 (97%)	233 (98%)	5 (2%)	47	37
1	B	240/246 (98%)	235 (98%)	5 (2%)	47	37
1	C	238/246 (97%)	233 (98%)	5 (2%)	47	37
1	D	239/246 (97%)	232 (97%)	7 (3%)	37	24
All	All	955/984 (97%)	933 (98%)	22 (2%)	51	33

All (22) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	117	GLU
1	A	126	ASP

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Mol	Chain	Res	Type
1	A	142	LEU
1	A	263[A]	VAL
1	A	263[B]	VAL
1	B	117	GLU
1	B	126	ASP
1	B	142	LEU
1	B	221[A]	GLN
1	B	221[B]	GLN
1	C	117	GLU
1	C	126	ASP
1	C	142	LEU
1	C	221[A]	GLN
1	C	221[B]	GLN
1	D	117	GLU
1	D	126	ASP
1	D	142	LEU
1	D	221[A]	GLN
1	D	221[B]	GLN
1	D	263[A]	VAL
1	D	263[B]	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (9) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	164	HIS
1	B	154	HIS
1	B	164	HIS
1	B	171	HIS
1	C	154	HIS
1	C	164	HIS
1	D	22	GLN
1	D	113	GLN
1	D	164	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 oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 16 ligands modelled in this entry, 4 are monoatomic - leaving 12 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
3	HQD	C	1277	-	14,14,14	1.40	2 (14%)	18,20,20	1.33	2 (11%)
3	HQD	A	1277	-	14,14,14	0.94	1 (7%)	18,20,20	1.66	2 (11%)
4	TAR	D	1280	-	9,9,9	1.20	0	12,12,12	2.03	4 (33%)
4	TAR	D	1279	-	9,9,9	1.32	1 (11%)	12,12,12	1.72	5 (41%)
4	TAR	C	1280	-	9,9,9	0.93	1 (11%)	12,12,12	1.53	2 (16%)
3	HQD	D	1277	-	14,14,14	0.93	1 (7%)	18,20,20	1.20	2 (11%)
4	TAR	C	1278	-	9,9,9	1.03	0	12,12,12	2.65	5 (41%)
3	HQD	B	1277	-	14,14,14	0.71	1 (7%)	18,20,20	2.30	2 (11%)
4	TAR	D	1278	-	9,9,9	1.05	0	12,12,12	2.20	5 (41%)
4	TAR	C	1279[A]	-	9,9,9	1.56	2 (22%)	12,12,12	1.50	4 (33%)
4	TAR	A	1278	-	9,9,9	1.00	0	12,12,12	1.24	1 (8%)
4	TAR	C	1279[B]	-	9,9,9	1.30	1 (11%)	12,12,12	1.28	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
3	HQD	C	1277	-	-	-	0/2/2/2
3	HQD	A	1277	-	-	-	0/2/2/2
4	TAR	D	1280	-	-	8/12/12/12	-
4	TAR	D	1279	-	-	5/12/12/12	-
4	TAR	C	1280	-	-	8/12/12/12	-
4	TAR	C	1278	-	-	12/12/12/12	-
3	HQD	D	1277	-	-	-	0/2/2/2
3	HQD	B	1277	-	-	-	0/2/2/2
4	TAR	D	1278	-	-	6/12/12/12	-
4	TAR	C	1279[A]	-	-	10/12/12/12	-
4	TAR	A	1278	-	-	10/12/12/12	-
4	TAR	C	1279[B]	-	-	8/12/12/12	-

All (10) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	1277	HQD	C2-N1	4.02	1.41	1.36
3	A	1277	HQD	C2-N1	3.34	1.40	1.36
4	C	1279[A]	TAR	O11-C1	-3.05	1.20	1.30
3	D	1277	HQD	C2-N1	2.85	1.39	1.36
3	C	1277	HQD	C3-C2	2.69	1.40	1.37
4	C	1279[B]	TAR	C2-C1	-2.54	1.49	1.52
3	B	1277	HQD	C3-C2	2.17	1.40	1.37
4	C	1279[A]	TAR	C2-C1	-2.11	1.49	1.52
4	C	1280	TAR	O41-C4	-2.03	1.24	1.30
4	D	1279	TAR	O3-C3	2.00	1.46	1.42

All (36) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	1277	HQD	O3-C3-C2	7.41	125.25	118.40
3	B	1277	HQD	C2-C3-C4	-6.02	118.58	122.33
3	A	1277	HQD	O3-C3-C2	5.95	123.90	118.40
4	C	1278	TAR	O41-C4-C3	5.09	127.44	113.31
4	D	1280	TAR	O41-C4-C3	4.31	125.30	113.31
3	C	1277	HQD	O3-C3-C2	4.31	122.38	118.40
4	C	1278	TAR	O4-C4-C3	-4.13	110.61	121.62
4	C	1278	TAR	O3-C3-C2	4.04	118.38	110.17
4	D	1278	TAR	O41-C4-C3	4.00	124.44	113.31
3	D	1277	HQD	C2-C3-C4	-3.68	120.03	122.33
4	D	1278	TAR	O4-C4-C3	-3.54	112.19	121.62

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	D	1280	TAR	O4-C4-C3	-3.25	112.96	121.62
4	D	1279	TAR	C3-C2-C1	3.25	117.02	109.82
4	D	1278	TAR	C2-C3-C4	3.14	116.78	109.82
3	A	1277	HQD	C2-C3-C4	-3.11	120.39	122.33
4	C	1278	TAR	O11-C1-C2	3.07	121.84	113.31
4	D	1279	TAR	O41-C4-C3	3.04	121.76	113.31
4	C	1280	TAR	O11-C1-C2	2.94	121.49	113.31
4	D	1278	TAR	C3-C2-C1	2.91	116.26	109.82
3	D	1277	HQD	O3-C3-C2	2.65	120.85	118.40
3	C	1277	HQD	C2-C3-C4	-2.59	120.71	122.33
4	D	1280	TAR	C3-C2-C1	2.48	115.31	109.82
4	C	1279[B]	TAR	O3-C3-C2	-2.32	105.44	110.17
4	C	1279[A]	TAR	O41-C4-C3	2.25	119.56	113.31
4	D	1278	TAR	O11-C1-C2	2.23	119.50	113.31
4	C	1279[A]	TAR	O2-C2-C1	-2.20	105.98	110.69
4	C	1280	TAR	O2-C2-C3	-2.20	105.68	110.17
4	D	1280	TAR	C2-C3-C4	2.19	114.68	109.82
4	C	1278	TAR	O1-C1-C2	-2.10	116.01	121.62
4	D	1279	TAR	O41-C4-O4	-2.10	119.31	124.08
4	D	1279	TAR	O2-C2-C3	-2.10	105.89	110.17
4	C	1279[A]	TAR	C2-C3-C4	-2.09	105.19	109.82
4	D	1279	TAR	O2-C2-C1	-2.05	106.32	110.69
4	C	1279[A]	TAR	O4-C4-C3	-2.03	116.21	121.62
4	A	1278	TAR	O41-C4-C3	2.03	118.94	113.31
4	C	1279[B]	TAR	O41-C4-C3	2.00	118.88	113.31

There are no chirality outliers.

All (67) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	1278	TAR	C1-C2-C3-C4
4	A	1278	TAR	O2-C2-C3-O3
4	C	1279[B]	TAR	O1-C1-C2-O2
4	C	1279[B]	TAR	O11-C1-C2-O2
4	C	1279[B]	TAR	C1-C2-C3-C4
4	C	1279[B]	TAR	O2-C2-C3-O3
4	C	1279[B]	TAR	O2-C2-C3-C4
4	C	1280	TAR	O3-C3-C4-O4
4	C	1280	TAR	O3-C3-C4-O41
4	D	1278	TAR	O1-C1-C2-O2
4	D	1279	TAR	C2-C3-C4-O4
4	D	1279	TAR	C2-C3-C4-O41

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Mol	Chain	Res	Type	Atoms
4	D	1280	TAR	O2-C2-C3-O3
4	C	1279[B]	TAR	C1-C2-C3-O3
4	C	1278	TAR	O2-C2-C3-O3
4	C	1279[A]	TAR	O2-C2-C3-O3
4	C	1280	TAR	O2-C2-C3-O3
4	C	1279[A]	TAR	C1-C2-C3-C4
4	C	1280	TAR	C1-C2-C3-C4
4	D	1280	TAR	C1-C2-C3-C4
4	D	1280	TAR	C1-C2-C3-O3
4	D	1280	TAR	O2-C2-C3-C4
4	A	1278	TAR	O3-C3-C4-O4
4	A	1278	TAR	O3-C3-C4-O41
4	C	1278	TAR	O3-C3-C4-O4
4	C	1278	TAR	O3-C3-C4-O41
4	C	1279[A]	TAR	O3-C3-C4-O4
4	C	1279[A]	TAR	O3-C3-C4-O41
4	C	1279[B]	TAR	O3-C3-C4-O4
4	C	1279[B]	TAR	O3-C3-C4-O41
4	C	1280	TAR	O1-C1-C2-O2
4	C	1280	TAR	O11-C1-C2-O2
4	D	1278	TAR	O11-C1-C2-O2
4	D	1279	TAR	O3-C3-C4-O4
4	D	1279	TAR	O3-C3-C4-O41
4	D	1280	TAR	O1-C1-C2-O2
4	D	1280	TAR	O11-C1-C2-O2
4	C	1278	TAR	C2-C3-C4-O4
4	C	1278	TAR	C2-C3-C4-O41
4	C	1280	TAR	C1-C2-C3-O3
4	A	1278	TAR	O2-C2-C3-C4
4	C	1278	TAR	C1-C2-C3-O3
4	C	1278	TAR	O2-C2-C3-C4
4	C	1279[A]	TAR	C1-C2-C3-O3
4	C	1279[A]	TAR	O2-C2-C3-C4
4	C	1280	TAR	O2-C2-C3-C4
4	A	1278	TAR	C1-C2-C3-O3
4	D	1280	TAR	O3-C3-C4-O4
4	D	1280	TAR	O3-C3-C4-O41
4	C	1278	TAR	C1-C2-C3-C4
4	A	1278	TAR	O11-C1-C2-O2
4	C	1278	TAR	O1-C1-C2-O2
4	A	1278	TAR	O1-C1-C2-O2
4	C	1278	TAR	O11-C1-C2-O2

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Mol	Chain	Res	Type	Atoms
4	D	1278	TAR	O2-C2-C3-O3
4	D	1278	TAR	C1-C2-C3-C4
4	D	1279	TAR	C1-C2-C3-O3
4	C	1279[A]	TAR	O11-C1-C2-C3
4	D	1278	TAR	C2-C3-C4-O4
4	A	1278	TAR	O1-C1-C2-C3
4	C	1278	TAR	O1-C1-C2-C3
4	C	1278	TAR	O11-C1-C2-C3
4	C	1279[A]	TAR	O1-C1-C2-C3
4	D	1278	TAR	C2-C3-C4-O41
4	C	1279[A]	TAR	O11-C1-C2-O2
4	A	1278	TAR	O11-C1-C2-C3
4	C	1279[A]	TAR	O1-C1-C2-O2

There are no ring outliers.

5 monomers are involved in 8 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	D	1279	TAR	2	0
4	C	1280	TAR	1	0
4	D	1278	TAR	1	0
4	C	1279[A]	TAR	1	0
4	C	1279[B]	TAR	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 [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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	273/287 (95%)	-1.10	0 100 100	14, 32, 46, 76	4 (1%)
1	B	273/287 (95%)	-1.11	0 100 100	11, 26, 44, 63	6 (2%)
1	C	273/287 (95%)	-1.12	0 100 100	15, 28, 47, 64	4 (1%)
1	D	272/287 (94%)	-1.12	0 100 100	14, 28, 44, 61	6 (2%)
All	All	1091/1148 (95%)	-1.11	0 100 100	11, 28, 46, 76	20 (1%)

There are no RSRZ outliers to report.

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(Å ²)	Q<0.9
4	TAR	A	1278	10/10	0.97	0.05	28,36,40,46	0
4	TAR	D	1279	10/10	0.98	0.05	30,32,37,39	0
3	HQD	B	1277	13/13	0.99	0.03	17,17,18,19	0
3	HQD	C	1277	13/13	0.99	0.03	16,17,18,19	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	HQD	D	1277	13/13	0.99	0.03	18,19,21,21	0
2	K	A	1276	1/1	0.99	0.05	33,33,33,33	0
4	TAR	C	1278	10/10	0.99	0.03	23,31,36,39	0
4	TAR	C	1279[A]	10/10	0.99	0.03	13,19,21,22	10
4	TAR	C	1279[B]	10/10	0.99	0.03	24,27,29,29	10
4	TAR	C	1280	10/10	0.99	0.04	24,30,33,36	0
4	TAR	D	1278	10/10	0.99	0.04	25,30,34,40	0
3	HQD	A	1277	13/13	0.99	0.03	21,22,24,24	0
4	TAR	D	1280	10/10	0.99	0.03	22,28,31,32	0
2	K	B	1276	1/1	1.00	0.05	25,25,25,25	0
2	K	C	1276	1/1	1.00	0.03	31,31,31,31	0
2	K	D	1276	1/1	1.00	0.03	28,28,28,28	0

6.5 Other polymers [i](#)

There are no such residues in this entry.