



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 08:02 AM GMT

PDB ID : 3D3E  
Title : Crystal Structure of Human 11-beta-Hydroxysteroid Dehydrogenase (HSD1)  
in Complex with Benzamide Inhibitor  
Authors : Wang, Z.; Sudom, A.; Liu, J.; Walker, N.P.  
Deposited on : 2008-05-09  
Resolution : 2.60 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

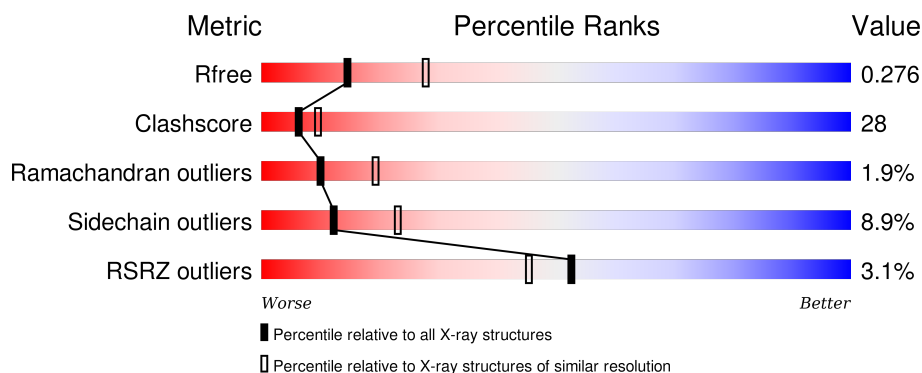
# 1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.60 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	2328 (2.60-2.60)
Clashscore	102246	2679 (2.60-2.60)
Ramachandran outliers	100387	2635 (2.60-2.60)
Sidechain outliers	100360	2635 (2.60-2.60)
RSRZ outliers	91569	2334 (2.60-2.60)

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>4%</div> <div>60% 27% 5% 8%</div> </div>
1	B	286	<div> <div>%</div> <div>60% 26% • 9%</div> </div>
1	C	286	<div> <div>4%</div> <div>58% 27% 6% 9%</div> </div>
1	D	286	<div> <div>3%</div> <div>57% 28% 5% 9%</div> </div>

## 2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 8318 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	262	Total	C	N	O	S	0	0	0
			2008	1282	338	374	14			
1	B	259	Total	C	N	O	S	0	0	0
			1983	1266	335	368	14			
1	C	259	Total	C	N	O	S	0	0	0
			1983	1266	335	368	14			
1	D	259	Total	C	N	O	S	0	0	0
			1983	1266	335	368	14			

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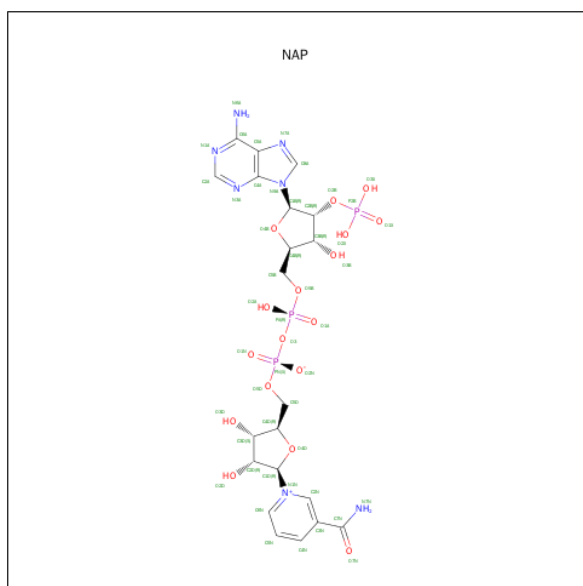
Chain	Residue	Modelled	Actual	Comment	Reference
B	10	GLN	-	EXPRESSION TAG	UNP P28845
B	11	HIS	-	EXPRESSION TAG	UNP P28845
B	12	GLN	-	EXPRESSION TAG	UNP P28845
B	13	HIS	-	EXPRESSION TAG	UNP P28845
B	14	GLN	-	EXPRESSION TAG	UNP P28845
B	15	HIS	-	EXPRESSION TAG	UNP P28845
B	16	GLN	-	EXPRESSION TAG	UNP P28845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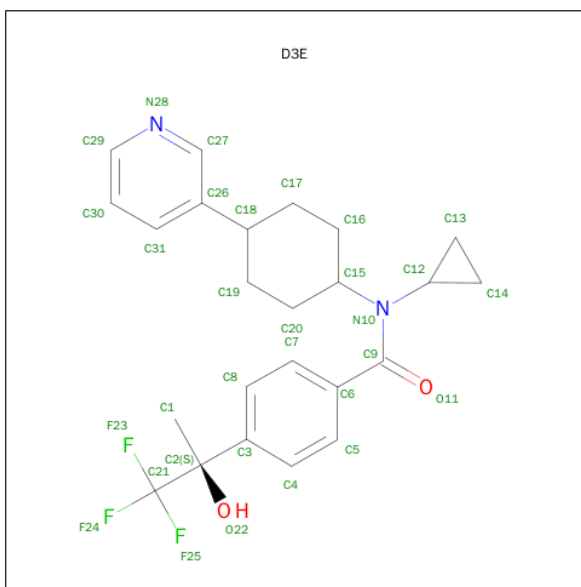
Chain	Residue	Modelled	Actual	Comment	Reference
D	16	GLN	-	EXPRESSION TAG	UNP P28845
D	17	HIS	-	EXPRESSION TAG	UNP P28845
D	18	GLN	-	EXPRESSION TAG	UNP P28845
D	19	HIS	-	EXPRESSION TAG	UNP P28845
D	20	GLN	-	EXPRESSION TAG	UNP P28845
D	21	GLN	-	EXPRESSION TAG	UNP P28845
D	22	PRO	-	EXPRESSION TAG	UNP P28845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

- Molecule 2 is NADP NICOTINAMIDE-ADENINE-DINUCLEOTIDE PHOSPHATE (three-letter code: NAP) (formula:  $C_{21}H_{28}N_7O_{17}P_3$ ).



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

- Molecule 3 is N-CYCLOPROPYL-N-(TRANS-4-PYRIDIN-3-YLCYCLOHEXYL)-4-[(1S)-2,2,2-TRIFLUORO-1-HYDROXY-1-METHYLETHYL]BENZAMIDE (three-letter code: D3E) (formula:  $C_{24}H_{27}F_3N_2O_2$ ).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	F	N	O	0	0
			31	24	3	2	2		
3	B	1	Total	C	F	N	O	0	0
			31	24	3	2	2		
3	C	1	Total	C	F	N	O	0	0
			31	24	3	2	2		
3	D	1	Total	C	F	N	O	0	0
			31	24	3	2	2		

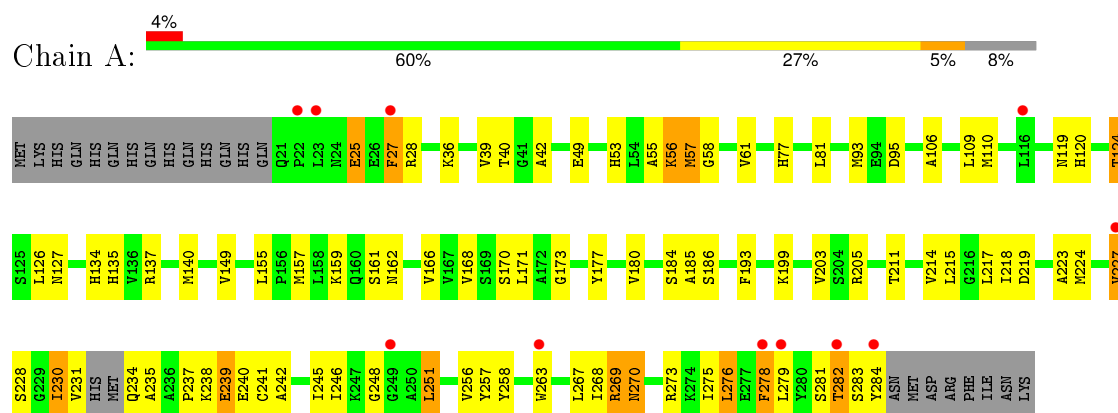
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	10	Total	O	0	0
			10	10		
4	B	19	Total	O	0	0
			19	19		
4	C	12	Total	O	0	0
			12	12		
4	D	4	Total	O	0	0
			4	4		

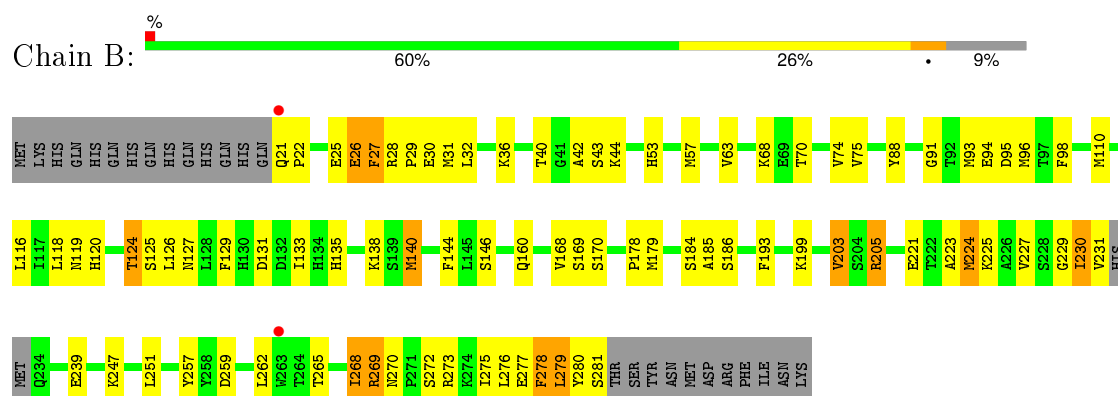
### 3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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.

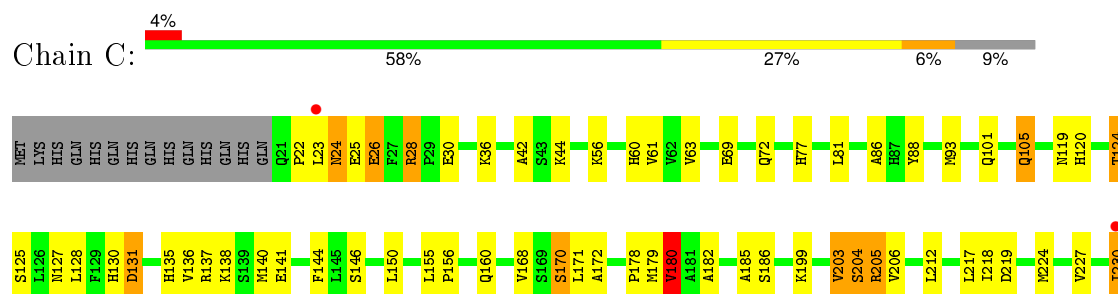
#### • Molecule 1: Corticosteroid 11-beta-dehydrogenase isozyme 1

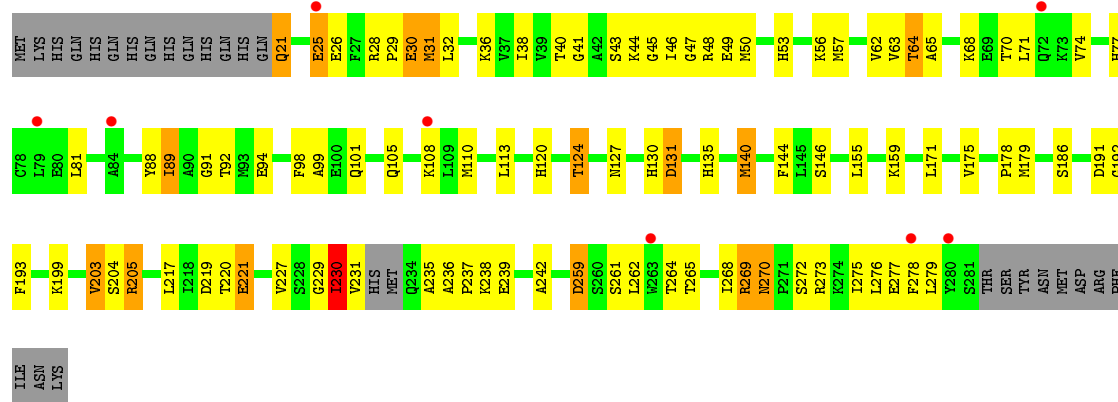


#### • Molecule 1: Corticosteroid 11-beta-dehydrogenase isozyme 1



#### • Molecule 1: Corticosteroid 11-beta-dehydrogenase isozyme 1







## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	56.70Å 152.85Å 73.71Å 90.00° 92.11° 90.00°	Depositor
Resolution (Å)	66.37 – 2.60 66.35 – 2.40	Depositor EDS
% Data completeness (in resolution range)	99.1 (66.37-2.60) 97.2 (66.35-2.40)	Depositor EDS
$R_{merge}$	0.04	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.82 (at 2.40Å)	Xtriage
Refinement program	REFMAC 5.4.0069	Depositor
R, $R_{free}$	0.227 , 0.283 0.226 , 0.276	Depositor DCC
$R_{free}$ test set	1924 reflections (5.31%)	DCC
Wilson B-factor (Å <sup>2</sup> )	55.2	Xtriage
Anisotropy	0.022	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.32 , 35.2	EDS
Estimated twinning fraction	0.058 for h,-k,-l	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.45$ , $\langle L^2 \rangle = 0.28$	Xtriage
Outliers	0 of 47581 reflections	Xtriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	8318	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	59.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.73% 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: NAP, D3E

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	0.35	0/2041	0.57	0/2756
1	B	0.37	0/2015	0.58	0/2720
1	C	0.36	0/2015	0.58	0/2720
1	D	0.33	0/2015	0.57	0/2720
All	All	0.35	0/8086	0.58	0/10916

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	2008	0	2055	116	0
1	B	1983	0	2034	107	0
1	C	1983	0	2034	132	0
1	D	1983	0	2034	116	0
2	A	48	0	25	2	0
2	B	48	0	25	3	0
2	C	48	0	25	1	0
2	D	48	0	25	1	0
3	A	31	0	27	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	B	31	0	27	2	0
3	C	31	0	27	1	0
3	D	31	0	27	1	0
4	A	10	0	0	0	0
4	B	19	0	0	0	0
4	C	12	0	0	0	0
4	D	4	0	0	0	0
All	All	8318	0	8365	462	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 28.

All (462) 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:A:275:ILE:CG2	1:A:279:LEU:HD11	1.51	1.38
1:D:28:ARG:HD2	1:D:30:GLU:OE2	1.37	1.25
1:A:267:LEU:HD21	1:C:275:ILE:CD1	1.69	1.21
1:A:275:ILE:HG23	1:A:279:LEU:CD1	1.73	1.18
1:B:140:MET:HE1	1:B:186:SER:HA	1.17	1.14
1:A:275:ILE:CG2	1:A:279:LEU:CD1	2.26	1.14
1:B:224:MET:CE	1:B:224:MET:HA	1.76	1.13
1:C:171:LEU:HD21	1:C:268:ILE:HD11	1.26	1.11
1:B:268:ILE:HD13	1:B:268:ILE:O	1.49	1.11
1:D:229:GLY:O	1:D:230:ILE:HG12	1.51	1.10
1:C:140:MET:HE1	1:C:186:SER:HA	1.26	1.08
1:A:267:LEU:HD21	1:C:275:ILE:HD11	1.28	1.07
1:D:140:MET:HE1	1:D:186:SER:HA	1.29	1.07
1:B:205:ARG:NH1	1:B:205:ARG:HG3	1.55	1.06
1:A:227:VAL:HA	1:A:230:ILE:CD1	1.85	1.06
1:D:217:LEU:HG	1:D:235:ALA:HB2	1.37	1.05
1:A:227:VAL:CA	1:A:230:ILE:HD11	1.85	1.05
1:B:205:ARG:CG	1:B:205:ARG:HH11	1.71	1.03
1:D:124:THR:HG23	1:D:135:HIS:CE1	1.95	1.01
1:B:224:MET:HE2	1:B:224:MET:HA	1.39	1.00
1:C:275:ILE:HG22	1:C:279:LEU:HD11	1.43	0.98
1:B:140:MET:CE	1:B:186:SER:HA	1.93	0.98
1:C:28:ARG:HH11	1:C:28:ARG:CG	1.75	0.98
1:D:229:GLY:O	1:D:230:ILE:CG1	2.11	0.98
1:D:276:LEU:O	1:D:279:LEU:HB2	1.63	0.98
1:A:219:ASP:OD1	1:A:237:PRO:HA	1.65	0.96

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:267:LEU:CD2	1:C:275:ILE:HD11	1.95	0.96
1:D:229:GLY:C	1:D:230:ILE:HG12	1.77	0.96
1:D:140:MET:CE	1:D:186:SER:HA	1.95	0.96
1:C:25:GLU:HG3	1:C:26:GLU:N	1.79	0.95
1:D:270:ASN:HD22	1:D:270:ASN:C	1.67	0.95
1:A:227:VAL:HA	1:A:230:ILE:HD11	0.95	0.95
1:D:270:ASN:ND2	1:D:273:ARG:H	1.67	0.93
1:C:25:GLU:HG3	1:C:26:GLU:H	1.33	0.91
1:D:269:ARG:HH21	1:D:269:ARG:HG2	1.32	0.91
1:A:270:ASN:HD22	1:A:270:ASN:C	1.71	0.91
1:B:272:SER:O	1:B:276:LEU:HG	1.71	0.90
1:C:140:MET:CE	1:C:186:SER:HA	2.01	0.90
1:D:269:ARG:HH21	1:D:269:ARG:CG	1.84	0.90
1:B:278:PHE:HD2	1:B:278:PHE:O	1.54	0.90
1:A:275:ILE:O	1:A:279:LEU:HG	1.72	0.90
1:A:223:ALA:O	1:A:227:VAL:HG22	1.72	0.89
1:D:229:GLY:O	1:D:230:ILE:CD1	2.21	0.89
1:C:268:ILE:O	1:C:268:ILE:HG22	1.71	0.88
1:C:264:THR:HA	1:C:267:LEU:HD12	1.57	0.86
1:A:268:ILE:CG2	1:A:269:ARG:N	2.37	0.86
1:C:263:TRP:O	1:C:267:LEU:HD12	1.73	0.86
1:D:130:HIS:CD2	1:D:131:ASP:OD1	2.30	0.84
1:A:275:ILE:HG22	1:A:279:LEU:CD1	2.06	0.84
1:A:275:ILE:HG23	1:A:279:LEU:HD11	0.84	0.84
1:C:171:LEU:HD21	1:C:268:ILE:CD1	2.07	0.84
1:B:91:GLY:HA3	1:B:98:PHE:CZ	2.12	0.84
1:C:275:ILE:O	1:C:279:LEU:HG	1.78	0.83
1:C:275:ILE:HG23	1:C:279:LEU:HD21	1.59	0.83
1:C:180:VAL:O	1:C:180:VAL:HG13	1.77	0.82
1:B:224:MET:HE3	1:B:224:MET:HA	1.59	0.82
1:D:227:VAL:CG1	1:D:227:VAL:O	2.27	0.82
1:D:270:ASN:HD21	1:D:273:ARG:H	1.26	0.82
1:B:40:THR:OG1	1:B:120:HIS:HD2	1.63	0.81
1:B:205:ARG:HG3	1:B:205:ARG:HH11	0.76	0.81
1:C:28:ARG:HG2	1:C:28:ARG:HH11	1.46	0.80
1:C:130:HIS:CD2	1:C:131:ASP:OD2	2.35	0.80
1:B:140:MET:HE1	1:B:186:SER:CA	2.08	0.79
1:A:40:THR:OG1	1:A:120:HIS:HD2	1.66	0.79
1:A:268:ILE:HG22	1:A:269:ARG:N	1.98	0.79
1:C:276:LEU:CA	1:C:279:LEU:HG	2.14	0.78
1:B:227:VAL:O	1:B:227:VAL:HG22	1.84	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:50:MET:HG2	1:D:242:ALA:HB1	1.66	0.77
1:C:28:ARG:HH11	1:C:28:ARG:HG3	1.48	0.77
1:D:77:HIS:CE1	1:D:81:LEU:HD11	2.20	0.77
1:D:278:PHE:O	1:D:278:PHE:CD1	2.37	0.76
1:C:171:LEU:CD2	1:C:268:ILE:HD11	2.12	0.76
1:C:275:ILE:C	1:C:279:LEU:HG	2.06	0.75
1:D:221:GLU:H	1:D:221:GLU:CD	1.84	0.75
1:C:101:GLN:O	1:C:105:GLN:HG2	1.86	0.75
1:A:270:ASN:ND2	1:A:270:ASN:C	2.35	0.75
1:C:263:TRP:O	1:C:267:LEU:CD1	2.35	0.75
1:C:275:ILE:CG2	1:C:279:LEU:HD21	2.16	0.75
1:C:105:GLN:HA	1:C:105:GLN:HE21	1.52	0.75
1:A:275:ILE:HG22	1:A:279:LEU:HD12	1.69	0.75
1:C:25:GLU:CG	1:C:26:GLU:N	2.49	0.75
1:A:119:ASN:HD22	1:A:168:VAL:HG21	1.50	0.74
1:C:276:LEU:HA	1:C:279:LEU:HG	1.70	0.74
1:C:224:MET:HA	1:C:224:MET:CE	2.18	0.74
1:D:124:THR:CG2	1:D:135:HIS:CE1	2.69	0.73
1:D:269:ARG:HG2	1:D:269:ARG:NH2	1.99	0.73
1:D:221:GLU:OE2	1:D:221:GLU:N	2.20	0.73
1:B:124:THR:HG23	1:B:135:HIS:CE1	2.23	0.73
1:B:224:MET:CE	1:B:224:MET:CA	2.61	0.73
1:D:70:THR:O	1:D:74:VAL:HG23	1.88	0.73
1:C:269:ARG:O	1:C:271:PRO:HD3	1.89	0.72
1:C:140:MET:HE1	1:C:186:SER:CA	2.15	0.72
1:D:124:THR:HG23	1:D:135:HIS:NE2	2.04	0.72
1:D:270:ASN:C	1:D:270:ASN:ND2	2.42	0.72
1:C:275:ILE:O	1:C:279:LEU:CD2	2.38	0.71
1:B:140:MET:HE3	1:B:186:SER:CB	2.20	0.71
1:A:140:MET:CE	1:A:186:SER:HA	2.20	0.71
3:C:293:D3E:O11	3:C:293:D3E:H14A	1.90	0.71
1:B:94:GLU:OE2	1:B:138:LYS:HE2	1.90	0.71
1:C:140:MET:HE2	1:C:144:PHE:HB3	1.72	0.71
1:C:264:THR:CA	1:C:267:LEU:HD12	2.21	0.71
1:C:275:ILE:CG2	1:C:279:LEU:HD11	2.19	0.70
1:D:229:GLY:O	1:D:230:ILE:HD13	1.92	0.70
1:A:140:MET:HE1	1:A:186:SER:HA	1.71	0.70
1:A:267:LEU:HD21	1:C:275:ILE:HD12	1.71	0.70
1:D:217:LEU:CG	1:D:235:ALA:HB2	2.19	0.70
1:B:140:MET:HE3	1:B:186:SER:HB2	1.74	0.69
1:C:140:MET:HE2	1:C:144:PHE:CB	2.22	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:70:THR:O	1:B:74:VAL:HG23	1.91	0.69
1:B:268:ILE:CD1	1:B:268:ILE:O	2.36	0.69
1:A:248:GLY:HA3	1:A:256:VAL:HG21	1.72	0.69
1:C:275:ILE:O	1:C:279:LEU:CG	2.41	0.69
1:D:50:MET:CG	1:D:242:ALA:HB1	2.22	0.69
1:C:140:MET:HE3	1:C:140:MET:HA	1.74	0.69
1:D:124:THR:CG2	1:D:135:HIS:HE1	2.06	0.68
1:B:278:PHE:CD2	1:B:278:PHE:O	2.44	0.68
1:A:77:HIS:HE1	1:A:81:LEU:HD11	1.57	0.68
1:D:88:TYR:O	1:D:89:ILE:HG12	1.93	0.68
1:A:275:ILE:HD11	1:C:266:LEU:HB3	1.76	0.68
1:A:77:HIS:CE1	1:A:81:LEU:HD11	2.28	0.68
1:C:275:ILE:HG22	1:C:279:LEU:CD1	2.21	0.68
1:A:257:TYR:CE2	1:A:268:ILE:HG21	2.30	0.67
1:D:88:TYR:O	1:D:89:ILE:CG1	2.42	0.67
1:A:224:MET:HA	1:A:224:MET:HE2	1.76	0.67
1:A:126:LEU:O	1:A:127:ASN:ND2	2.28	0.67
1:D:140:MET:HE2	1:D:144:PHE:HB3	1.75	0.67
1:C:264:THR:OG1	1:C:265:THR:N	2.26	0.66
1:D:269:ARG:HH21	1:D:269:ARG:CB	2.09	0.66
1:C:124:THR:HG23	1:C:135:HIS:CE1	2.30	0.66
1:C:268:ILE:CG2	1:C:268:ILE:O	2.44	0.66
1:B:257:TYR:CD2	1:B:268:ILE:CG2	2.79	0.66
1:B:268:ILE:C	1:B:268:ILE:HD13	2.15	0.66
1:C:227:VAL:HG23	1:C:227:VAL:O	1.96	0.65
1:D:140:MET:HE2	1:D:144:PHE:CB	2.27	0.65
1:C:264:THR:O	1:C:265:THR:C	2.34	0.65
1:D:227:VAL:HG12	1:D:227:VAL:O	1.95	0.65
1:C:28:ARG:HG3	1:C:28:ARG:NH1	2.09	0.65
1:A:224:MET:HE1	1:A:227:VAL:CG2	2.26	0.65
1:B:53:HIS:O	1:B:57:MET:HG3	1.97	0.65
1:C:30:GLU:CD	1:C:30:GLU:H	2.01	0.64
1:C:276:LEU:HD23	1:C:280:TYR:HE2	1.62	0.64
1:C:230:ILE:HG13	1:C:230:ILE:O	1.98	0.64
1:B:259:ASP:HB3	1:B:265:THR:HG22	1.80	0.64
1:A:224:MET:HE1	1:A:227:VAL:HG21	1.80	0.64
1:C:264:THR:HA	1:C:267:LEU:CD1	2.27	0.64
1:C:178:PRO:O	1:C:179:MET:HB2	1.96	0.64
1:D:92:THR:OG1	1:D:94:GLU:HB2	1.98	0.64
1:A:214:VAL:HG11	1:A:268:ILE:HD11	1.79	0.64
1:A:268:ILE:HG22	1:A:269:ARG:H	1.63	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:27:PHE:HB2	1:A:251:LEU:HD11	1.78	0.63
1:B:268:ILE:O	1:B:269:ARG:C	2.34	0.63
1:B:140:MET:CE	1:B:186:SER:CA	2.72	0.63
1:D:29:PRO:O	1:D:30:GLU:C	2.36	0.63
1:D:270:ASN:O	1:D:270:ASN:ND2	2.31	0.63
1:C:180:VAL:O	1:C:180:VAL:CG1	2.47	0.63
1:A:219:ASP:OD2	1:A:238:LYS:HB3	1.99	0.62
1:B:91:GLY:HA3	1:B:98:PHE:CE1	2.33	0.62
1:C:105:GLN:CA	1:C:105:GLN:NE2	2.61	0.62
1:C:105:GLN:HA	1:C:105:GLN:NE2	2.14	0.62
1:C:248:GLY:HA3	1:C:256:VAL:HG21	1.81	0.62
1:A:36:LYS:HD3	1:A:110:MET:O	2.00	0.62
1:A:268:ILE:O	1:A:269:ARG:O	2.18	0.62
1:A:268:ILE:HG23	1:A:269:ARG:N	2.14	0.61
1:D:217:LEU:HG	1:D:235:ALA:CB	2.22	0.61
1:D:265:THR:HA	1:D:268:ILE:HD12	1.83	0.61
1:D:227:VAL:HG13	1:D:227:VAL:O	1.99	0.61
1:C:140:MET:HG2	1:D:140:MET:HG2	1.83	0.61
1:A:224:MET:CE	1:A:227:VAL:HG21	2.30	0.61
1:A:270:ASN:ND2	1:A:273:ARG:H	1.99	0.61
1:A:185:ALA:HB2	1:B:193:PHE:HB2	1.82	0.61
1:C:251:LEU:HD12	1:C:253:GLN:HE21	1.65	0.61
1:B:28:ARG:O	1:B:30:GLU:N	2.33	0.61
1:D:269:ARG:CG	1:D:269:ARG:NH2	2.55	0.61
1:A:257:TYR:CD2	1:A:268:ILE:HG21	2.35	0.60
1:A:278:PHE:C	1:A:278:PHE:CD1	2.74	0.60
1:A:218:ILE:HD12	1:A:241:CYS:SG	2.42	0.60
1:C:171:LEU:CD2	1:C:268:ILE:CD1	2.75	0.60
1:C:140:MET:HE3	1:C:186:SER:CB	2.31	0.60
1:B:36:LYS:HD3	1:B:110:MET:O	2.02	0.60
1:B:27:PHE:C	1:B:27:PHE:CD2	2.75	0.60
1:B:229:GLY:O	1:B:230:ILE:HD13	2.01	0.60
1:B:276:LEU:O	1:B:279:LEU:HB2	2.02	0.59
1:B:272:SER:O	1:B:276:LEU:CG	2.49	0.59
1:B:28:ARG:HG3	1:B:30:GLU:HB2	1.83	0.59
1:C:275:ILE:O	1:C:279:LEU:HD23	2.02	0.59
1:D:275:ILE:O	1:D:279:LEU:HG	2.03	0.59
1:D:40:THR:OG1	1:D:120:HIS:HD2	1.85	0.59
1:A:124:THR:HG23	1:A:135:HIS:CE1	2.37	0.59
1:A:55:ALA:C	1:A:57:MET:H	2.05	0.59
1:A:193:PHE:HB2	1:B:185:ALA:HB2	1.85	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:230:ILE:O	1:A:231:VAL:C	2.41	0.59
1:A:55:ALA:O	1:A:57:MET:N	2.35	0.58
1:A:224:MET:HA	1:A:224:MET:CE	2.33	0.58
1:D:231:VAL:HG12	1:D:231:VAL:O	2.03	0.58
1:D:120:HIS:HE1	1:D:146:SER:OG	1.85	0.58
1:C:276:LEU:HD23	1:C:280:TYR:CE2	2.39	0.58
1:C:119:ASN:ND2	2:C:3:NAP:H4D	2.18	0.58
1:B:224:MET:HE3	1:B:224:MET:CA	2.30	0.58
1:B:93:MET:HG3	1:B:120:HIS:CE1	2.39	0.58
1:C:251:LEU:HD12	1:C:253:GLN:NE2	2.19	0.58
1:C:248:GLY:HA3	1:C:256:VAL:CG2	2.34	0.57
1:B:227:VAL:HG23	1:B:231:VAL:HG23	1.87	0.57
1:A:27:PHE:CD2	1:A:27:PHE:C	2.77	0.57
1:A:166:VAL:HG22	1:A:211:THR:HB	1.87	0.57
1:D:140:MET:HA	1:D:140:MET:HE3	1.86	0.57
1:A:27:PHE:CB	1:A:251:LEU:HD11	2.35	0.57
1:B:169:SER:O	2:B:2:NAP:H6N	2.05	0.56
1:C:265:THR:O	1:C:267:LEU:N	2.38	0.56
1:D:261:SER:O	1:D:264:THR:N	2.38	0.56
1:D:269:ARG:HH21	1:D:269:ARG:HB3	1.70	0.56
1:A:224:MET:CE	1:A:227:VAL:CG2	2.83	0.56
1:B:268:ILE:CD1	1:B:268:ILE:C	2.75	0.56
1:A:270:ASN:HD21	1:A:273:ARG:H	1.52	0.56
1:B:116:LEU:HD21	1:B:118:LEU:HD21	1.88	0.55
1:B:28:ARG:HD2	1:B:30:GLU:OE1	2.06	0.55
1:D:29:PRO:O	1:D:31:MET:N	2.39	0.55
1:D:45:GLY:O	1:D:48:ARG:N	2.39	0.55
1:A:55:ALA:O	1:A:58:GLY:N	2.35	0.55
1:A:283:SER:O	1:A:284:TYR:CB	2.55	0.55
1:A:170:SER:O	1:A:214:VAL:HG13	2.07	0.55
1:C:224:MET:HA	1:C:224:MET:HE2	1.87	0.55
1:A:278:PHE:O	1:A:278:PHE:CD1	2.60	0.55
1:A:283:SER:O	1:A:284:TYR:HB3	2.07	0.55
1:D:49:GLU:HG3	1:D:238:LYS:HG3	1.89	0.55
1:C:276:LEU:N	1:C:279:LEU:HG	2.22	0.55
1:D:264:THR:O	1:D:268:ILE:HG13	2.07	0.55
1:B:68:LYS:HE3	1:B:88:TYR:CE1	2.41	0.55
1:A:93:MET:HG3	1:A:120:HIS:CE1	2.42	0.55
1:A:39:VAL:HG12	1:A:42:ALA:HB2	1.87	0.55
1:B:227:VAL:CG2	1:B:231:VAL:CG2	2.85	0.54
1:B:221:GLU:HG2	1:B:225:LYS:NZ	2.21	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:199:LYS:O	1:C:203:VAL:HG13	2.07	0.54
1:B:124:THR:HG23	1:B:135:HIS:HE1	1.71	0.54
1:C:217:LEU:O	1:C:218:ILE:HD13	2.08	0.54
1:C:77:HIS:CE1	1:C:81:LEU:HD11	2.43	0.54
1:A:270:ASN:ND2	1:A:270:ASN:O	2.41	0.54
1:D:130:HIS:HD2	1:D:131:ASP:OD1	1.85	0.54
1:A:281:SER:OG	1:A:282:THR:N	2.41	0.54
1:A:40:THR:OG1	1:A:120:HIS:CD2	2.54	0.54
1:D:63:VAL:HG23	1:D:63:VAL:O	2.07	0.54
1:A:268:ILE:C	1:A:269:ARG:O	2.46	0.54
1:B:140:MET:CE	1:B:186:SER:CB	2.86	0.54
1:D:140:MET:CE	1:D:140:MET:HA	2.37	0.54
1:C:265:THR:O	1:C:268:ILE:N	2.40	0.53
1:D:278:PHE:O	1:D:278:PHE:CG	2.61	0.53
1:A:27:PHE:HB2	1:A:251:LEU:CD1	2.38	0.53
3:B:293:D3E:O11	3:B:293:D3E:H14A	2.07	0.53
1:B:140:MET:HA	1:B:140:MET:HE3	1.89	0.53
1:B:205:ARG:CG	1:B:205:ARG:NH1	2.42	0.53
1:A:134:HIS:ND1	1:A:135:HIS:N	2.56	0.53
3:D:293:D3E:O11	3:D:293:D3E:H14A	2.06	0.53
1:A:119:ASN:ND2	2:A:1:NAP:H4D	2.24	0.53
1:D:62:VAL:HG23	1:D:110:MET:SD	2.47	0.53
1:C:276:LEU:HA	1:C:279:LEU:CG	2.39	0.53
1:C:23:LEU:HB2	1:C:251:LEU:O	2.09	0.53
1:C:130:HIS:NE2	1:C:131:ASP:OD2	2.42	0.52
1:D:178:PRO:O	1:D:179:MET:HB2	2.09	0.52
1:B:68:LYS:HE3	1:B:88:TYR:HE1	1.75	0.52
1:C:276:LEU:O	1:C:279:LEU:HB2	2.09	0.52
1:A:224:MET:CA	1:A:224:MET:HE2	2.40	0.52
1:C:267:LEU:O	1:C:269:ARG:N	2.38	0.52
1:B:257:TYR:CD2	1:B:268:ILE:HG23	2.44	0.52
1:B:276:LEU:HD23	1:B:276:LEU:N	2.24	0.52
1:B:275:ILE:HG22	1:B:276:LEU:HD23	1.92	0.52
1:C:204:SER:O	1:C:205:ARG:C	2.47	0.52
1:A:268:ILE:O	1:A:269:ARG:C	2.46	0.52
1:D:199:LYS:O	1:D:203:VAL:HG12	2.10	0.52
1:D:140:MET:HE3	1:D:186:SER:CB	2.40	0.51
1:C:204:SER:HB2	1:C:206:VAL:HG23	1.91	0.51
1:C:140:MET:CE	1:C:140:MET:HA	2.39	0.51
1:B:178:PRO:O	1:B:179:MET:HB2	2.11	0.51
1:D:217:LEU:O	1:D:235:ALA:HB1	2.11	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:130:HIS:CG	1:C:131:ASP:OD2	2.63	0.51
1:A:124:THR:HG23	1:A:135:HIS:HE1	1.76	0.51
1:B:27:PHE:CE2	1:B:247:LYS:HG2	2.46	0.51
1:A:281:SER:C	1:A:283:SER:H	2.14	0.51
1:C:105:GLN:CA	1:C:105:GLN:HE21	2.14	0.51
1:B:27:PHE:CD2	1:B:247:LYS:HG2	2.46	0.51
1:D:120:HIS:CE1	1:D:146:SER:OG	2.63	0.51
1:C:262:LEU:N	1:C:262:LEU:HD23	2.26	0.51
1:D:65:ALA:HB3	1:D:71:LEU:HD11	1.93	0.51
1:A:227:VAL:HG12	1:A:230:ILE:CD1	2.41	0.50
1:C:224:MET:HA	1:C:224:MET:HE3	1.93	0.50
1:C:280:TYR:CD2	1:C:280:TYR:N	2.79	0.50
1:B:140:MET:HA	1:B:140:MET:CE	2.41	0.50
1:C:124:THR:CG2	1:C:135:HIS:CE1	2.94	0.50
1:B:126:LEU:O	1:B:127:ASN:ND2	2.45	0.50
1:B:27:PHE:CE2	1:B:247:LYS:HE2	2.45	0.50
1:C:170:SER:HB3	1:C:172:ALA:H	1.77	0.50
1:A:239:GLU:CD	1:A:239:GLU:H	2.13	0.50
1:D:46:ILE:HG13	1:D:220:THR:HG21	1.94	0.50
1:A:275:ILE:O	1:A:279:LEU:CG	2.53	0.50
1:C:140:MET:CE	1:C:186:SER:CA	2.81	0.50
1:A:49:GLU:O	1:A:53:HIS:HD2	1.95	0.50
1:B:278:PHE:HD2	1:B:281:SER:HG	1.58	0.50
1:C:124:THR:CG2	1:C:135:HIS:HE1	2.25	0.50
1:A:219:ASP:CG	1:A:238:LYS:H	2.15	0.50
1:A:227:VAL:HG12	1:A:230:ILE:HD12	1.93	0.50
1:C:24:ASN:CG	1:C:24:ASN:O	2.51	0.50
1:D:92:THR:C	1:D:94:GLU:H	2.14	0.49
1:A:55:ALA:C	1:A:57:MET:N	2.63	0.49
1:D:155:LEU:HG	1:D:159:LYS:HE3	1.94	0.49
1:B:257:TYR:CD2	1:B:268:ILE:HG21	2.47	0.49
1:A:219:ASP:OD2	1:A:238:LYS:N	2.42	0.49
1:A:219:ASP:OD2	1:A:238:LYS:CB	2.60	0.49
1:D:77:HIS:HE1	1:D:81:LEU:HD11	1.73	0.49
1:D:28:ARG:NE	1:D:30:GLU:HB2	2.28	0.49
1:D:178:PRO:O	1:D:179:MET:CB	2.61	0.49
1:B:129:PHE:C	1:B:129:PHE:CD2	2.86	0.49
1:A:240:GLU:HB3	1:A:258:TYR:OH	2.13	0.49
1:B:223:ALA:O	1:B:227:VAL:HG12	2.12	0.49
1:B:40:THR:OG1	1:B:120:HIS:CD2	2.53	0.49
1:C:128:LEU:CD2	1:C:179:MET:CE	2.91	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:124:THR:HG22	1:B:125:SER:H	1.78	0.48
1:A:106:ALA:O	1:A:109:LEU:HB3	2.13	0.48
1:D:26:GLU:OE1	1:D:26:GLU:HA	2.13	0.48
1:A:171:LEU:HD23	1:A:214:VAL:HG12	1.94	0.48
1:A:257:TYR:CD2	1:A:268:ILE:HD13	2.48	0.48
1:D:270:ASN:HD21	1:D:273:ARG:N	2.03	0.48
1:A:215:LEU:HD11	1:A:245:ILE:HD11	1.95	0.48
1:B:42:ALA:HB3	1:B:63:VAL:HB	1.95	0.48
1:D:64:THR:HG23	1:D:65:ALA:N	2.22	0.48
1:B:28:ARG:C	1:B:30:GLU:N	2.67	0.48
1:A:199:LYS:O	1:A:203:VAL:HG13	2.13	0.48
1:C:22:PRO:O	1:C:23:LEU:C	2.52	0.48
1:B:199:LYS:O	1:B:203:VAL:HG13	2.13	0.48
1:C:239:GLU:HG3	1:C:240:GLU:N	2.29	0.48
1:D:53:HIS:O	1:D:57:MET:HG3	2.14	0.48
1:B:140:MET:HE2	1:B:144:PHE:CB	2.44	0.47
1:B:273:ARG:O	1:B:277:GLU:HG3	2.14	0.47
1:B:178:PRO:O	1:B:179:MET:CB	2.61	0.47
1:D:21:GLN:N	1:D:21:GLN:OE1	2.47	0.47
1:D:25:GLU:OE2	1:D:31:MET:CE	2.62	0.47
1:D:279:LEU:HD23	1:D:279:LEU:HA	1.67	0.47
1:C:185:ALA:HB2	1:D:193:PHE:HB2	1.96	0.47
1:D:41:GLY:O	1:D:47:GLY:HA3	2.14	0.47
1:A:155:LEU:HG	1:A:159:LYS:HE3	1.97	0.47
1:C:137:ARG:O	1:C:141:GLU:HG2	2.14	0.47
1:B:43:SER:HB2	1:B:70:THR:CG2	2.44	0.47
1:D:101:GLN:O	1:D:105:GLN:HB3	2.15	0.47
1:C:269:ARG:C	1:C:271:PRO:HD3	2.35	0.47
1:D:28:ARG:HG2	1:D:28:ARG:HH11	1.79	0.47
1:C:146:SER:O	1:C:150:LEU:HG	2.15	0.47
1:D:264:THR:HG22	1:D:268:ILE:HD11	1.97	0.46
1:D:91:GLY:HA3	1:D:98:PHE:CZ	2.50	0.46
1:B:27:PHE:HA	1:B:31:MET:SD	2.56	0.46
1:D:230:ILE:O	1:D:231:VAL:C	2.54	0.46
1:B:120:HIS:HE1	1:B:146:SER:OG	1.99	0.46
1:C:263:TRP:C	1:C:267:LEU:HD12	2.36	0.46
1:C:93:MET:HG3	1:C:120:HIS:CE1	2.51	0.46
1:B:268:ILE:O	1:B:269:ARG:O	2.32	0.46
1:C:178:PRO:O	1:C:179:MET:CB	2.62	0.46
1:D:140:MET:CE	1:D:186:SER:CA	2.82	0.46
1:B:278:PHE:CD2	1:B:278:PHE:C	2.89	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:219:ASP:OD2	1:D:238:LYS:HE2	2.16	0.46
1:C:61:VAL:O	1:C:86:ALA:HA	2.16	0.46
1:A:217:LEU:HG	1:A:235:ALA:HB2	1.97	0.46
1:C:227:VAL:HB	1:C:230:ILE:CG2	2.46	0.46
1:C:88:TYR:C	1:C:88:TYR:CD1	2.89	0.46
1:B:227:VAL:HG21	1:B:231:VAL:CG2	2.46	0.45
1:B:227:VAL:HG21	1:B:231:VAL:HB	1.99	0.45
1:C:119:ASN:HD22	1:C:168:VAL:HG21	1.82	0.45
1:C:170:SER:HB3	1:C:172:ALA:N	2.31	0.45
1:C:140:MET:CE	1:C:186:SER:CB	2.94	0.45
1:A:93:MET:C	1:A:95:ASP:H	2.20	0.45
1:D:262:LEU:N	1:D:262:LEU:HD23	2.31	0.45
1:B:257:TYR:CE2	1:B:268:ILE:HG23	2.52	0.45
1:D:269:ARG:HB3	1:D:269:ARG:NH2	2.30	0.45
1:C:30:GLU:CD	1:C:30:GLU:N	2.69	0.45
1:D:92:THR:OG1	1:D:94:GLU:CB	2.65	0.45
1:B:95:ASP:OD1	1:B:95:ASP:C	2.55	0.45
1:C:42:ALA:HB3	1:C:63:VAL:HB	1.98	0.45
1:B:257:TYR:HD2	1:B:268:ILE:HG21	1.82	0.45
1:C:234:GLN:O	1:C:260:SER:OG	2.31	0.45
1:C:224:MET:CA	1:C:224:MET:CE	2.92	0.45
1:B:28:ARG:HB2	1:B:30:GLU:OE1	2.17	0.45
1:A:180:VAL:HG23	1:A:184:SER:HG	1.82	0.45
1:B:262:LEU:HA	1:B:262:LEU:HD23	1.66	0.44
1:A:137:ARG:HH22	1:B:96:MET:HG3	1.81	0.44
1:B:227:VAL:CG2	1:B:231:VAL:HG23	2.46	0.44
1:C:128:LEU:CD2	1:C:179:MET:HE1	2.47	0.44
1:D:236:ALA:HB1	1:D:237:PRO:HD2	1.99	0.44
1:A:224:MET:HE1	1:A:227:VAL:HG23	1.97	0.44
1:D:259:ASP:OD1	1:D:259:ASP:C	2.56	0.44
1:D:92:THR:C	1:D:94:GLU:N	2.71	0.44
1:C:136:VAL:HG22	1:C:182:ALA:HB2	1.98	0.44
1:B:227:VAL:CG2	1:B:231:VAL:HB	2.48	0.44
1:B:221:GLU:HG2	1:B:225:LYS:HZ2	1.82	0.44
1:D:108:LYS:HB3	1:D:108:LYS:HE2	1.87	0.44
1:A:278:PHE:C	1:A:278:PHE:HD1	2.18	0.44
3:A:293:D3E:H14A	3:A:293:D3E:O11	2.16	0.44
1:A:267:LEU:O	1:A:268:ILE:C	2.56	0.43
1:D:32:LEU:HD23	1:D:57:MET:SD	2.58	0.43
1:D:191:ASP:O	1:D:192:GLY:C	2.55	0.43
1:D:28:ARG:HE	1:D:30:GLU:HB2	1.81	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:272:SER:O	1:B:276:LEU:CD2	2.66	0.43
1:D:77:HIS:ND1	1:D:81:LEU:HD11	2.32	0.43
1:D:63:VAL:CG2	1:D:63:VAL:O	2.67	0.43
1:D:44:LYS:HG3	2:D:4:NAP:H3B	2.01	0.43
1:A:227:VAL:HA	1:A:230:ILE:CG1	2.47	0.43
1:B:116:LEU:CD2	1:B:118:LEU:HD21	2.48	0.43
1:D:38:ILE:HG13	1:D:113:LEU:CD1	2.48	0.43
1:A:77:HIS:CE1	1:A:81:LEU:CD1	2.98	0.43
1:D:88:TYR:O	1:D:89:ILE:HG13	2.18	0.43
1:A:161:SER:O	1:A:162:ASN:C	2.55	0.43
1:A:149:VAL:HG22	1:B:133:ILE:HD13	2.01	0.43
1:C:265:THR:OG1	1:C:266:LEU:N	2.48	0.43
1:C:265:THR:O	1:C:266:LEU:C	2.56	0.43
1:D:277:GLU:C	1:D:279:LEU:H	2.22	0.43
1:B:70:THR:O	1:B:70:THR:HG22	2.18	0.43
1:C:36:LYS:HA	1:C:60:HIS:HB2	2.01	0.43
1:C:199:LYS:NZ	1:C:278:PHE:CZ	2.87	0.42
1:C:217:LEU:C	1:C:218:ILE:HD13	2.39	0.42
1:D:171:LEU:HD23	1:D:171:LEU:HA	1.82	0.42
1:C:155:LEU:HB3	1:C:156:PRO:HD3	2.00	0.42
1:D:268:ILE:O	1:D:269:ARG:C	2.57	0.42
1:B:119:ASN:ND2	2:B:2:NAP:H4D	2.34	0.42
1:A:93:MET:HG2	2:A:1:NAP:H2A	2.00	0.42
1:C:140:MET:CG	1:D:140:MET:HG2	2.49	0.42
1:C:128:LEU:HD23	1:C:179:MET:HE2	2.01	0.42
1:A:134:HIS:CG	1:A:135:HIS:N	2.87	0.42
1:B:91:GLY:CA	1:B:98:PHE:CZ	2.94	0.42
1:B:119:ASN:HD22	1:B:168:VAL:HG21	1.84	0.42
1:A:171:LEU:C	1:A:173:GLY:H	2.22	0.42
1:C:130:HIS:CE1	1:C:131:ASP:OD2	2.72	0.42
1:B:28:ARG:C	1:B:30:GLU:H	2.23	0.42
1:D:43:SER:O	1:D:48:ARG:HD3	2.20	0.42
1:B:75:VAL:HG21	1:B:88:TYR:CD2	2.54	0.42
1:C:241:CYS:HB2	1:C:258:TYR:CE1	2.55	0.42
1:C:140:MET:HG2	1:D:140:MET:CG	2.48	0.42
1:B:93:MET:HG2	2:B:2:NAP:H2A	2.02	0.42
1:D:98:PHE:O	1:D:99:ALA:C	2.58	0.42
1:C:224:MET:CA	1:C:224:MET:HE3	2.50	0.42
1:B:21:GLN:HA	1:B:22:PRO:HD3	1.79	0.42
3:B:293:D3E:H13	3:B:293:D3E:H16	2.01	0.42
1:A:155:LEU:HD12	1:A:155:LEU:HA	1.81	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:268:ILE:C	1:B:269:ARG:O	2.53	0.42
1:A:134:HIS:C	1:A:134:HIS:ND1	2.71	0.41
1:A:171:LEU:HB3	1:A:177:TYR:OH	2.20	0.41
1:A:257:TYR:CE2	1:A:268:ILE:CG2	3.02	0.41
1:D:36:LYS:HD3	1:D:110:MET:O	2.20	0.41
1:A:275:ILE:HG22	1:A:276:LEU:N	2.36	0.41
1:B:278:PHE:CD2	1:B:281:SER:OG	2.73	0.41
1:A:25:GLU:O	1:A:251:LEU:CD2	2.69	0.41
1:B:27:PHE:CB	1:B:251:LEU:HD21	2.50	0.41
1:D:62:VAL:HG23	1:D:110:MET:CE	2.51	0.41
1:D:29:PRO:C	1:D:31:MET:N	2.73	0.41
1:C:275:ILE:C	1:C:279:LEU:CG	2.82	0.41
1:B:275:ILE:HG22	1:B:276:LEU:N	2.36	0.41
1:C:227:VAL:O	1:C:227:VAL:CG2	2.67	0.41
1:C:212:LEU:O	1:C:255:GLU:HA	2.21	0.41
1:A:56:LYS:NZ	1:A:81:LEU:HD22	2.36	0.41
1:B:129:PHE:CD2	1:B:129:PHE:O	2.74	0.41
1:A:170:SER:HB3	3:A:293:D3E:H14A	2.03	0.41
1:C:128:LEU:HD21	1:C:179:MET:HE1	2.03	0.40
1:D:77:HIS:CE1	1:D:81:LEU:CD1	2.98	0.40
1:C:105:GLN:CD	1:C:105:GLN:N	2.73	0.40
1:A:215:LEU:HD13	1:A:241:CYS:SG	2.62	0.40
1:A:248:GLY:HA3	1:A:256:VAL:CG2	2.46	0.40
1:C:219:ASP:OD1	1:C:237:PRO:HA	2.22	0.40
1:C:277:GLU:HG3	1:D:175:VAL:HB	2.02	0.40
1:A:242:ALA:O	1:A:246:ILE:HG13	2.21	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	258/286 (90%)	231 (90%)	22 (8%)	5 (2%)	10	19
1	B	255/286 (89%)	229 (90%)	23 (9%)	3 (1%)	16	33
1	C	255/286 (89%)	223 (88%)	25 (10%)	7 (3%)	6	10
1	D	255/286 (89%)	216 (85%)	35 (14%)	4 (2%)	12	24
All	All	1023/1144 (89%)	899 (88%)	105 (10%)	19 (2%)	10	19

All (19) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	269	ARG
1	C	264	THR
1	C	265	THR
1	C	268	ILE
1	D	205	ARG
1	D	230	ILE
1	A	56	LYS
1	A	227	VAL
1	C	180	VAL
1	C	266	LEU
1	A	228	SER
1	A	282	THR
1	B	26	GLU
1	C	131	ASP
1	B	29	PRO
1	B	269	ARG
1	D	30	GLU
1	C	230	ILE
1	D	89	ILE

### 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	219/243 (90%)	203 (93%)	16 (7%)	17	35
1	B	216/243 (89%)	195 (90%)	21 (10%)	10	19

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	C	216/243 (89%)	196 (91%)	20 (9%)	11	21
1	D	216/243 (89%)	196 (91%)	20 (9%)	11	21
All	All	867/972 (89%)	790 (91%)	77 (9%)	12	23

All (77) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	25	GLU
1	A	27	PHE
1	A	28	ARG
1	A	57	MET
1	A	61	VAL
1	A	124	THR
1	A	157	MET
1	A	205	ARG
1	A	230	ILE
1	A	234	GLN
1	A	239	GLU
1	A	251	LEU
1	A	263	TRP
1	A	270	ASN
1	A	276	LEU
1	A	278	PHE
1	B	25	GLU
1	B	26	GLU
1	B	27	PHE
1	B	32	LEU
1	B	44	LYS
1	B	124	THR
1	B	131	ASP
1	B	140	MET
1	B	160	GLN
1	B	170	SER
1	B	184	SER
1	B	203	VAL
1	B	205	ARG
1	B	224	MET
1	B	230	ILE
1	B	239	GLU
1	B	268	ILE
1	B	270	ASN

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Mol	Chain	Res	Type
1	B	278	PHE
1	B	279	LEU
1	B	280	TYR
1	C	24	ASN
1	C	26	GLU
1	C	28	ARG
1	C	44	LYS
1	C	56	LYS
1	C	69	GLU
1	C	72	GLN
1	C	105	GLN
1	C	124	THR
1	C	125	SER
1	C	127	ASN
1	C	138	LYS
1	C	160	GLN
1	C	170	SER
1	C	180	VAL
1	C	203	VAL
1	C	204	SER
1	C	205	ARG
1	C	274	LYS
1	C	276	LEU
1	D	21	GLN
1	D	25	GLU
1	D	31	MET
1	D	56	LYS
1	D	64	THR
1	D	68	LYS
1	D	124	THR
1	D	127	ASN
1	D	131	ASP
1	D	140	MET
1	D	203	VAL
1	D	204	SER
1	D	205	ARG
1	D	221	GLU
1	D	230	ILE
1	D	239	GLU
1	D	259	ASP
1	D	269	ARG
1	D	270	ASN

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Mol	Chain	Res	Type
1	D	272	SER

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (35) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	24	ASN
1	A	53	HIS
1	A	72	GLN
1	A	77	HIS
1	A	87	HIS
1	A	119	ASN
1	A	120	HIS
1	A	127	ASN
1	A	130	HIS
1	A	135	HIS
1	A	270	ASN
1	B	119	ASN
1	B	120	HIS
1	B	127	ASN
1	B	135	HIS
1	B	253	GLN
1	B	270	ASN
1	C	72	GLN
1	C	105	GLN
1	C	119	ASN
1	C	120	HIS
1	C	127	ASN
1	C	130	HIS
1	C	134	HIS
1	C	135	HIS
1	C	253	GLN
1	D	87	HIS
1	D	105	GLN
1	D	119	ASN
1	D	120	HIS
1	D	127	ASN
1	D	130	HIS
1	D	134	HIS
1	D	135	HIS
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	NAP	A	1	-	42,52,52	1.54	3 (7%)	54,80,80	2.01	6 (11%)
3	D3E	A	293	-	33,34,34	0.74	1 (3%)	45,51,51	2.22	6 (13%)
2	NAP	B	2	-	42,52,52	1.57	3 (7%)	54,80,80	1.99	5 (9%)
3	D3E	B	293	-	33,34,34	0.80	2 (6%)	45,51,51	2.42	4 (8%)
3	D3E	C	293	-	33,34,34	0.79	1 (3%)	45,51,51	2.44	3 (6%)
2	NAP	C	3	-	42,52,52	1.54	3 (7%)	54,80,80	1.89	5 (9%)
3	D3E	D	293	-	33,34,34	0.77	2 (6%)	45,51,51	2.23	4 (8%)
2	NAP	D	4	-	42,52,52	1.59	3 (7%)	54,80,80	1.89	5 (9%)

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	NAP	A	1	-	-	0/27/67/67	0/5/5/5
3	D3E	A	293	-	-	0/33/47/47	0/3/4/4
2	NAP	B	2	-	-	0/27/67/67	0/5/5/5
3	D3E	B	293	-	-	0/33/47/47	0/3/4/4
3	D3E	C	293	-	-	0/33/47/47	0/3/4/4
2	NAP	C	3	-	-	0/27/67/67	0/5/5/5
3	D3E	D	293	-	-	0/33/47/47	0/3/4/4
2	NAP	D	4	-	-	0/27/67/67	0/5/5/5

All (18) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	293	D3E	C12-N10	-2.76	1.44	1.48
3	B	293	D3E	C12-N10	-2.56	1.44	1.48
3	B	293	D3E	C6-C9	-2.12	1.46	1.50
3	D	293	D3E	C12-N10	-2.10	1.45	1.48
2	A	1	NAP	C2A-N1A	2.03	1.37	1.33
2	B	2	NAP	C2A-N1A	2.18	1.38	1.33
3	A	293	D3E	C9-N10	2.19	1.39	1.36
2	C	3	NAP	C2A-N1A	2.23	1.38	1.33
3	D	293	D3E	C9-N10	2.39	1.40	1.36
2	D	4	NAP	C2A-N1A	2.41	1.38	1.33
2	A	1	NAP	C2A-N3A	3.04	1.37	1.32
2	B	2	NAP	C2A-N3A	3.33	1.38	1.32
2	C	3	NAP	C2A-N3A	3.33	1.38	1.32
2	D	4	NAP	C2A-N3A	3.33	1.38	1.32
2	C	3	NAP	O7N-C7N	7.76	1.40	1.24
2	A	1	NAP	O7N-C7N	8.04	1.41	1.24
2	B	2	NAP	O7N-C7N	8.05	1.41	1.24
2	D	4	NAP	O7N-C7N	8.14	1.41	1.24

All (38) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	293	D3E	C13-C12-N10	-13.20	99.95	118.91
3	C	293	D3E	C13-C12-N10	-12.97	100.28	118.91
2	B	2	NAP	N3A-C2A-N1A	-12.19	119.56	128.89
2	A	1	NAP	N3A-C2A-N1A	-12.04	119.67	128.89
3	A	293	D3E	C13-C12-N10	-11.85	101.88	118.91
2	D	4	NAP	N3A-C2A-N1A	-11.46	120.12	128.89
2	C	3	NAP	N3A-C2A-N1A	-11.25	120.28	128.89
3	D	293	D3E	C13-C12-N10	-10.94	103.20	118.91
3	C	293	D3E	C14-C12-N10	-8.44	106.78	118.91

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	293	D3E	C14-C12-N10	-7.35	108.34	118.91
3	B	293	D3E	C14-C12-N10	-6.64	109.37	118.91
3	A	293	D3E	C14-C12-N10	-4.65	112.23	118.91
3	A	293	D3E	O22-C2-C21	-4.15	99.68	106.21
3	D	293	D3E	O22-C2-C21	-3.43	100.82	106.21
2	A	1	NAP	C1B-N9A-C4A	-3.34	121.90	126.94
3	D	293	D3E	C20-C15-N10	-3.24	106.60	112.65
2	A	1	NAP	PN-O3-PA	-3.09	124.05	132.73
3	B	293	D3E	C20-C15-N10	-2.84	107.35	112.65
2	D	4	NAP	C1B-N9A-C4A	-2.61	123.00	126.94
2	C	3	NAP	PN-O3-PA	-2.58	125.49	132.73
3	C	293	D3E	O22-C2-C21	-2.48	102.31	106.21
3	B	293	D3E	C8-C3-C2	-2.38	118.85	121.51
2	C	3	NAP	O7N-C7N-C3N	-2.31	117.06	119.59
2	B	2	NAP	O7N-C7N-C3N	-2.29	117.09	119.59
3	A	293	D3E	C20-C15-N10	-2.18	108.58	112.65
2	D	4	NAP	PN-O3-PA	-2.18	126.62	132.73
2	C	3	NAP	O3D-C3D-C2D	-2.08	105.06	111.83
3	A	293	D3E	C6-C9-N10	2.06	122.13	118.43
2	A	1	NAP	C3N-C7N-N7N	2.10	120.12	117.82
3	A	293	D3E	C21-C2-C3	2.15	112.56	109.53
2	B	2	NAP	O4B-C1B-N9A	2.16	112.63	108.10
2	B	2	NAP	C2N-C3N-C4N	2.38	120.94	118.29
2	A	1	NAP	O4D-C1D-N1N	2.39	110.76	108.13
2	A	1	NAP	O4B-C1B-N9A	2.50	113.34	108.10
2	D	4	NAP	C3N-C7N-N7N	2.51	120.56	117.82
2	B	2	NAP	O4D-C1D-N1N	2.98	111.40	108.13
2	C	3	NAP	C3N-C7N-N7N	3.22	121.34	117.82
2	D	4	NAP	O4D-C1D-N1N	3.25	111.70	108.13

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

8 monomers are involved in 13 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	1	NAP	2	0
3	A	293	D3E	2	0
2	B	2	NAP	3	0
3	B	293	D3E	2	0
3	C	293	D3E	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	C	3	NAP	1	0
3	D	293	D3E	1	0
2	D	4	NAP	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 ⓘ

### 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	262/286 (91%)	0.00	11 (4%) 40 32	38, 58, 91, 101	0
1	B	259/286 (90%)	-0.07	2 (0%) 87 85	33, 48, 72, 86	0
1	C	259/286 (90%)	-0.06	11 (4%) 40 32	32, 54, 88, 91	0
1	D	259/286 (90%)	0.06	8 (3%) 52 45	36, 70, 87, 95	0
All	All	1039/1144 (90%)	-0.02	32 (3%) 52 45	32, 56, 87, 101	0

All (32) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	23	LEU	7.3
1	C	263	TRP	4.4
1	C	268	ILE	4.3
1	A	279	LEU	4.3
1	D	25	GLU	3.8
1	C	266	LEU	3.3
1	C	230	ILE	3.2
1	A	284	TYR	3.2
1	D	263	TRP	3.0
1	B	263	TRP	2.9
1	A	278	PHE	2.8
1	A	227	VAL	2.8
1	B	21	GLN	2.8
1	A	263	TRP	2.6
1	A	22	PRO	2.6
1	D	278	PHE	2.6
1	A	282	THR	2.4
1	C	278	PHE	2.3
1	C	279	LEU	2.3
1	A	116	LEU	2.2
1	C	269	ARG	2.2

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Mol	Chain	Res	Type	RSRZ
1	D	108	LYS	2.2
1	C	265	THR	2.2
1	C	257	TYR	2.2
1	C	23	LEU	2.1
1	C	267	LEU	2.1
1	D	84	ALA	2.1
1	A	27	PHE	2.1
1	D	280	TYR	2.0
1	D	79	LEU	2.0
1	A	249	GLY	2.0
1	D	72	GLN	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
3	D3E	C	293	31/31	0.93	0.20	0.28	73,74,77,77	0
3	D3E	B	293	31/31	0.90	0.19	0.13	60,61,65,65	0
3	D3E	A	293	31/31	0.93	0.17	-0.12	54,55,57,57	0
3	D3E	D	293	31/31	0.96	0.15	-0.15	69,70,71,71	0
2	NAP	A	1	48/48	0.97	0.13	-0.36	39,44,47,48	0
2	NAP	D	4	48/48	0.97	0.13	-0.89	53,55,59,61	0
2	NAP	C	3	48/48	0.97	0.14	-0.96	33,38,42,44	0
2	NAP	B	2	48/48	0.97	0.13	-0.97	27,39,43,44	0



## 6.5 Other polymers [i](#)

There are no such residues in this entry.