



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 07:04 AM UTC

PDB ID : 3JS3 / pdb_00003js3
Title : Crystal structure of type I 3-dehydroquinatase (aroD) from *Clostridium difficile* with covalent reaction intermediate
Authors : Minasov, G.; Light, S.H.; Shuvalova, L.; Dubrovska, I.; Winsor, J.; Peterson, S.N.; Anderson, W.F.; Center for Structural Genomics of Infectious Diseases (CSGID)
Deposited on : 2009-09-09
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 : 4-5-2 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

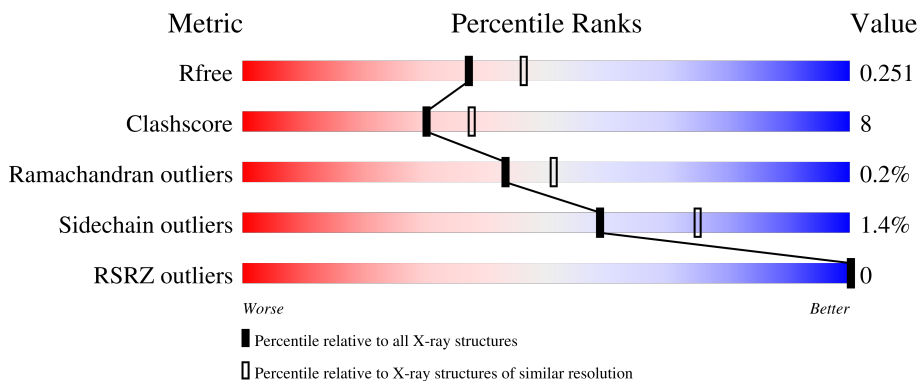
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 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}	180053	6164 (2.20-2.20)
Clashscore	190562	6851 (2.20-2.20)
Ramachandran outliers	187476	6768 (2.20-2.20)
Sidechain outliers	187428	6769 (2.20-2.20)
RSRZ outliers	180081	6166 (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 $\leq 5\%$. 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	258	
1	B	258	
1	C	258	
1	D	258	

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	DHS	A	301	X	-	-	-

2 Entry composition [i](#)

There are 3 unique types of molecules in this entry. The entry contains 8482 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.

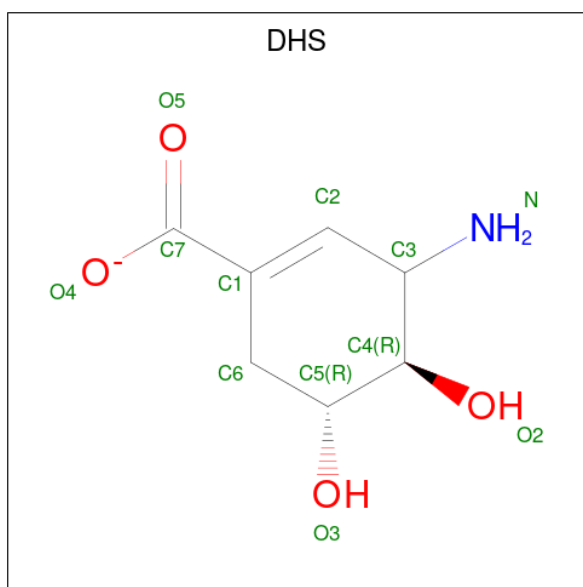
- Molecule 1 is a protein called 3-dehydroquinate dehydratase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	253	2053	1312	343	386	12	0	5	0
1	B	253	2023	1294	337	379	13	0	2	0
1	C	253	2024	1297	338	377	12	0	2	0
1	D	253	2016	1290	336	378	12	0	1	0

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-2	SER	-	expression tag	UNP Q186A6
A	-1	ASN	-	expression tag	UNP Q186A6
A	0	ALA	-	expression tag	UNP Q186A6
B	-2	SER	-	expression tag	UNP Q186A6
B	-1	ASN	-	expression tag	UNP Q186A6
B	0	ALA	-	expression tag	UNP Q186A6
C	-2	SER	-	expression tag	UNP Q186A6
C	-1	ASN	-	expression tag	UNP Q186A6
C	0	ALA	-	expression tag	UNP Q186A6
D	-2	SER	-	expression tag	UNP Q186A6
D	-1	ASN	-	expression tag	UNP Q186A6
D	0	ALA	-	expression tag	UNP Q186A6

- Molecule 2 is 3-AMINO-4,5-DIHYDROXY-CYCLOHEX-1-ENECARBOXYLATE (CCD ID: DHS) (formula: C₇H₁₀NO₄).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total C O 11 7 4	0	0
2	B	1	Total C O 11 7 4	0	0
2	C	1	Total C O 11 7 4	0	0
2	D	1	Total C O 11 7 4	0	0

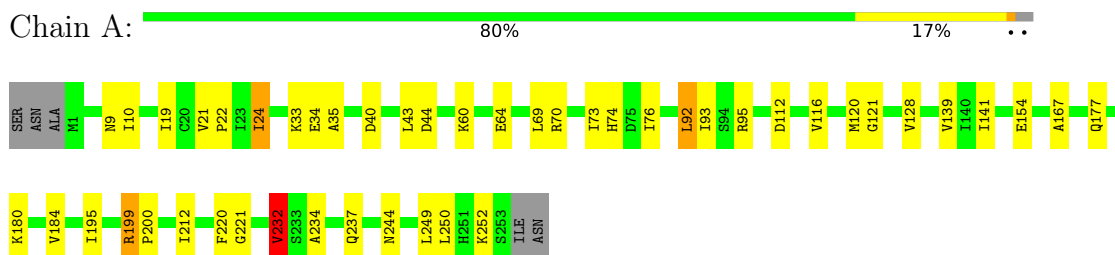
- Molecule 3 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	83	Total O 85 85	0	3
3	B	66	Total O 66 66	0	0
3	C	85	Total O 86 86	0	1
3	D	84	Total O 85 85	0	1

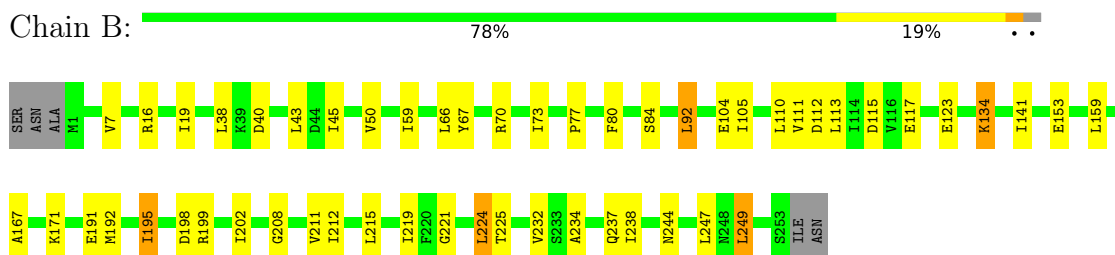
3 Residue-property plots [i](#)

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.

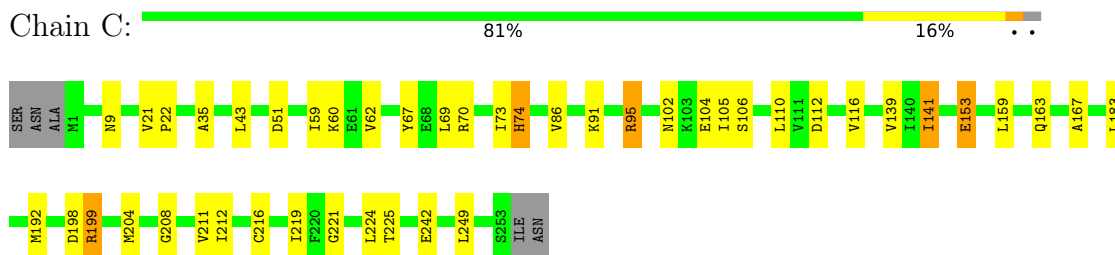
- Molecule 1: 3-dehydroquinatate dehydratase



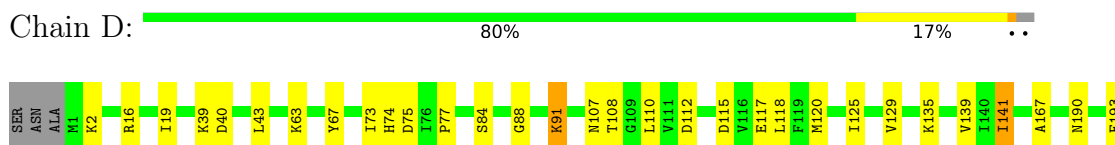
- Molecule 1: 3-dehydroquinatate dehydratase



- Molecule 1: 3-dehydroquinatate dehydratase



- Molecule 1: 3-dehydroquinatate dehydratase





4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	60.47Å 139.62Å 66.77Å 90.00° 90.63° 90.00°	Depositor
Resolution (Å)	29.55 – 2.20 29.55 – 2.20	Depositor EDS
% Data completeness (in resolution range)	99.8 (29.55-2.20) 96.6 (29.55-2.20)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.38 (at 2.20Å)	Xtrriage
Refinement program	REFMAC 5.5.0102	Depositor
R, R_{free}	0.189 , 0.241 0.201 , 0.251	Depositor DCC
R_{free} test set	2839 reflections (5.06%)	wwPDB-VP
Wilson B-factor (Å ²)	42.2	Xtrriage
Anisotropy	0.258	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 29.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtrriage
Estimated twinning fraction	0.209 for h,-k,-l	Xtrriage
F_o, F_c correlation	0.97	EDS
Total number of atoms	8482	wwPDB-VP
Average B, all atoms (Å ²)	26.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 10.35% 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 [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: DHS

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	0.75	0/2082	1.03	7/2799 (0.3%)
1	B	0.73	0/2052	0.99	3/2759 (0.1%)
1	C	0.78	0/2053	1.01	4/2760 (0.1%)
1	D	0.74	0/2045	0.99	5/2750 (0.2%)
All	All	0.75	0/8232	1.00	19/11068 (0.2%)

There are no bond length outliers.

All (19) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	121	GLY	N-CA-C	9.51	120.98	111.95
1	B	195	ILE	N-CA-C	6.86	118.18	111.67
1	B	16	ARG	CB-CA-C	-5.89	100.21	109.52
1	A	221	GLY	N-CA-C	5.74	121.31	114.48
1	C	139	VAL	N-CA-C	5.65	116.08	108.17
1	A	232	VAL	N-CA-C	5.65	116.86	109.58
1	A	177	GLN	N-CA-C	-5.57	106.48	113.72
1	D	196	TYR	N-CA-C	5.41	120.01	113.41
1	A	195	ILE	N-CA-C	5.40	116.80	111.67
1	B	221	GLY	N-CA-C	5.35	122.08	114.85
1	A	139	VAL	N-CA-C	5.35	115.60	108.11
1	D	221	GLY	N-CA-C	5.34	122.07	114.85
1	C	221	GLY	N-CA-C	5.33	122.04	114.85
1	A	220	PHE	N-CA-C	5.23	119.71	113.23
1	D	88	GLY	N-CA-C	5.20	121.92	114.64
1	C	141	ILE	N-CA-C	-5.19	100.28	107.80
1	C	199	ARG	CB-CA-C	-5.13	103.35	110.37
1	D	39	LYS	N-CA-C	5.06	117.18	111.11
1	D	141	ILE	N-CA-C	-5.03	100.51	107.80

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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	2053	0	2122	37	0
1	B	2023	0	2096	46	0
1	C	2024	0	2107	36	0
1	D	2016	0	2090	34	0
2	A	11	0	7	0	0
2	B	11	0	7	1	0
2	C	11	0	7	0	0
2	D	11	0	7	0	0
3	A	85	0	0	4	0
3	B	66	0	0	3	0
3	C	86	0	0	2	0
3	D	85	0	0	3	0
All	All	8482	0	8443	139	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 8.

All (139) 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:249:LEU:C	1:B:249:LEU:HD23	1.99	0.88
1:C:59:ILE:HD11	1:C:104:GLU:HB2	1.71	0.73
1:D:43:LEU:HD12	1:D:43:LEU:C	2.15	0.71
1:A:73:ILE:HG23	1:A:76:ILE:HB	1.74	0.70
1:C:60:LYS:HA	1:C:60:LYS:HE2	1.73	0.69
1:B:191:GLU:HG3	1:B:195:ILE:HD12	1.72	0.69
1:A:10:ILE:HD11	3:A:266:HOH:O	1.94	0.67
1:D:120:MET:HE2	1:D:120:MET:HA	1.76	0.67
1:A:73:ILE:CG2	1:A:76:ILE:HB	2.25	0.66
1:A:70:ARG:NH2	1:A:112:ASP:OD2	2.28	0.66
1:B:73:ILE:O	1:B:73:ILE:HG13	1.96	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:249:LEU:HD11	1:B:238:ILE:HG23	1.79	0.65
1:B:45:ILE:HD12	1:B:224:LEU:HD11	1.80	0.64
1:B:92:LEU:HD12	1:B:92:LEU:O	1.99	0.63
1:A:43:LEU:C	1:A:43:LEU:HD12	2.23	0.62
1:C:211[A]:VAL:HG21	1:D:250:LEU:HD22	1.81	0.62
1:A:232:VAL:HG13	1:A:234:ALA:O	2.00	0.62
1:C:204:MET:HE3	3:C:276:HOH:O	1.99	0.62
1:B:141:ILE:HD12	1:B:167:ALA:HB2	1.81	0.61
1:A:141:ILE:HD12	1:A:167:ALA:HB2	1.82	0.61
1:B:249:LEU:C	1:B:249:LEU:CD2	2.70	0.61
1:C:211[B]:VAL:HG11	1:D:250:LEU:HD22	1.82	0.61
1:B:134:LYS:HE3	1:B:134:LYS:CA	2.30	0.60
1:C:35:ALA:HB2	1:C:69:LEU:CD1	2.32	0.60
1:C:59:ILE:HD11	1:C:104:GLU:CB	2.32	0.59
1:B:134:LYS:HE3	1:B:134:LYS:HA	1.83	0.59
1:B:198:ASP:HB3	1:B:199:ARG:HE	1.68	0.58
1:D:73:ILE:HG13	1:D:73:ILE:O	2.02	0.58
1:B:66:LEU:HD11	1:B:105:ILE:HG23	1.85	0.58
1:B:232:VAL:HG12	1:B:237:GLN:HB2	1.85	0.58
1:C:212:ILE:HD13	1:D:216:CYS:HB3	1.86	0.58
1:B:134:LYS:HA	1:B:134:LYS:CE	2.34	0.58
1:A:92:LEU:C	1:A:92:LEU:HD23	2.29	0.57
1:A:95[A]:ARG:HG3	1:A:120:MET:HE3	1.86	0.57
1:C:67:TYR:CD1	1:C:110:LEU:HD11	2.40	0.57
1:C:70:ARG:NH2	1:C:112:ASP:OD2	2.37	0.57
1:B:67:TYR:CE1	1:B:110:LEU:HD11	2.40	0.56
1:C:208:GLY:O	1:C:211[A]:VAL:HG13	2.04	0.56
1:C:51:ASP:O	1:C:91[A]:LYS:HD2	2.05	0.56
1:A:232:VAL:HG22	1:A:237:GLN:HG3	1.86	0.56
1:B:219:ILE:HD13	3:B:263:HOH:O	2.06	0.56
1:A:24:ILE:H	1:A:24:ILE:HD13	1.71	0.55
1:C:183:LEU:HD21	1:D:220:PHE:CE1	2.41	0.55
1:D:74:HIS:ND1	1:D:75:ASP:OD1	2.39	0.55
1:A:199:ARG:HB2	1:A:200:PRO:CD	2.37	0.54
1:C:212:ILE:HD11	1:D:212:ILE:HG13	1.89	0.54
1:D:19:ILE:HD11	1:D:244:ASN:HA	1.89	0.54
1:D:43:LEU:HD12	1:D:43:LEU:O	2.08	0.54
1:A:60:LYS:O	1:A:64[A]:GLU:HG3	2.08	0.54
1:B:92:LEU:O	1:B:92:LEU:CD1	2.56	0.54
1:D:107:ASN:HA	1:D:135:LYS:HD3	1.89	0.54
1:B:234:ALA:HB2	2:B:301:DHS:H62	1.91	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:215:LEU:HD21	1:B:238:ILE:CD1	2.39	0.52
1:C:67:TYR:CE1	1:C:110:LEU:HD11	2.44	0.51
1:A:92:LEU:HD23	1:A:93:ILE:N	2.26	0.51
1:D:190:ASN:O	1:D:194:LYS:HG2	2.10	0.51
1:C:163:GLN:HG3	1:C:199:ARG:HD2	1.93	0.51
1:D:141:ILE:HD12	1:D:167:ALA:HB2	1.93	0.51
1:B:7:VAL:O	1:B:7:VAL:HG23	2.11	0.50
1:C:159:LEU:HB3	1:C:192:MET:HE2	1.92	0.50
1:C:249:LEU:HD21	1:D:238:ILE:HD12	1.94	0.50
1:B:59:ILE:HD13	1:B:104:GLU:HG3	1.94	0.50
1:B:123:GLU:HB2	3:B:269:HOH:O	2.12	0.49
1:D:129:VAL:HG22	1:D:139:VAL:HG11	1.94	0.49
1:B:115:ASP:OD1	1:B:115:ASP:C	2.56	0.49
1:A:73:ILE:HG22	1:A:73:ILE:O	2.13	0.49
1:C:102:ASN:O	1:C:106:SER:HB2	2.13	0.49
1:D:16:ARG:NH2	3:D:314:HOH:O	2.45	0.48
1:D:43:LEU:C	1:D:43:LEU:CD1	2.83	0.48
1:A:10:ILE:CD1	1:A:44:ASP:O	2.62	0.48
1:B:159:LEU:HD13	1:B:192:MET:HG3	1.96	0.47
1:B:249:LEU:HD23	1:B:249:LEU:O	2.11	0.47
1:B:70:ARG:HG3	1:B:110:LEU:HD22	1.96	0.47
1:C:95:ARG:HE	1:C:95:ARG:HB2	1.47	0.47
1:B:171:LYS:HA	1:B:202:ILE:O	2.15	0.47
1:D:208:GLY:O	1:D:211:VAL:HG23	2.14	0.47
1:B:43:LEU:C	1:B:43:LEU:HD12	2.40	0.47
1:D:77:PRO:HA	1:D:112:ASP:OD2	2.15	0.46
1:C:116:VAL:O	1:C:141:ILE:HA	2.16	0.46
1:B:111:VAL:CG1	1:B:113:LEU:O	2.63	0.46
1:C:216:CYS:HB3	1:D:212:ILE:HD13	1.97	0.46
1:C:62:VAL:HG12	1:C:105:ILE:HD11	1.97	0.46
1:B:153:GLU:HG3	3:B:257:HOH:O	2.16	0.46
1:A:116[B]:VAL:O	1:A:141:ILE:HA	2.16	0.46
1:D:199:ARG:HB2	1:D:200:PRO:CD	2.46	0.46
1:A:35:ALA:HB2	1:A:69:LEU:CD1	2.45	0.45
1:B:40:ASP:HB3	1:C:9:ASN:O	2.16	0.45
1:A:234:ALA:O	1:A:237:GLN:HG2	2.16	0.45
1:C:224:LEU:HD23	1:C:225:THR:N	2.31	0.45
1:D:2:LYS:NZ	1:D:193:PHE:O	2.49	0.45
1:A:116[A]:VAL:O	1:A:141:ILE:HA	2.17	0.44
1:C:242:GLU:CD	1:D:249:LEU:HD13	2.42	0.44
1:A:141:ILE:CD1	1:A:167:ALA:HB2	2.46	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:63:LYS:HD2	1:D:108:THR:HG22	1.99	0.44
1:A:24:ILE:HD13	1:A:34:GLU:OE1	2.18	0.44
1:B:84:SER:OG	1:B:117:GLU:OE1	2.30	0.43
1:B:38:LEU:HB3	1:B:43:LEU:HD21	1.99	0.43
1:B:77:PRO:HA	1:B:112:ASP:OD2	2.19	0.43
1:B:141:ILE:CD1	1:B:167:ALA:HB2	2.47	0.43
1:B:208:GLY:HA2	1:B:211:VAL:HG23	2.00	0.43
1:D:225:THR:HG23	1:D:243:LEU:HD21	2.00	0.43
1:B:159:LEU:CD1	1:B:192:MET:HG3	2.48	0.43
1:A:40:ASP:HB2	3:A:299:HOH:O	2.18	0.43
1:D:84:SER:OG	1:D:117:GLU:OE1	2.31	0.42
1:C:43:LEU:HD12	1:C:43:LEU:C	2.44	0.42
1:C:73:ILE:O	1:C:74:HIS:C	2.62	0.42
1:C:198:ASP:OD1	1:C:199:ARG:HG3	2.19	0.42
1:D:115:ASP:OD1	1:D:115:ASP:C	2.62	0.42
1:C:141:ILE:HD12	1:C:167:ALA:HB2	2.00	0.42
1:C:153:GLU:H	1:C:153:GLU:CD	2.27	0.42
1:A:212:ILE:HD11	1:B:212:ILE:HG12	2.02	0.42
1:A:154[A]:GLU:OE1	3:A:297[A]:HOH:O	2.22	0.42
1:B:19:ILE:HD11	1:B:244:ASN:HA	2.00	0.41
1:A:180:LYS:NZ	3:A:292:HOH:O	2.52	0.41
1:A:116[A]:VAL:CG2	1:A:128:VAL:HG11	2.50	0.41
1:B:70:ARG:NH1	1:B:73:ILE:O	2.52	0.41
1:D:118:LEU:HA	1:D:125:ILE:HD11	2.01	0.41
1:B:70:ARG:HA	1:B:70:ARG:HD3	1.86	0.41
1:A:250:LEU:HD21	1:B:215:LEU:HD11	2.02	0.41
1:C:67:TYR:CG	1:C:110:LEU:HD11	2.55	0.41
1:A:19:ILE:HD11	1:A:244:ASN:HA	2.02	0.41
1:A:21:VAL:HA	1:A:22:PRO:HD3	1.91	0.41
1:B:225:THR:HG21	1:B:247:LEU:HD11	2.03	0.41
1:D:63:LYS:HD2	1:D:108:THR:CG2	2.51	0.41
1:A:199:ARG:HB2	1:A:200:PRO:HD3	2.02	0.41
1:C:219:ILE:HG12	3:C:282:HOH:O	2.19	0.41
1:A:24:ILE:HD13	1:A:24:ILE:N	2.34	0.41
1:B:67:TYR:CD1	1:B:110:LEU:HD11	2.56	0.41
1:D:67:TYR:CE1	1:D:110:LEU:HD11	2.56	0.41
1:A:9:ASN:O	1:D:40:ASP:OD1	2.39	0.40
1:A:199:ARG:CB	1:A:200:PRO:CD	2.99	0.40
1:C:105:ILE:HD13	1:C:105:ILE:HA	1.95	0.40
1:C:21:VAL:HA	1:C:22:PRO:HD3	1.92	0.40
1:C:86:VAL:O	1:C:86:VAL:HG12	2.20	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:212:ILE:HB	3:D:332:HOH:O	2.20	0.40
1:A:180:LYS:O	1:A:184:VAL:HG23	2.21	0.40
1:A:249:LEU:HD11	1:B:238:ILE:CG2	2.49	0.40
1:B:50:VAL:HG11	1:B:80:PHE:CZ	2.56	0.40
1:D:91:LYS:HG3	3:D:264:HOH:O	2.20	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	256/258 (99%)	249 (97%)	6 (2%)	1 (0%)	30	34
1	B	253/258 (98%)	245 (97%)	8 (3%)	0	100	100
1	C	253/258 (98%)	248 (98%)	4 (2%)	1 (0%)	30	34
1	D	252/258 (98%)	246 (98%)	6 (2%)	0	100	100
All	All	1014/1032 (98%)	988 (97%)	24 (2%)	2 (0%)	43	51

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	74	HIS
1	C	74	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	233/232 (100%)	227 (97%)	6 (3%)	40	55
1	B	230/232 (99%)	226 (98%)	4 (2%)	53	69
1	C	230/232 (99%)	228 (99%)	2 (1%)	70	84
1	D	229/232 (99%)	228 (100%)	1 (0%)	84	92
All	All	922/928 (99%)	909 (99%)	13 (1%)	59	75

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

Mol	Chain	Res	Type
1	A	24	ILE
1	A	33	LYS
1	A	92	LEU
1	A	199	ARG
1	A	232	VAL
1	A	252	LYS
1	B	92	LEU
1	B	134	LYS
1	B	224	LEU
1	B	249	LEU
1	C	95	ARG
1	C	153	GLU
1	D	91	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	107	ASN
1	D	107	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](#)

4 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	DHS	C	301	1	11,11,12	1.20	1 (9%)	13,15,17	1.34	1 (7%)
2	DHS	A	301	1	11,11,12	0.96	0	13,15,17	1.50	3 (23%)
2	DHS	D	301	1	11,11,12	1.05	0	13,15,17	1.21	2 (15%)
2	DHS	B	301	1	11,11,12	0.69	0	13,15,17	1.73	4 (30%)

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	DHS	C	301	1	-	4/4/17/20	0/1/1/1
2	DHS	A	301	1	1/1/4/6	4/4/17/20	0/1/1/1
2	DHS	D	301	1	-	4/4/17/20	0/1/1/1
2	DHS	B	301	1	-	4/4/17/20	0/1/1/1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	301	DHS	C3-C4	2.82	1.55	1.52

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	301	DHS	O4-C7-C1	3.54	122.92	115.43
2	A	301	DHS	O4-C7-C1	2.95	121.66	115.43
2	C	301	DHS	O4-C7-C1	2.82	121.38	115.43
2	B	301	DHS	O5-C7-C1	-2.59	117.09	121.64
2	D	301	DHS	O5-C7-C1	-2.57	117.13	121.64
2	A	301	DHS	O5-C7-C1	-2.33	117.55	121.64
2	B	301	DHS	C3-C4-C5	2.31	113.63	110.69
2	D	301	DHS	O4-C7-C1	2.29	120.28	115.43
2	B	301	DHS	C5-C6-C1	2.18	115.97	111.77
2	A	301	DHS	O3-C5-C6	-2.05	104.84	109.38

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
2	A	301	DHS	C3

All (16) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	301	DHS	C6-C1-C7-O4
2	A	301	DHS	C6-C1-C7-O5
2	A	301	DHS	C2-C1-C7-O4
2	A	301	DHS	C2-C1-C7-O5
2	B	301	DHS	C6-C1-C7-O4
2	B	301	DHS	C6-C1-C7-O5
2	B	301	DHS	C2-C1-C7-O4
2	B	301	DHS	C2-C1-C7-O5
2	C	301	DHS	C6-C1-C7-O4
2	C	301	DHS	C6-C1-C7-O5
2	C	301	DHS	C2-C1-C7-O4
2	C	301	DHS	C2-C1-C7-O5
2	D	301	DHS	C6-C1-C7-O4
2	D	301	DHS	C6-C1-C7-O5
2	D	301	DHS	C2-C1-C7-O4
2	D	301	DHS	C2-C1-C7-O5

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	301	DHS	1	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	253/258 (98%)	-1.42	0 100 100	8, 24, 34, 50	5 (1%)
1	B	253/258 (98%)	-1.33	0 100 100	12, 28, 39, 57	2 (0%)
1	C	253/258 (98%)	-1.46	0 100 100	11, 24, 33, 45	2 (0%)
1	D	253/258 (98%)	-1.42	0 100 100	15, 27, 38, 56	1 (0%)
All	All	1012/1032 (98%)	-1.41	0 100 100	8, 26, 37, 57	10 (0%)

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
2	DHS	B	301	11/12	0.98	0.06	31,38,40,40	11
2	DHS	D	301	11/12	0.98	0.04	30,36,39,40	11
2	DHS	C	301	11/12	0.99	0.03	31,36,39,40	0
2	DHS	A	301	11/12	0.99	0.03	35,38,41,43	0

6.5 Other polymers [i](#)

There are no such residues in this entry.