



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 12:01 PM GMT

PDB ID : 3QQP  
Title : Crystal Structure of 11beta-Hydroxysteroid Dehydrogenase 1 (11b-HSD1) in Complex with Urea Inhibitor  
Authors : Loenze, P.; Schimanski-Breves, S.; Engel, C.K.  
Deposited on : 2011-02-16  
Resolution : 2.72 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](mailto:validation@mail.wwpdb.org)  
A user guide is available at  
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>  
with specific help available everywhere you see the ⓘ symbol.

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The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467  
Mogul : 1.7 (RC4), CSD as536be (2015)  
Xtriage (Phenix) : 1.9-1692  
EDS : rb-20026688  
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)  
Refmac : 5.8.0135  
CCP4 : 6.5.0  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : trunk26865

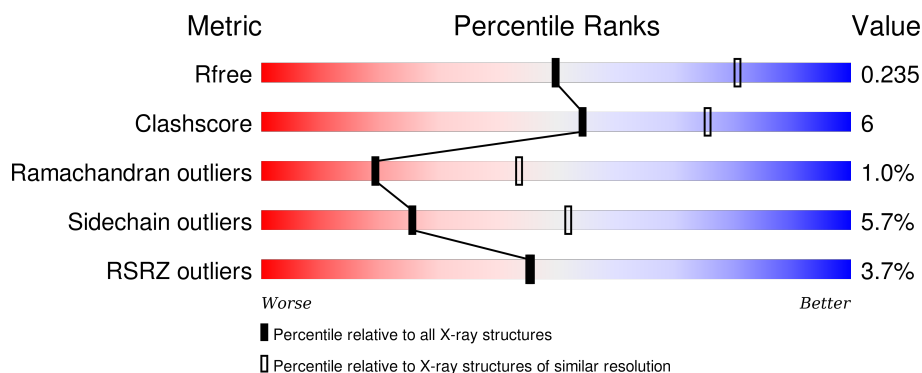
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.72 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))
$R_{free}$	91344	2439 (2.74-2.70)
Clashscore	102246	2771 (2.74-2.70)
Ramachandran outliers	100387	2726 (2.74-2.70)
Sidechain outliers	100360	2727 (2.74-2.70)
RSRZ outliers	91569	2443 (2.74-2.70)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria. 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	286	<div> <div>5%</div> <div>81% 14% 6%</div> </div>
1	B	286	<div> <div>5%</div> <div>78% 13% 7%</div> </div>
1	C	286	<div> <div>2%</div> <div>78% 12% 8%</div> </div>
1	D	286	<div> <div>2%</div> <div>77% 13% 10%</div> </div>

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	S05	A	1	-	-	-	X
2	S05	B	2	-	-	-	X
2	S05	C	3	-	-	-	X

## 2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 8650 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 Corticosteroid 11-beta-dehydrogenase isozyme 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	270	Total	C	N	O	S	0	5	0
			2092	1332	353	391	16			
1	B	266	Total	C	N	O	S	0	7	0
			2074	1322	350	386	16			
1	C	262	Total	C	N	O	S	0	3	0
			2020	1288	343	374	15			
1	D	258	Total	C	N	O	S	0	5	0
			1985	1261	338	371	15			

There are 72 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	7	MET	-	EXPRESSION TAG	UNP P28845
A	8	LYS	-	EXPRESSION TAG	UNP P28845
A	9	HIS	-	EXPRESSION TAG	UNP P28845
A	10	GLN	-	EXPRESSION TAG	UNP P28845
A	11	HIS	-	EXPRESSION TAG	UNP P28845
A	12	GLN	-	EXPRESSION TAG	UNP P28845
A	13	HIS	-	EXPRESSION TAG	UNP P28845
A	14	GLN	-	EXPRESSION TAG	UNP P28845
A	15	HIS	-	EXPRESSION TAG	UNP P28845
A	16	GLN	-	EXPRESSION TAG	UNP P28845
A	17	HIS	-	EXPRESSION TAG	UNP P28845
A	18	GLN	-	EXPRESSION TAG	UNP P28845
A	19	HIS	-	EXPRESSION TAG	UNP P28845
A	20	GLN	-	EXPRESSION TAG	UNP P28845
A	21	GLN	-	EXPRESSION TAG	UNP P28845
A	22	PRO	-	EXPRESSION TAG	UNP P28845
A	23	LEU	-	EXPRESSION TAG	UNP P28845
A	272	SER	CYS	ENGINEERED MUTATION	UNP P28845
B	7	MET	-	EXPRESSION TAG	UNP P28845
B	8	LYS	-	EXPRESSION TAG	UNP P28845
B	9	HIS	-	EXPRESSION TAG	UNP P28845

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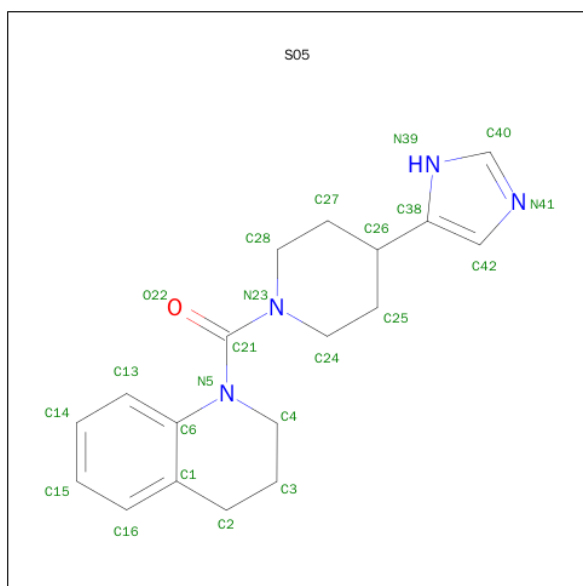
Chain	Residue	Modelled	Actual	Comment	Reference
B	10	GLN	-	EXPRESSION TAG	UNP P28845
B	11	HIS	-	EXPRESSION TAG	UNP P28845
B	12	GLN	-	EXPRESSION TAG	UNP P28845
B	13	HIS	-	EXPRESSION TAG	UNP P28845
B	14	GLN	-	EXPRESSION TAG	UNP P28845
B	15	HIS	-	EXPRESSION TAG	UNP P28845
B	16	GLN	-	EXPRESSION TAG	UNP P28845
B	17	HIS	-	EXPRESSION TAG	UNP P28845
B	18	GLN	-	EXPRESSION TAG	UNP P28845
B	19	HIS	-	EXPRESSION TAG	UNP P28845
B	20	GLN	-	EXPRESSION TAG	UNP P28845
B	21	GLN	-	EXPRESSION TAG	UNP P28845
B	22	PRO	-	EXPRESSION TAG	UNP P28845
B	23	LEU	-	EXPRESSION TAG	UNP P28845
B	272	SER	CYS	ENGINEERED MUTATION	UNP P28845
C	7	MET	-	EXPRESSION TAG	UNP P28845
C	8	LYS	-	EXPRESSION TAG	UNP P28845
C	9	HIS	-	EXPRESSION TAG	UNP P28845
C	10	GLN	-	EXPRESSION TAG	UNP P28845
C	11	HIS	-	EXPRESSION TAG	UNP P28845
C	12	GLN	-	EXPRESSION TAG	UNP P28845
C	13	HIS	-	EXPRESSION TAG	UNP P28845
C	14	GLN	-	EXPRESSION TAG	UNP P28845
C	15	HIS	-	EXPRESSION TAG	UNP P28845
C	16	GLN	-	EXPRESSION TAG	UNP P28845
C	17	HIS	-	EXPRESSION TAG	UNP P28845
C	18	GLN	-	EXPRESSION TAG	UNP P28845
C	19	HIS	-	EXPRESSION TAG	UNP P28845
C	20	GLN	-	EXPRESSION TAG	UNP P28845
C	21	GLN	-	EXPRESSION TAG	UNP P28845
C	22	PRO	-	EXPRESSION TAG	UNP P28845
C	23	LEU	-	EXPRESSION TAG	UNP P28845
C	272	SER	CYS	ENGINEERED MUTATION	UNP P28845
D	7	MET	-	EXPRESSION TAG	UNP P28845
D	8	LYS	-	EXPRESSION TAG	UNP P28845
D	9	HIS	-	EXPRESSION TAG	UNP P28845
D	10	GLN	-	EXPRESSION TAG	UNP P28845
D	11	HIS	-	EXPRESSION TAG	UNP P28845
D	12	GLN	-	EXPRESSION TAG	UNP P28845
D	13	HIS	-	EXPRESSION TAG	UNP P28845
D	14	GLN	-	EXPRESSION TAG	UNP P28845
D	15	HIS	-	EXPRESSION TAG	UNP P28845

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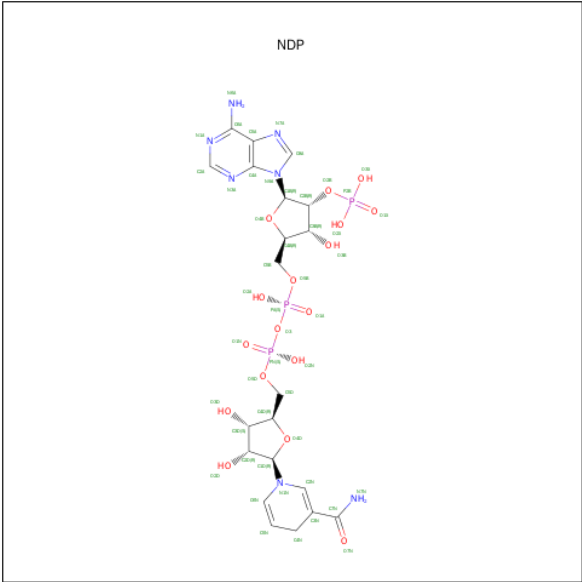
Chain	Residue	Modelled	Actual	Comment	Reference
D	16	GLN	-	EXPRESSION TAG	UNP P28845
D	17	HIS	-	EXPRESSION TAG	UNP P28845
D	18	GLN	-	EXPRESSION TAG	UNP P28845
D	19	HIS	-	EXPRESSION TAG	UNP P28845
D	20	GLN	-	EXPRESSION TAG	UNP P28845
D	21	GLN	-	EXPRESSION TAG	UNP P28845
D	22	PRO	-	EXPRESSION TAG	UNP P28845
D	23	LEU	-	EXPRESSION TAG	UNP P28845
D	272	SER	CYS	ENGINEERED MUTATION	UNP P28845

- Molecule 2 is 3,4-DIHYDROQUINOLIN-1(2H)-YL[4-(1H-IMIDAZOL-5-YL)PIPERIDIN-1-YL]METHANONE (three-letter code: S05) (formula: C<sub>18</sub>H<sub>22</sub>N<sub>4</sub>O).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	N	O	0	0
			23	18	4	1		
2	B	1	Total	C	N	O	0	0
			23	18	4	1		
2	C	1	Total	C	N	O	0	0
			23	18	4	1		
2	D	1	Total	C	N	O	0	0
			23	18	4	1		

- Molecule 3 is NADPH DIHYDRO-NICOTINAMIDE-ADENINE-DINUCLEOTIDE PHOSPHATE (three-letter code: NDP) (formula: C<sub>21</sub>H<sub>30</sub>N<sub>7</sub>O<sub>17</sub>P<sub>3</sub>).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	N	O	P	0	0
			48	21	7	17	3		
3	B	1	Total	C	N	O	P	0	0
			48	21	7	17	3		
3	C	1	Total	C	N	O	P	0	0
			48	21	7	17	3		
3	D	1	Total	C	N	O	P	0	0
			48	21	7	17	3		

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	63	Total	O	0	0
			63	63		
4	B	37	Total	O	0	0
			37	37		
4	C	57	Total	O	0	0
			57	57		
4	D	38	Total	O	0	0
			38	38		







## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	56.93 Å 153.38 Å 74.18 Å 90.00° 93.46° 90.00°	Depositor
Resolution (Å)	36.71 – 2.72 74.04 – 2.72	Depositor EDS
% Data completeness (in resolution range)	99.8 (36.71-2.72) 99.8 (74.04-2.72)	Depositor EDS
$R_{merge}$	0.12	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	4.08 (at 2.73 Å)	Xtriage
Refinement program	BUSTER 2.9.7	Depositor
R, $R_{free}$	0.164 , 0.234 0.169 , 0.235	Depositor DCC
$R_{free}$ test set	1683 reflections (5.20%)	DCC
Wilson B-factor (Å <sup>2</sup> )	25.9	Xtriage
Anisotropy	0.616	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.33 , 47.5	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.31$	Xtriage
Outliers	0 of 34037 reflections	Xtriage
$F_o, F_c$ correlation	0.93	EDS
Total number of atoms	8650	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	29.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.82% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical values of  $\langle |L| \rangle$ ,  $\langle L^2 \rangle$  for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 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: NDP, S05

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	0.50	0/2148	0.70	0/2900
1	B	0.49	0/2134	0.70	0/2882
1	C	0.49	0/2067	0.70	0/2791
1	D	0.48	0/2037	0.70	0/2750
All	All	0.49	0/8386	0.70	0/11323

There are no bond length outliers.

There are no bond angle outliers.

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	2092	0	2128	17	0
1	B	2074	0	2110	51	0
1	C	2020	0	2064	26	0
1	D	1985	0	2031	29	0
2	A	23	0	22	0	0
2	B	23	0	22	0	0
2	C	23	0	22	1	0
2	D	23	0	22	0	0
3	A	48	0	26	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	B	48	0	26	3	0
3	C	48	0	26	2	0
3	D	48	0	26	9	0
4	A	63	0	0	1	0
4	B	37	0	0	1	0
4	C	57	0	0	0	0
4	D	38	0	0	0	0
All	All	8650	0	8525	108	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 6.

All (108) 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:274:LYS:HD2	1:D:266:LEU:HD13	1.21	1.15
1:B:278:PHE:CD2	1:B:279:LEU:CD2	2.30	1.14
1:C:265:THR:O	1:C:268:ILE:HG22	1.64	0.98
1:B:278:PHE:CD2	1:B:279:LEU:HD22	1.97	0.97
1:B:274:LYS:HE3	1:D:266:LEU:HD22	1.53	0.90
1:B:279:LEU:HD23	1:B:279:LEU:H	1.39	0.88
1:C:265:THR:O	1:C:268:ILE:CG2	2.22	0.88
1:B:274:LYS:HD2	1:D:266:LEU:CD1	2.02	0.87
1:B:275:ILE:HG23	1:B:279:LEU:HG	1.61	0.81
1:B:279:LEU:O	1:B:280:TYR:CD2	2.33	0.81
1:C:214:VAL:HG11	1:C:268:ILE:CD1	2.11	0.81
1:B:278:PHE:CD2	1:B:279:LEU:HD21	2.15	0.79
1:B:121:ILE:HG12	3:B:293:NDP:H3D	1.64	0.79
1:B:263:TRP:HD1	1:B:263:TRP:H	1.25	0.79
1:B:271:PRO:HA	1:B:274:LYS:HG2	1.65	0.78
1:B:263:TRP:CD1	1:B:263:TRP:N	2.51	0.77
1:B:279:LEU:HD23	1:B:279:LEU:N	2.00	0.76
1:C:257:TYR:CE2	1:C:268:ILE:HG12	2.20	0.76
1:B:261:SER:O	1:B:262:LEU:HD23	1.85	0.75
1:B:274:LYS:CE	1:D:266:LEU:HD22	2.18	0.74
1:B:279:LEU:N	1:B:279:LEU:CD2	2.50	0.73
1:C:214:VAL:HG11	1:C:268:ILE:HD11	1.74	0.70
1:B:278:PHE:CE2	1:B:279:LEU:HD22	2.29	0.68
1:D:155:LEU:HD21	1:D:201:TYR:OH	1.94	0.68
1:C:257:TYR:CD2	1:C:268:ILE:HG12	2.30	0.67
1:C:265:THR:C	1:C:268:ILE:HG22	2.16	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:155:LEU:HD21	1:C:201:TYR:OH	1.97	0.64
1:B:278:PHE:O	1:B:280:TYR:N	2.30	0.62
1:A:151:THR:HG23	1:A:165:ILE:HD13	1.85	0.58
1:C:248:GLY:HA3	1:C:256:VAL:HG21	1.85	0.58
1:B:204:SER:HB2	1:B:206:VAL:HG23	1.86	0.58
1:B:271:PRO:O	1:B:274:LYS:HG3	2.05	0.56
1:D:170:SER:CB	3:D:293:NDP:H5N	2.35	0.56
1:B:279:LEU:CD2	1:B:279:LEU:H	2.11	0.56
1:A:265:THR:O	1:A:268:ILE:HG22	2.06	0.55
1:C:149:VAL:HG22	1:D:133:ILE:HD12	1.87	0.55
1:B:278:PHE:C	1:B:280:TYR:H	2.09	0.55
1:B:68:LYS:O	1:B:72[B]:GLN:HB3	2.07	0.54
1:B:278:PHE:CE2	1:B:279:LEU:CD2	2.87	0.54
1:B:261:SER:C	1:B:262:LEU:HD23	2.27	0.53
1:B:216:GLY:O	3:B:293:NDP:H42N	2.09	0.53
1:A:193:PHE:HB2	1:B:185:ALA:HB2	1.90	0.53
1:D:126:LEU:HD11	1:D:227:VAL:HG12	1.92	0.52
1:B:278:PHE:HD2	1:B:279:LEU:HD21	1.69	0.52
1:A:149:VAL:HG22	1:B:133:ILE:HD13	1.91	0.52
1:D:170:SER:HB3	3:D:293:NDP:C5N	2.41	0.51
1:B:278:PHE:HD2	1:B:279:LEU:CD2	2.12	0.51
1:D:170:SER:HB3	3:D:293:NDP:H5N	1.93	0.50
1:D:119:ASN:HD22	1:D:168:VAL:HG21	1.76	0.50
1:D:243:LEU:HG	1:D:247:LYS:HE3	1.92	0.49
1:D:119:ASN:ND2	3:D:293:NDP:H4D	2.28	0.49
1:C:216:GLY:O	3:C:293:NDP:H42N	2.12	0.49
1:A:248:GLY:HA3	1:A:256:VAL:HG21	1.95	0.49
1:D:240:GLU:O	1:D:244:GLU:HG2	2.13	0.49
1:C:278:PHE:HD2	1:C:278:PHE:C	2.16	0.49
1:B:278:PHE:C	1:B:278:PHE:CD1	2.86	0.48
1:B:278:PHE:CG	1:B:279:LEU:CD2	2.93	0.48
1:D:121:ILE:HG12	3:D:293:NDP:H3D	1.95	0.48
1:C:278:PHE:CD2	1:C:278:PHE:C	2.87	0.48
1:B:40:THR:O	1:B:119:ASN:HB3	2.15	0.47
1:B:275:ILE:HD11	1:D:266:LEU:HB2	1.95	0.47
1:A:267:LEU:O	1:B:272:SER:HB3	2.15	0.47
1:A:279:LEU:HD22	1:C:263:TRP:CD1	2.50	0.47
1:C:214:VAL:HG11	1:C:268:ILE:HD13	1.94	0.47
1:B:278:PHE:CG	1:B:279:LEU:HD22	2.49	0.46
1:A:264:THR:HG23	1:B:276:LEU:HD11	1.97	0.46
1:C:216:GLY:HA3	1:C:259:ASP:OD2	2.14	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:267:LEU:O	1:D:272:SER:HB3	2.16	0.46
1:B:279:LEU:O	1:B:280:TYR:CG	2.69	0.46
1:C:270:ASN:C	1:C:270:ASN:HD22	2.20	0.46
1:D:170:SER:HB3	3:D:293:NDP:C6N	2.45	0.46
1:C:278:PHE:HD2	1:C:278:PHE:O	1.99	0.46
1:D:37:VAL:HG13	1:D:115:MET:HB3	1.98	0.46
1:C:119:ASN:HD22	1:C:168:VAL:HG21	1.80	0.45
1:D:141:GLU:HA	1:D:145:LEU:HB2	1.97	0.45
1:B:263:TRP:N	1:B:263:TRP:HD1	1.97	0.45
1:B:126:LEU:HD23	1:B:180:VAL:HG13	1.98	0.45
2:C:3:S05:H4A	3:C:293:NDP:H41N	1.99	0.45
1:C:42:ALA:HB3	1:C:63:VAL:HB	1.98	0.44
1:B:119:ASN:ND2	3:B:293:NDP:H4D	2.32	0.44
1:B:36:LYS:HG2	1:B:110:MET:HB3	2.00	0.44
1:B:278:PHE:C	1:B:280:TYR:N	2.71	0.43
1:C:270:ASN:ND2	1:C:273:ARG:H	2.16	0.43
1:C:230:ILE:HD12	1:C:231:VAL:O	2.18	0.43
1:A:284:TYR:HB3	1:B:231:VAL:HG22	2.01	0.43
1:B:274:LYS:CD	1:D:266:LEU:HD13	2.15	0.42
1:A:144:PHE:O	1:A:147:TYR:HB2	2.19	0.42
1:A:119:ASN:HD22	1:A:168:VAL:HG21	1.84	0.42
1:D:216:GLY:O	3:D:293:NDP:H42N	2.19	0.42
1:D:130:HIS:O	1:D:131:ASP:HB2	2.19	0.42
1:C:148:VAL:HG13	1:C:193:PHE:CZ	2.54	0.42
1:D:170:SER:HB3	3:D:293:NDP:H6N	2.02	0.41
1:A:133:ILE:HD11	1:B:152:VAL:HG21	2.02	0.41
1:A:155:LEU:HD12	1:A:155:LEU:HA	1.88	0.41
1:D:243:LEU:HA	1:D:246:ILE:HD12	2.01	0.41
1:B:28:ARG:HG2	1:B:31:MET:HG3	2.02	0.41
1:A:37:VAL:HG22	1:A:115:MET:HB3	2.03	0.41
1:D:20:GLN:HG2	1:D:254:GLU:HG2	2.02	0.41
1:A:215:LEU:HD11	1:A:245:ILE:HD11	2.03	0.41
1:D:131:ASP:O	1:D:133:ILE:N	2.54	0.41
1:A:216:GLY:HA3	1:A:259:ASP:OD2	2.20	0.41
1:C:155:LEU:N	1:C:156:PRO:CD	2.84	0.41
1:D:170:SER:HB2	3:D:293:NDP:H5N	2.02	0.41
4:A:337:HOH:O	1:B:273:ARG:NH1	2.53	0.41
1:B:87:HIS:HD2	4:B:299:HOH:O	2.04	0.40
1:D:198:ARG:NH2	1:D:254:GLU:O	2.55	0.40
1:C:123:ASN:H	1:C:123:ASN:ND2	2.19	0.40
1:A:137:ARG:HH22	1:B:96:MET:HG3	1.87	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	273/286 (96%)	261 (96%)	10 (4%)	2 (1%)	26	54
1	B	271/286 (95%)	247 (91%)	20 (7%)	4 (2%)	13	31
1	C	263/286 (92%)	251 (95%)	10 (4%)	2 (1%)	24	50
1	D	261/286 (91%)	247 (95%)	12 (5%)	2 (1%)	24	50
All	All	1068/1144 (93%)	1006 (94%)	52 (5%)	10 (1%)	19	47

All (10) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	280	TYR
1	B	279	LEU
1	D	132	ASP
1	D	219	ASP
1	A	287	ASP
1	A	219	ASP
1	C	67	SER
1	B	219	ASP
1	B	264	THR
1	C	219	ASP

### 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	232/243 (96%)	220 (95%)	12 (5%)	29	56
1	B	230/243 (95%)	216 (94%)	14 (6%)	23	48
1	C	222/243 (91%)	208 (94%)	14 (6%)	22	47
1	D	220/243 (90%)	209 (95%)	11 (5%)	30	59
All	All	904/972 (93%)	853 (94%)	51 (6%)	25	53

All (51) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	23	LEU
1	A	145	LEU
1	A	160	GLN
1	A	184	SER
1	A	221	GLU
1	A	230	ILE
1	A	262	LEU
1	A	269	ARG
1	A	270	ASN
1	A	274	LYS
1	A	288	ARG
1	A	289	PHE
1	B	21	GLN
1	B	108	LYS
1	B	121	ILE
1	B	145	LEU
1	B	184	SER
1	B	202	SER
1	B	204	SER
1	B	228	SER
1	B	263	TRP
1	B	268	ILE
1	B	270	ASN
1	B	274	LYS
1	B	279	LEU
1	B	284	TYR
1	C	21	GLN
1	C	124	THR
1	C	138	LYS
1	C	145	LEU
1	C	225	LYS
1	C	230	ILE
1	C	233	MET

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Mol	Chain	Res	Type
1	C	239	GLU
1	C	262	LEU
1	C	268	ILE
1	C	269	ARG
1	C	270	ASN
1	C	278	PHE
1	C	279	LEU
1	D	76[A]	SER
1	D	76[B]	SER
1	D	108	LYS
1	D	109	LEU
1	D	155	LEU
1	D	160	GLN
1	D	255	GLU
1	D	269	ARG
1	D	270	ASN
1	D	274	LYS
1	D	276	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (17) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	33	GLN
1	A	87	HIS
1	A	119	ASN
1	A	127	ASN
1	A	234	GLN
1	B	87	HIS
1	B	119	ASN
1	B	127	ASN
1	B	270	ASN
1	C	119	ASN
1	C	123	ASN
1	C	135	HIS
1	C	270	ASN
1	D	105	GLN
1	D	119	ASN
1	D	160	GLN
1	D	270	ASN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

## 5.6 Ligand geometry ⓘ

8 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	S05	A	1	-	22,26,26	1.23	3 (13%)	29,36,36	1.72	6 (20%)
3	NDP	A	293	-	42,52,52	1.30	3 (7%)	55,80,80	1.39	9 (16%)
2	S05	B	2	-	22,26,26	1.06	2 (9%)	29,36,36	1.51	5 (17%)
3	NDP	B	293	-	42,52,52	1.17	2 (4%)	55,80,80	1.41	6 (10%)
3	NDP	C	293	-	42,52,52	1.27	4 (9%)	55,80,80	1.24	4 (7%)
2	S05	C	3	-	22,26,26	1.22	4 (18%)	29,36,36	1.59	7 (24%)
3	NDP	D	293	-	42,52,52	1.01	1 (2%)	55,80,80	1.28	6 (10%)
2	S05	D	4	-	22,26,26	1.21	3 (13%)	29,36,36	1.57	6 (20%)

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	S05	A	1	-	-	0/9/32/32	0/4/4/4
3	NDP	A	293	-	-	0/30/77/77	0/5/5/5
2	S05	B	2	-	-	0/9/32/32	1/4/4/4
3	NDP	B	293	-	-	0/30/77/77	0/5/5/5
3	NDP	C	293	-	-	0/30/77/77	0/5/5/5
2	S05	C	3	-	-	0/9/32/32	1/4/4/4
3	NDP	D	293	-	-	0/30/77/77	0/5/5/5
2	S05	D	4	-	-	0/9/32/32	0/4/4/4

All (22) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	293	NDP	P2B-O2B	2.00	1.66	1.60
2	B	2	S05	C28-N23	2.07	1.50	1.47
3	C	293	NDP	C7N-N7N	2.07	1.39	1.33
2	D	4	S05	C4-N5	2.07	1.51	1.47
2	B	2	S05	C24-N23	2.07	1.50	1.47
3	A	293	NDP	C2A-N1A	2.13	1.37	1.33
2	A	1	S05	C28-N23	2.14	1.50	1.47
2	C	3	S05	C2-C1	2.14	1.55	1.51
2	C	3	S05	C28-N23	2.17	1.50	1.47
2	C	3	S05	C4-N5	2.32	1.51	1.47
2	D	4	S05	C24-N23	2.33	1.51	1.47
3	B	293	NDP	O4B-C1B	2.33	1.44	1.41
2	D	4	S05	C2-C1	2.37	1.55	1.51
2	A	1	S05	C4-N5	2.52	1.51	1.47
2	C	3	S05	C6-N5	2.72	1.46	1.41
2	A	1	S05	C24-N23	3.09	1.52	1.47
3	B	293	NDP	C2A-N3A	3.11	1.37	1.32
3	C	293	NDP	C2A-N3A	3.37	1.38	1.32
3	D	293	NDP	C2A-N3A	3.68	1.38	1.32
3	A	293	NDP	C2A-N3A	4.14	1.39	1.32
3	A	293	NDP	O4B-C1B	4.40	1.46	1.41
3	C	293	NDP	O4B-C1B	5.20	1.47	1.41

All (49) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	293	NDP	O2B-P2B-O1X	-5.01	94.61	107.11
2	B	2	S05	O22-C21-N23	-3.27	116.45	123.72
3	B	293	NDP	N3A-C2A-N1A	-3.25	126.40	128.89
3	A	293	NDP	O3B-C3B-C4B	-3.25	101.30	111.05
2	A	1	S05	O22-C21-N23	-3.17	116.68	123.72

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	293	NDP	N3A-C2A-N1A	-2.83	126.73	128.89
2	D	4	S05	O22-C21-N23	-2.69	117.73	123.72
2	C	3	S05	O22-C21-N23	-2.69	117.75	123.72
3	B	293	NDP	O3-PN-O5D	-2.68	95.81	102.94
3	D	293	NDP	O2B-P2B-O1X	-2.43	101.03	107.11
3	C	293	NDP	O3-PA-O5B	-2.35	96.71	102.94
3	A	293	NDP	C4D-O4D-C1D	-2.32	104.41	109.52
2	D	4	S05	C42-C38-C26	-2.26	126.18	129.28
2	A	1	S05	C42-C38-C26	-2.17	126.29	129.28
3	A	293	NDP	C2D-C3D-C4D	-2.08	98.34	102.61
3	A	293	NDP	C2D-C1D-N1N	-2.06	107.78	113.34
3	C	293	NDP	C4B-O4B-C1B	-2.04	107.48	109.72
3	C	293	NDP	O5B-C5B-C4B	-2.04	101.60	109.12
2	B	2	S05	C28-C27-C26	2.00	113.53	110.97
2	B	2	S05	C27-C26-C25	2.05	113.85	109.31
3	B	293	NDP	O4B-C1B-N9A	2.11	112.52	108.10
2	D	4	S05	C27-C26-C25	2.12	113.99	109.31
2	C	3	S05	C2-C1-C6	2.15	123.82	119.44
3	D	293	NDP	O2N-PN-O1N	2.15	124.16	112.53
3	A	293	NDP	O2N-PN-O1N	2.18	124.36	112.53
2	A	1	S05	C27-C26-C25	2.18	114.14	109.31
3	A	293	NDP	O3D-C3D-C4D	2.20	117.64	111.05
3	D	293	NDP	O3X-P2B-O1X	2.23	117.77	110.58
2	C	3	S05	C42-N41-C40	2.25	109.27	105.71
3	A	293	NDP	O3X-P2B-O1X	2.30	117.99	110.58
2	C	3	S05	C28-C27-C26	2.42	114.07	110.97
3	D	293	NDP	C4A-C5A-N7A	2.50	111.78	109.48
3	C	293	NDP	O4D-C1D-N1N	2.61	113.58	108.07
2	C	3	S05	C27-C26-C25	2.65	115.17	109.31
3	A	293	NDP	O4D-C1D-N1N	2.71	113.78	108.07
2	A	1	S05	C24-C25-C26	2.75	114.48	110.97
2	B	2	S05	C24-C25-C26	2.76	114.50	110.97
2	D	4	S05	C28-C27-C26	2.80	114.55	110.97
2	C	3	S05	C24-C25-C26	2.81	114.56	110.97
2	D	4	S05	C24-C25-C26	2.94	114.72	110.97
3	B	293	NDP	O3X-P2B-O1X	3.04	120.37	110.58
3	B	293	NDP	O3X-P2B-O2X	3.20	119.57	107.38
2	A	1	S05	C25-C24-N23	3.32	115.89	111.07
3	D	293	NDP	O4D-C1D-N1N	3.56	115.59	108.07
2	C	3	S05	C28-N23-C24	3.67	119.36	112.56
2	B	2	S05	C28-N23-C24	3.86	119.72	112.56
3	A	293	NDP	C4A-C5A-N7A	4.07	113.22	109.48

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	4	S05	C28-N23-C24	4.38	120.68	112.56
2	A	1	S05	C28-N23-C24	5.17	122.15	112.56

There are no chirality outliers.

There are no torsion outliers.

All (2) ring outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	C	3	S05	C24-C25-C26-C27-C28-N23
2	B	2	S05	C24-C25-C26-C27-C28-N23

4 monomers are involved in 14 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	293	NDP	3	0
3	C	293	NDP	2	0
2	C	3	S05	1	0
3	D	293	NDP	9	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<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	270/286 (94%)	-0.14	13 (4%) 34 33	10, 23, 72, 100	0
1	B	266/286 (93%)	-0.14	14 (5%) 30 29	10, 25, 65, 113	0
1	C	262/286 (91%)	-0.29	5 (1%) 70 71	8, 20, 49, 62	0
1	D	258/286 (90%)	-0.07	7 (2%) 58 58	13, 29, 64, 87	0
All	All	1056/1144 (92%)	-0.16	39 (3%) 45 46	8, 24, 62, 113	0

All (39) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	279	LEU	6.0
1	A	229	GLY	5.3
1	B	280	TYR	5.0
1	A	284	TYR	4.4
1	B	263	TRP	4.2
1	D	263	TRP	4.2
1	C	263	TRP	4.1
1	B	285	ASN	3.7
1	C	279	LEU	3.6
1	D	23	LEU	3.4
1	A	263	TRP	3.4
1	B	20	GLN	3.2
1	B	284	TYR	3.2
1	A	233	MET	3.1
1	B	262	LEU	3.1
1	D	24	ASN	2.9
1	D	266	LEU	2.8
1	A	230	ILE	2.8
1	C	20	GLN	2.7
1	A	232	HIS	2.7
1	A	231	VAL	2.6

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Mol	Chain	Res	Type	RSRZ
1	A	24	ASN	2.6
1	A	23	LEU	2.5
1	A	279	LEU	2.4
1	B	267	LEU	2.4
1	B	276	LEU	2.4
1	B	282	THR	2.4
1	A	280	TYR	2.4
1	A	25	GLU	2.3
1	B	261	SER	2.3
1	D	61	VAL	2.2
1	C	265	THR	2.2
1	B	23	LEU	2.2
1	A	234	GLN	2.1
1	D	20	GLN	2.1
1	C	280	TYR	2.1
1	B	283	SER	2.0
1	D	21	GLN	2.0
1	B	266	LEU	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 carbohydrates 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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95<sup>th</sup> 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	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
2	S05	A	1	23/23	0.84	0.27	3.00	49,56,64,65	0
2	S05	B	2	23/23	0.85	0.27	2.58	55,64,67,67	0
2	S05	C	3	23/23	0.81	0.25	2.33	45,50,53,53	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
2	S05	D	4	23/23	0.88	0.26	1.55	56,60,62,62	0
3	NDP	C	293	48/48	0.99	0.12	-0.49	15,18,21,22	0
3	NDP	A	293	48/48	0.98	0.13	-0.50	15,17,18,19	0
3	NDP	B	293	48/48	0.98	0.13	-0.63	18,19,22,23	0
3	NDP	D	293	48/48	0.98	0.13	-0.91	18,23,26,27	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.