



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 07:53 AM GMT

PDB ID : 3CH6
Title : Crystal Structure of 11beta-HSD1 Double Mutant (L262R, F278E) Complexed with (3,3-dimethylpiperidin-1-yl)(6-(3-fluoro-4-methylphenyl)pyridin-2-yl)methanone
Authors : Sheriff, S.
Deposited on : 2008-03-07
Resolution : 2.35 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
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

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

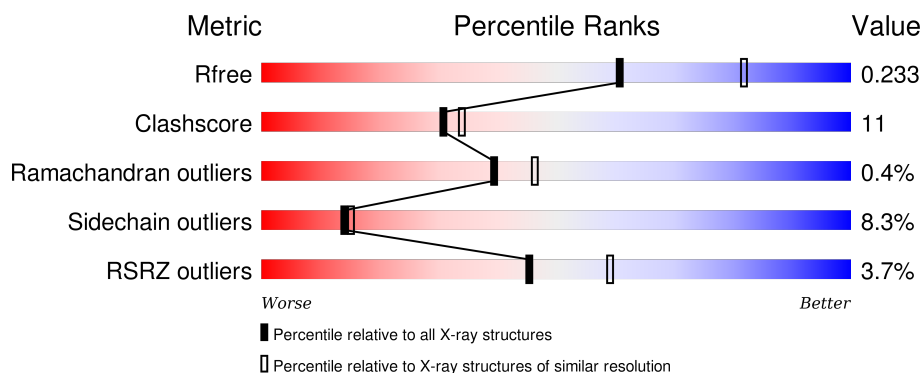
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.35 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	1352 (2.38-2.34)
Clashscore	102246	1456 (2.38-2.34)
Ramachandran outliers	100387	1435 (2.38-2.34)
Sidechain outliers	100360	1436 (2.38-2.34)
RSRZ outliers	91569	1358 (2.38-2.34)

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 ≥ 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	 3% 73% 15% • 8%
1	B	286	 3% 76% 17% 5% •
1	D	286	 3% 76% 16% • 5%
1	E	286	 4% 73% 16% • 8%

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
3	311	E	604	-	X	-	-

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 8775 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	264	Total	C	N	O	S	0	2	0
			2036	1292	351	376	17			
1	B	279	Total	C	N	O	S	0	1	0
			2125	1341	364	400	20			
1	D	273	Total	C	N	O	S	0	1	0
			2072	1312	354	388	18			
1	E	263	Total	C	N	O	S	0	1	0
			2019	1282	343	377	17			

There are 76 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	7	GLY	-	EXPRESSION TAG	UNP P28845
A	8	SER	-	EXPRESSION TAG	UNP P28845
A	9	HIS	-	EXPRESSION TAG	UNP P28845
A	10	MET	-	EXPRESSION TAG	UNP P28845
A	11	ALA	-	EXPRESSION TAG	UNP P28845
A	12	SER	-	EXPRESSION TAG	UNP P28845
A	13	MET	-	EXPRESSION TAG	UNP P28845
A	14	THR	-	EXPRESSION TAG	UNP P28845
A	15	GLY	-	EXPRESSION TAG	UNP P28845
A	16	GLY	-	EXPRESSION TAG	UNP P28845
A	17	GLN	-	EXPRESSION TAG	UNP P28845
A	18	GLN	-	EXPRESSION TAG	UNP P28845
A	19	MET	-	EXPRESSION TAG	UNP P28845
A	20	GLY	-	EXPRESSION TAG	UNP P28845
A	21	ARG	-	EXPRESSION TAG	UNP P28845
A	22	GLY	-	EXPRESSION TAG	UNP P28845
A	23	SER	-	EXPRESSION TAG	UNP P28845
A	262	ARG	LEU	ENGINEERED	UNP P28845
A	278	GLU	PHE	ENGINEERED	UNP P28845
B	7	GLY	-	EXPRESSION TAG	UNP P28845
B	8	SER	-	EXPRESSION TAG	UNP P28845

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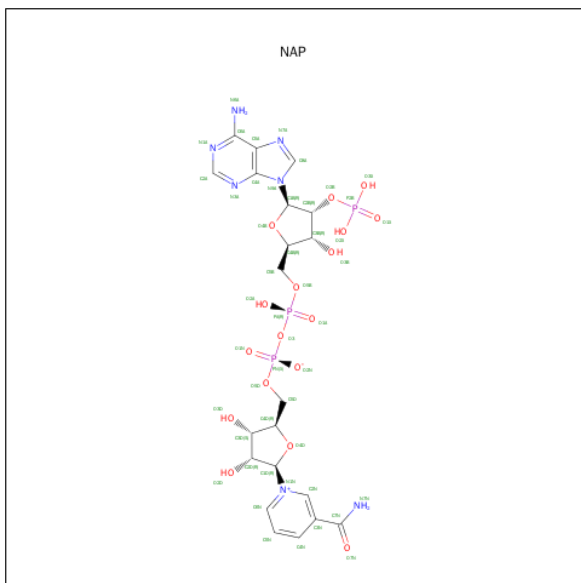
Chain	Residue	Modelled	Actual	Comment	Reference
B	9	HIS	-	EXPRESSION TAG	UNP P28845
B	10	MET	-	EXPRESSION TAG	UNP P28845
B	11	ALA	-	EXPRESSION TAG	UNP P28845
B	12	SER	-	EXPRESSION TAG	UNP P28845
B	13	MET	-	EXPRESSION TAG	UNP P28845
B	14	THR	-	EXPRESSION TAG	UNP P28845
B	15	GLY	-	EXPRESSION TAG	UNP P28845
B	16	GLY	-	EXPRESSION TAG	UNP P28845
B	17	GLN	-	EXPRESSION TAG	UNP P28845
B	18	GLN	-	EXPRESSION TAG	UNP P28845
B	19	MET	-	EXPRESSION TAG	UNP P28845
B	20	GLY	-	EXPRESSION TAG	UNP P28845
B	21	ARG	-	EXPRESSION TAG	UNP P28845
B	22	GLY	-	EXPRESSION TAG	UNP P28845
B	23	SER	-	EXPRESSION TAG	UNP P28845
B	262	ARG	LEU	ENGINEERED	UNP P28845
B	278	GLU	PHE	ENGINEERED	UNP P28845
D	7	GLY	-	EXPRESSION TAG	UNP P28845
D	8	SER	-	EXPRESSION TAG	UNP P28845
D	9	HIS	-	EXPRESSION TAG	UNP P28845
D	10	MET	-	EXPRESSION TAG	UNP P28845
D	11	ALA	-	EXPRESSION TAG	UNP P28845
D	12	SER	-	EXPRESSION TAG	UNP P28845
D	13	MET	-	EXPRESSION TAG	UNP P28845
D	14	THR	-	EXPRESSION TAG	UNP P28845
D	15	GLY	-	EXPRESSION TAG	UNP P28845
D	16	GLY	-	EXPRESSION TAG	UNP P28845
D	17	GLN	-	EXPRESSION TAG	UNP P28845
D	18	GLN	-	EXPRESSION TAG	UNP P28845
D	19	MET	-	EXPRESSION TAG	UNP P28845
D	20	GLY	-	EXPRESSION TAG	UNP P28845
D	21	ARG	-	EXPRESSION TAG	UNP P28845
D	22	GLY	-	EXPRESSION TAG	UNP P28845
D	23	SER	-	EXPRESSION TAG	UNP P28845
D	262	ARG	LEU	ENGINEERED	UNP P28845
D	278	GLU	PHE	ENGINEERED	UNP P28845
E	7	GLY	-	EXPRESSION TAG	UNP P28845
E	8	SER	-	EXPRESSION TAG	UNP P28845
E	9	HIS	-	EXPRESSION TAG	UNP P28845
E	10	MET	-	EXPRESSION TAG	UNP P28845
E	11	ALA	-	EXPRESSION TAG	UNP P28845
E	12	SER	-	EXPRESSION TAG	UNP P28845

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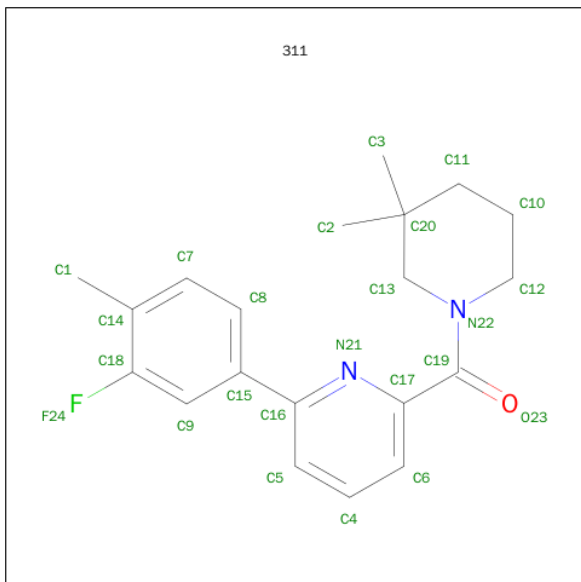
Chain	Residue	Modelled	Actual	Comment	Reference
E	13	MET	-	EXPRESSION TAG	UNP P28845
E	14	THR	-	EXPRESSION TAG	UNP P28845
E	15	GLY	-	EXPRESSION TAG	UNP P28845
E	16	GLY	-	EXPRESSION TAG	UNP P28845
E	17	GLN	-	EXPRESSION TAG	UNP P28845
E	18	GLN	-	EXPRESSION TAG	UNP P28845
E	19	MET	-	EXPRESSION TAG	UNP P28845
E	20	GLY	-	EXPRESSION TAG	UNP P28845
E	21	ARG	-	EXPRESSION TAG	UNP P28845
E	22	GLY	-	EXPRESSION TAG	UNP P28845
E	23	SER	-	EXPRESSION TAG	UNP P28845
E	262	ARG	LEU	ENGINEERED	UNP P28845
E	278	GLU	PHE	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 48	C 21	N 7	O 17	P 3	0	0
2	B	1	Total 48	C 21	N 7	O 17	P 3	0	0
2	D	1	Total 48	C 21	N 7	O 17	P 3	0	0
2	E	1	Total 48	C 21	N 7	O 17	P 3	0	0

- Molecule 3 is (3,3-DIMETHYLPIPERIDIN-1-YL)(6-(3-FLUORO-4-METHYLPHENYL)PYRIDIN-2-YL)METHANONE (three-letter code: 311) (formula: $C_{20}H_{23}FN_2O$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	F	N	O	0	0
			24	20	1	2	1		
3	B	1	Total	C	F	N	O	0	0
			24	20	1	2	1		
3	D	1	Total	C	F	N	O	0	0
			24	20	1	2	1		
3	E	1	Total	C	F	N	O	0	0
			24	20	1	2	1		

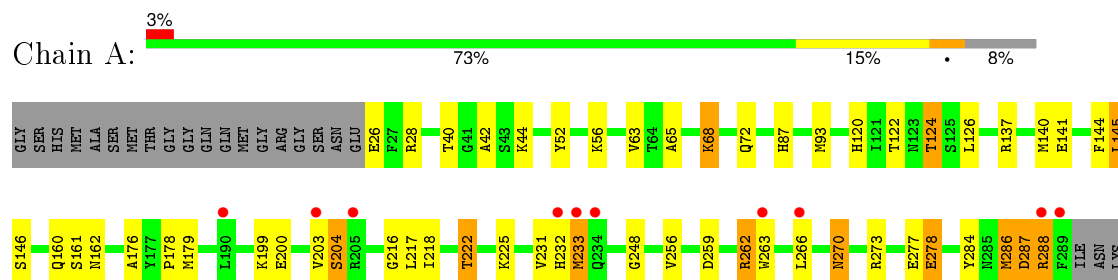
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	55	Total	O	0	0
			55	55		
4	B	65	Total	O	0	0
			65	65		
4	D	60	Total	O	0	0
			60	60		
4	E	55	Total	O	0	0
			55	55		

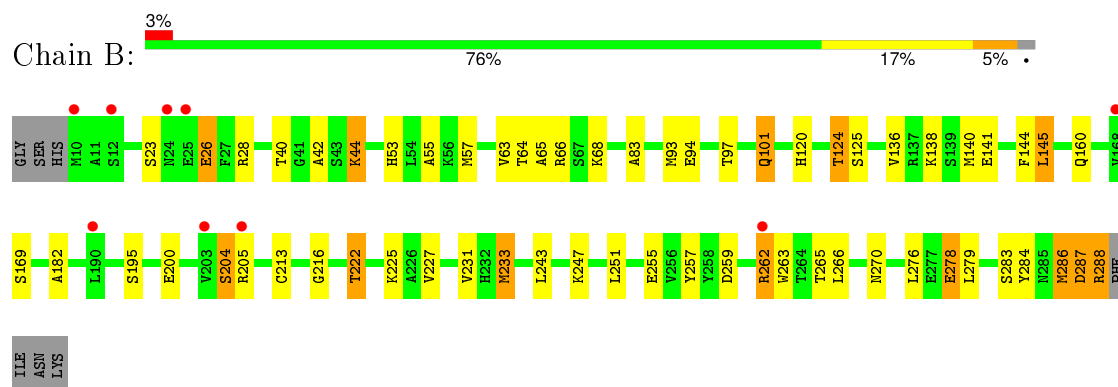
3 Residue-property plots

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.

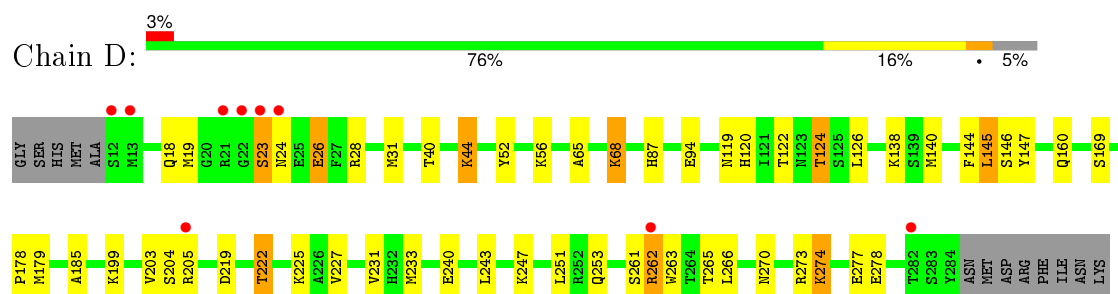
- Molecule 1: Corticosteroid 11-beta-dehydrogenase isozyme 1



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

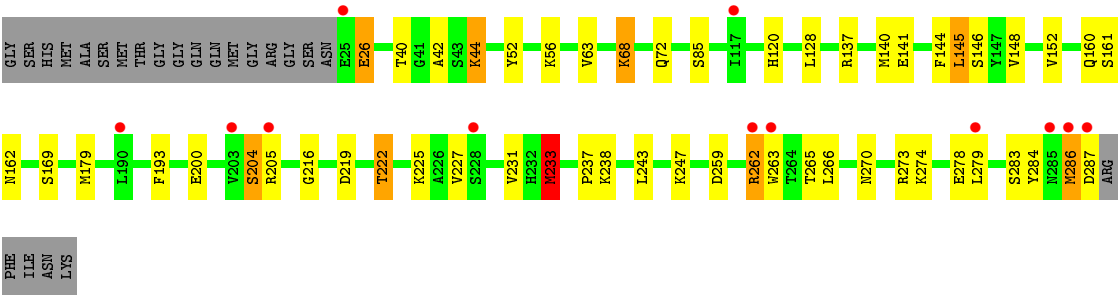


- Molecule 1: Corticosteroid 11-beta-dehydrogenase isozyme 1



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





4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	74.50 Å 94.30 Å 167.00 Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	50.00 – 2.35 32.00 – 2.34	Depositor EDS
% Data completeness (in resolution range)	89.3 (50.00-2.35) 89.2 (32.00-2.34)	Depositor EDS
R_{merge}	0.04	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	7.47 (at 2.34 Å)	Xtriage
Refinement program	BUSTER-TNT 2.1.1	Depositor
R, R_{free}	0.187 , 0.230 0.187 , 0.233	Depositor DCC
R_{free} test set	1061 reflections (2.44%)	DCC
Wilson B-factor (Å ²)	30.4	Xtriage
Anisotropy	0.444	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 47.9	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.46$, $\langle L^2 \rangle = 0.29$	Xtriage
Outliers	0 of 44683 reflections	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	8775	wwPDB-VP
Average B, all atoms (Å ²)	32.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.26% 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, 0.375 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: 311, NAP

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	0.69	0/2081	0.77	0/2808
1	B	0.70	0/2163	0.76	0/2915
1	D	0.73	0/2110	0.76	0/2846
1	E	0.72	1/2057 (0.0%)	0.78	2/2776 (0.1%)
All	All	0.71	1/8411 (0.0%)	0.77	2/11345 (0.0%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	E	233	MET	CG-SD	5.55	1.95	1.81

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	273	ARG	NE-CZ-NH2	-8.22	116.19	120.30
1	E	273	ARG	NE-CZ-NH1	6.18	123.39	120.30

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	2036	0	2073	52	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	B	2125	0	2152	57	0
1	D	2072	0	2099	43	0
1	E	2019	0	2056	49	0
2	A	48	0	25	1	0
2	B	48	0	25	4	0
2	D	48	0	25	4	0
2	E	48	0	25	3	0
3	A	24	0	23	1	0
3	B	24	0	23	1	0
3	D	24	0	23	0	0
3	E	24	0	23	2	0
4	A	55	0	0	2	0
4	B	65	0	0	2	0
4	D	60	0	0	2	0
4	E	55	0	0	1	0
All	All	8775	0	8572	186	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 11.

All (186) 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:262:ARG:HB2	1:B:262:ARG:HH11	1.05	1.12
1:E:262:ARG:HH11	1:E:262:ARG:HB2	1.14	1.08
1:D:231:VAL:HG12	1:D:233:MET:HG2	1.40	0.98
1:D:19:MET:HE3	1:D:23:SER:HB2	1.47	0.96
1:B:284:TYR:CD2	1:B:286:MET:HE1	2.07	0.89
1:D:122:THR:O	1:D:124:THR:HG22	1.76	0.86
1:B:262:ARG:HH11	1:B:262:ARG:CB	1.89	0.85
1:D:262:ARG:HH11	1:D:262:ARG:HA	1.44	0.83
1:B:262:ARG:NH1	1:B:262:ARG:HB2	1.91	0.83
1:E:262:ARG:HH11	1:E:262:ARG:CB	1.93	0.80
1:E:284:TYR:CD2	1:E:286:MET:HE1	2.15	0.80
1:A:68:LYS:O	1:A:72:GLN:HG3	1.82	0.80
1:E:231:VAL:HG12	1:E:233:MET:HG2	1.64	0.79
1:D:231:VAL:CG1	1:D:233:MET:HG2	2.15	0.76
1:B:44:LYS:HG3	2:B:502:NAP:H3B	1.68	0.75
1:B:124:THR:HG21	4:B:858:HOH:O	1.86	0.75
1:A:137:ARG:NH2	1:B:145:LEU:HD22	2.04	0.73
1:A:140:MET:HE3	1:A:140:MET:HA	1.70	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:68:LYS:HG2	1:A:72:GLN:HE21	1.57	0.70
1:E:284:TYR:CE2	1:E:286:MET:HE1	2.27	0.70
1:E:26:GLU:HA	1:E:26:GLU:OE1	1.93	0.68
1:E:231:VAL:HG12	1:E:233:MET:CG	2.24	0.68
1:A:126:LEU:HD23	1:A:126:LEU:N	2.08	0.68
1:D:262:ARG:HH11	1:D:262:ARG:CA	2.06	0.67
1:E:40:THR:OG1	1:E:120:HIS:HD2	1.78	0.67
1:A:124:THR:HG21	4:A:975:HOH:O	1.94	0.66
1:A:231:VAL:HG12	1:A:233:MET:HG2	1.78	0.66
1:A:262:ARG:HH11	1:A:262:ARG:CB	2.10	0.64
1:A:68:LYS:HG2	1:A:72:GLN:NE2	2.13	0.64
1:E:222:THR:HG21	2:E:504:NAP:O2A	1.98	0.64
1:A:262:ARG:NH1	1:A:262:ARG:HB2	2.12	0.64
1:D:40:THR:OG1	1:D:120:HIS:HD2	1.79	0.64
1:B:26:GLU:HA	1:B:26:GLU:OE1	1.97	0.63
1:B:222:THR:HG21	2:B:502:NAP:O2A	1.98	0.63
1:B:263:TRP:CH2	1:E:279:LEU:HD21	2.34	0.63
1:A:262:ARG:HH11	1:A:262:ARG:HB2	1.63	0.63
1:A:284:TYR:CE2	1:A:286:MET:HE1	2.34	0.63
1:B:93:MET:HG3	1:B:120:HIS:CE1	2.33	0.63
1:E:243:LEU:HG	1:E:247:LYS:HE3	1.80	0.63
1:B:284:TYR:HD2	1:B:286:MET:HE1	1.62	0.61
1:A:26:GLU:HA	1:A:26:GLU:OE1	2.00	0.61
1:A:262:ARG:HH11	1:A:262:ARG:HA	1.65	0.60
1:E:169:SER:O	2:E:504:NAP:H6N	2.01	0.60
1:D:262:ARG:HH11	1:D:262:ARG:CB	2.14	0.60
1:B:263:TRP:HH2	1:E:279:LEU:CD2	2.15	0.60
1:D:87:HIS:HD2	4:D:916:HOH:O	1.84	0.59
1:E:179:MET:HE3	3:E:604:311:H1B	1.84	0.59
1:B:243:LEU:HG	1:B:247:LYS:HE3	1.85	0.59
1:E:44:LYS:HG3	2:E:504:NAP:H3B	1.85	0.58
1:B:40:THR:OG1	1:B:120:HIS:HD2	1.86	0.58
1:E:140:MET:HA	1:E:140:MET:HE3	1.86	0.58
1:B:284:TYR:CE2	1:B:286:MET:HE1	2.39	0.57
1:A:222:THR:HG21	2:A:501:NAP:O2A	2.04	0.57
1:B:263:TRP:HH2	1:E:279:LEU:HD21	1.68	0.57
1:B:279:LEU:HD21	1:E:263:TRP:CH2	2.39	0.57
1:B:279:LEU:CD2	1:E:263:TRP:HH2	2.18	0.57
1:A:263:TRP:N	1:A:263:TRP:CD1	2.69	0.57
1:D:273:ARG:O	1:D:277:GLU:HG3	2.05	0.57
1:E:284:TYR:CD2	1:E:286:MET:CE	2.89	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:94:GLU:OE1	1:B:138:LYS:HE2	2.05	0.56
1:A:288:ARG:HG2	1:A:288:ARG:O	2.06	0.56
1:E:262:ARG:NH1	1:E:262:ARG:HB2	2.00	0.56
1:A:178:PRO:O	1:A:179:MET:HB2	2.06	0.56
1:D:263:TRP:N	1:D:263:TRP:CD1	2.72	0.56
1:E:243:LEU:O	1:E:247:LYS:HG3	2.06	0.56
1:A:120:HIS:HE1	1:A:146:SER:OG	1.89	0.55
1:B:23:SER:O	1:B:251:LEU:HD22	2.06	0.55
1:A:87:HIS:HD2	4:A:1025:HOH:O	1.88	0.55
1:E:274:LYS:HD3	4:E:1003:HOH:O	2.06	0.55
1:B:140:MET:HE3	1:B:140:MET:HA	1.88	0.55
1:D:262:ARG:HB2	1:D:262:ARG:NH1	2.21	0.55
1:A:68:LYS:CG	1:A:72:GLN:HE21	2.19	0.55
1:E:140:MET:HE3	1:E:144:PHE:HB3	1.89	0.54
1:A:231:VAL:HG12	1:A:233:MET:CG	2.38	0.54
1:D:145:LEU:HD22	1:E:137:ARG:NH2	2.23	0.54
1:A:40:THR:OG1	1:A:120:HIS:HD2	1.91	0.54
1:D:222:THR:HG21	2:D:503:NAP:O2A	2.08	0.54
1:A:262:ARG:HH11	1:A:262:ARG:CA	2.20	0.53
1:B:243:LEU:O	1:B:247:LYS:HG3	2.08	0.53
1:E:200:GLU:O	1:E:204:SER:OG	2.26	0.53
1:B:255:GLU:OE2	1:B:257:TYR:OH	2.22	0.53
1:D:119:ASN:ND2	2:D:503:NAP:H4D	2.25	0.52
1:D:126:LEU:N	1:D:126:LEU:HD23	2.24	0.52
1:D:140:MET:HA	1:D:140:MET:HE3	1.91	0.52
1:E:219:ASP:OD2	1:E:238:LYS:HG2	2.10	0.52
1:B:169:SER:O	2:B:502:NAP:H6N	2.09	0.51
1:B:55:ALA:HA	1:B:83:ALA:HB2	1.93	0.51
1:D:18:GLN:O	1:D:28:ARG:NH2	2.44	0.51
1:A:270:ASN:HD22	1:A:270:ASN:C	2.13	0.51
1:D:23:SER:O	1:D:251:LEU:HD22	2.10	0.51
1:E:231:VAL:CG1	1:E:233:MET:HG2	2.37	0.50
1:D:26:GLU:OE1	1:D:26:GLU:HA	2.11	0.50
1:D:140:MET:HE3	1:D:144:PHE:HB3	1.93	0.50
1:B:97:THR:O	1:B:101:GLN:HG3	2.11	0.50
1:A:42:ALA:HB3	1:A:63:VAL:HB	1.93	0.50
1:D:68:LYS:HB3	4:D:941:HOH:O	2.10	0.50
1:D:243:LEU:O	1:D:247:LYS:HG3	2.11	0.50
1:A:122:THR:O	1:A:124:THR:HG22	2.12	0.50
1:A:179:MET:CE	1:B:286:MET:SD	3.00	0.50
1:B:200:GLU:O	1:B:204:SER:OG	2.28	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:44:LYS:HG3	2:D:503:NAP:H3B	1.94	0.49
1:A:140:MET:CA	1:A:140:MET:HE3	2.39	0.49
1:E:120:HIS:HE1	1:E:146:SER:OG	1.96	0.49
1:A:278:GLU:HG2	1:D:266:LEU:HD21	1.95	0.48
1:D:261:SER:O	1:D:265:THR:HG23	2.13	0.48
1:B:227:VAL:HB	1:B:231:VAL:HB	1.95	0.48
1:B:231:VAL:HG12	1:B:233:MET:CG	2.44	0.48
1:B:279:LEU:HD21	1:E:263:TRP:HH2	1.77	0.48
1:E:216:GLY:HA3	1:E:259:ASP:OD2	2.13	0.48
1:E:262:ARG:O	1:E:262:ARG:HG3	2.14	0.48
1:D:243:LEU:HG	1:D:247:LYS:HE3	1.96	0.48
1:D:233:MET:CE	1:E:283:SER:HB2	2.44	0.48
1:B:216:GLY:HA3	1:B:259:ASP:OD2	2.13	0.48
1:A:68:LYS:HD3	1:A:72:GLN:NE2	2.28	0.48
1:D:231:VAL:HG12	1:D:233:MET:CG	2.29	0.47
1:A:93:MET:HG3	1:A:120:HIS:CE1	2.49	0.47
1:B:279:LEU:CD2	1:E:263:TRP:CH2	2.97	0.47
1:A:263:TRP:N	1:A:263:TRP:HD1	2.13	0.47
1:D:169:SER:O	2:D:503:NAP:H6N	2.14	0.47
1:B:53:HIS:O	1:B:57:MET:HG3	2.14	0.47
1:B:136:VAL:HG22	1:B:182:ALA:HB2	1.97	0.47
1:B:42:ALA:HB3	1:B:63:VAL:HB	1.97	0.47
1:A:233:MET:CE	1:B:283:SER:HB2	2.45	0.46
1:B:64:THR:O	1:B:65:ALA:HB2	2.15	0.46
1:A:217:LEU:O	1:A:218:ILE:HD13	2.16	0.46
1:D:120:HIS:HE1	1:D:146:SER:OG	1.97	0.46
1:B:263:TRP:CD1	1:B:263:TRP:N	2.80	0.46
1:E:52:TYR:O	1:E:56:LYS:HG3	2.16	0.46
1:E:141:GLU:HA	1:E:145:LEU:HB2	1.97	0.46
1:A:137:ARG:NH2	1:B:145:LEU:CD2	2.76	0.46
1:A:126:LEU:CD2	1:A:126:LEU:N	2.77	0.46
1:B:287:ASP:N	1:B:287:ASP:OD2	2.38	0.46
1:A:52:TYR:O	1:A:56:LYS:HG3	2.16	0.46
1:E:227:VAL:HB	1:E:231:VAL:HB	1.98	0.46
1:E:179:MET:CE	3:E:604:311:H1B	2.45	0.46
1:D:178:PRO:O	1:D:179:MET:HB2	2.15	0.45
1:A:216:GLY:HA3	1:A:259:ASP:OD2	2.16	0.45
1:B:284:TYR:HD2	1:B:286:MET:CE	2.26	0.45
3:B:602:311:H2A	3:B:602:311:H10	1.64	0.45
1:B:141:GLU:HA	1:B:145:LEU:HB2	1.98	0.45
1:B:231:VAL:HG12	1:B:233:MET:HG2	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:40:THR:CB	1:E:120:HIS:HD2	2.29	0.45
1:B:136:VAL:HA	1:B:182:ALA:HB1	1.99	0.45
1:B:262:ARG:O	1:B:262:ARG:HG3	2.15	0.44
1:D:94:GLU:OE1	1:D:138:LYS:HE2	2.16	0.44
1:D:274:LYS:HG2	1:D:274:LYS:H	1.61	0.44
1:B:276:LEU:HA	1:B:276:LEU:HD23	1.83	0.44
1:E:68:LYS:HD2	1:E:72:GLN:NE2	2.32	0.44
1:B:66:ARG:HB2	2:B:502:NAP:O2X	2.17	0.44
1:A:140:MET:O	1:A:144:PHE:HB3	2.17	0.44
1:D:199:LYS:O	1:D:203:VAL:HG13	2.17	0.44
1:B:278:GLU:HG2	1:E:263:TRP:HZ2	1.82	0.43
1:A:200:GLU:O	1:A:204:SER:OG	2.36	0.43
1:E:231:VAL:CG1	1:E:233:MET:CG	2.95	0.43
1:D:227:VAL:HB	1:D:231:VAL:HB	2.01	0.43
1:D:262:ARG:HH11	1:D:262:ARG:HB2	1.77	0.43
1:A:140:MET:HE3	1:A:144:PHE:HB3	2.00	0.42
1:A:284:TYR:CD2	1:A:286:MET:HE1	2.54	0.42
1:B:287:ASP:O	1:B:288:ARG:CB	2.67	0.42
1:D:19:MET:SD	1:D:31:MET:CE	3.08	0.42
1:E:219:ASP:OD1	1:E:237:PRO:HA	2.19	0.42
1:E:284:TYR:HD2	1:E:286:MET:CE	2.32	0.42
1:D:144:PHE:O	1:D:147:TYR:HB2	2.20	0.42
1:A:248:GLY:HA3	1:A:256:VAL:HG21	2.02	0.42
1:B:40:THR:CB	1:B:120:HIS:HD2	2.32	0.42
1:B:125:SER:HB2	4:B:926:HOH:O	2.19	0.42
1:E:161:SER:O	1:E:162:ASN:HB2	2.20	0.41
1:A:273:ARG:O	1:A:277:GLU:HG3	2.21	0.41
1:E:42:ALA:HB3	1:E:63:VAL:HB	2.03	0.41
1:B:169:SER:N	1:B:213:CYS:O	2.45	0.41
1:A:176:ALA:HB2	1:B:195:SER:HB3	2.02	0.41
1:A:140:MET:CE	1:A:140:MET:HA	2.47	0.41
1:A:161:SER:O	1:A:162:ASN:HB2	2.20	0.41
1:A:199:LYS:O	1:A:203:VAL:HG13	2.21	0.41
1:B:287:ASP:O	1:B:288:ARG:HB3	2.20	0.41
1:E:286:MET:HE3	1:E:286:MET:HB2	1.79	0.41
1:D:263:TRP:HD1	1:D:263:TRP:N	2.19	0.41
1:B:140:MET:HE3	1:B:144:PHE:HB3	2.03	0.41
1:E:148:VAL:O	1:E:152:VAL:HG23	2.21	0.41
3:A:601:311:H10	3:A:601:311:H2A	1.82	0.41
1:A:287:ASP:N	1:A:287:ASP:OD2	2.54	0.41
1:D:251:LEU:HD12	1:D:253:GLN:HE21	1.86	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:120:HIS:CE1	1:A:146:SER:OG	2.73	0.41
1:D:52:TYR:O	1:D:56:LYS:HG3	2.21	0.40
1:A:141:GLU:HA	1:A:145:LEU:HB2	2.03	0.40
1:D:185:ALA:HB2	1:E:193:PHE:HB2	2.03	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	264/286 (92%)	253 (96%)	9 (3%)	2 (1%)	24	26
1	B	278/286 (97%)	265 (95%)	13 (5%)	0	100	100
1	D	272/286 (95%)	261 (96%)	9 (3%)	2 (1%)	26	29
1	E	262/286 (92%)	252 (96%)	10 (4%)	0	100	100
All	All	1076/1144 (94%)	1031 (96%)	41 (4%)	4 (0%)	39	46

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	288	ARG
1	D	219	ASP
1	A	65	ALA
1	D	65	ALA

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	222/237 (94%)	205 (92%)	17 (8%)	16	17
1	B	230/237 (97%)	209 (91%)	21 (9%)	12	11
1	D	223/237 (94%)	206 (92%)	17 (8%)	16	18
1	E	220/237 (93%)	201 (91%)	19 (9%)	13	13
All	All	895/948 (94%)	821 (92%)	74 (8%)	14	15

All (74) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	28	ARG
1	A	44	LYS
1	A	68	LYS
1	A	124	THR
1	A	145	LEU
1	A	160	GLN
1	A	204	SER
1	A	222	THR
1	A	225	LYS
1	A	232	HIS
1	A	233	MET
1	A	262	ARG
1	A	266	LEU
1	A	270	ASN
1	A	278	GLU
1	A	286	MET
1	A	287	ASP
1	B	26	GLU
1	B	28	ARG
1	B	44	LYS
1	B	68	LYS
1	B	101	GLN
1	B	124	THR
1	B	145	LEU
1	B	160	GLN
1	B	204	SER
1	B	205	ARG
1	B	222	THR
1	B	225	LYS
1	B	233	MET

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Mol	Chain	Res	Type
1	B	262	ARG
1	B	265	THR
1	B	266	LEU
1	B	270	ASN
1	B	278	GLU
1	B	286	MET
1	B	287	ASP
1	B	288	ARG
1	D	23	SER
1	D	24	ASN
1	D	26	GLU
1	D	44	LYS
1	D	68	LYS
1	D	124	THR
1	D	145	LEU
1	D	160	GLN
1	D	204	SER
1	D	205	ARG
1	D	222	THR
1	D	225	LYS
1	D	240	GLU
1	D	262	ARG
1	D	270	ASN
1	D	274	LYS
1	D	278	GLU
1	E	26	GLU
1	E	44	LYS
1	E	68	LYS
1	E	85	SER
1	E	128	LEU
1	E	145	LEU
1	E	160	GLN
1	E	204	SER
1	E	205	ARG
1	E	222	THR
1	E	225	LYS
1	E	233	MET
1	E	262	ARG
1	E	265	THR
1	E	266	LEU
1	E	270	ASN
1	E	278	GLU

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Mol	Chain	Res	Type
1	E	286	MET
1	E	287	ASP

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	72	GLN
1	A	87	HIS
1	A	119	ASN
1	A	120	HIS
1	A	270	ASN
1	B	119	ASN
1	B	120	HIS
1	B	270	ASN
1	D	24	ASN
1	D	87	HIS
1	D	119	ASN
1	D	120	HIS
1	D	253	GLN
1	D	270	ASN
1	E	119	ASN
1	E	120	HIS
1	E	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	501	-	42,52,52	1.15	2 (4%)	54,80,80	1.22	4 (7%)
3	311	A	601	-	26,26,26	2.02	10 (38%)	35,38,38	2.57	12 (34%)
2	NAP	B	502	-	42,52,52	1.29	3 (7%)	54,80,80	1.22	2 (3%)
3	311	B	602	-	26,26,26	2.17	9 (34%)	35,38,38	2.30	13 (37%)
2	NAP	D	503	-	42,52,52	0.86	1 (2%)	54,80,80	1.14	3 (5%)
3	311	D	603	-	26,26,26	2.18	9 (34%)	35,38,38	2.51	13 (37%)
2	NAP	E	504	-	42,52,52	1.02	2 (4%)	54,80,80	1.31	6 (11%)
3	311	E	604	-	26,26,26	2.56	15 (57%)	35,38,38	3.35	22 (62%)

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	501	-	-	0/27/67/67	0/5/5/5
3	311	A	601	-	-	0/12/24/24	0/3/3/3
2	NAP	B	502	-	-	0/27/67/67	0/5/5/5
3	311	B	602	-	-	0/12/24/24	0/3/3/3
2	NAP	D	503	-	-	0/27/67/67	0/5/5/5
3	311	D	603	-	-	0/12/24/24	0/3/3/3
2	NAP	E	504	-	-	0/27/67/67	0/5/5/5
3	311	E	604	-	-	0/12/24/24	0/3/3/3

All (51) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	D	603	311	C15-C16	-2.94	1.44	1.48
3	E	604	311	C4-C6	-2.69	1.33	1.38
3	E	604	311	C6-C17	-2.68	1.33	1.39
3	A	601	311	F24-C18	-2.65	1.29	1.35
2	B	502	NAP	C7N-N7N	2.00	1.37	1.33
3	B	602	311	C8-C7	2.01	1.42	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	E	504	NAP	O4D-C1D	2.02	1.43	1.41
3	E	604	311	C9-C15	2.06	1.43	1.39
3	A	601	311	C4-C6	2.07	1.43	1.38
3	E	604	311	O23-C19	2.15	1.27	1.22
3	A	601	311	C13-C20	2.16	1.56	1.52
3	D	603	311	C2-C20	2.30	1.58	1.53
3	A	601	311	O23-C19	2.32	1.27	1.22
2	B	502	NAP	O4D-C1D	2.33	1.44	1.41
3	D	603	311	C9-C18	2.36	1.41	1.37
3	B	602	311	C3-C20	2.36	1.58	1.53
3	E	604	311	C1-C14	2.42	1.55	1.51
3	D	603	311	C8-C7	2.51	1.43	1.38
3	B	602	311	C13-N22	2.53	1.49	1.46
3	E	604	311	C15-C16	2.62	1.52	1.48
3	E	604	311	C2-C20	2.71	1.58	1.53
3	E	604	311	C17-N21	2.75	1.38	1.34
3	B	602	311	C9-C18	2.84	1.42	1.37
2	A	501	NAP	C7N-N7N	2.95	1.39	1.33
3	B	602	311	C13-C20	2.98	1.58	1.52
3	A	601	311	C12-N22	3.00	1.52	1.47
3	A	601	311	C8-C15	3.02	1.45	1.39
3	A	601	311	C13-N22	3.08	1.49	1.46
3	A	601	311	C15-C16	3.10	1.53	1.48
3	E	604	311	C11-C20	3.14	1.59	1.53
3	E	604	311	C12-N22	3.17	1.52	1.47
2	D	503	NAP	O4B-C1B	3.19	1.45	1.41
3	B	602	311	C19-N22	3.20	1.42	1.34
2	E	504	NAP	O4B-C1B	3.21	1.45	1.41
3	D	603	311	C3-C20	3.23	1.59	1.53
3	E	604	311	C8-C15	3.43	1.46	1.39
3	B	602	311	C14-C18	3.56	1.41	1.37
3	D	603	311	C13-N22	3.61	1.50	1.46
3	D	603	311	C6-C17	3.63	1.46	1.39
3	A	601	311	C8-C7	3.85	1.45	1.38
3	E	604	311	C16-N21	3.95	1.40	1.34
3	E	604	311	C13-C20	4.02	1.60	1.52
3	D	603	311	C12-N22	4.05	1.54	1.47
3	B	602	311	C11-C10	4.06	1.63	1.52
3	E	604	311	C8-C7	4.10	1.46	1.38
3	A	601	311	C17-N21	4.42	1.41	1.34
2	A	501	NAP	O4B-C1B	4.51	1.46	1.41
3	D	603	311	C11-C20	4.67	1.61	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	E	604	311	C7-C14	4.89	1.51	1.39
3	B	602	311	C2-C20	4.94	1.63	1.53
2	B	502	NAP	O4B-C1B	5.37	1.48	1.41

All (75) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	E	604	311	C1-C14-C18	-9.43	116.27	121.68
3	A	601	311	C1-C14-C18	-8.92	116.56	121.68
3	B	602	311	C1-C14-C18	-7.79	117.21	121.68
3	D	603	311	C1-C14-C18	-7.50	117.38	121.68
3	E	604	311	C8-C7-C14	-6.35	113.17	122.00
3	A	601	311	C8-C7-C14	-5.38	114.52	122.00
3	E	604	311	C9-C15-C16	-5.30	113.61	120.54
3	E	604	311	C5-C16-N21	-4.44	115.88	122.01
3	B	602	311	C11-C20-C13	-4.06	106.00	108.12
3	E	604	311	C3-C20-C2	-3.83	102.59	109.38
3	D	603	311	C19-C17-N21	-3.72	109.57	117.40
3	E	604	311	C10-C12-N22	-3.69	103.03	110.65
3	B	602	311	C11-C10-C12	-3.38	105.74	110.72
3	A	601	311	C8-C15-C9	-3.18	113.94	118.17
3	D	603	311	C9-C15-C16	-3.11	116.47	120.54
3	D	603	311	C15-C16-N21	-3.02	112.11	116.13
2	E	504	NAP	N3A-C2A-N1A	-3.01	126.59	128.89
3	E	604	311	F24-C18-C9	-2.99	112.98	118.59
2	A	501	NAP	O2B-P2B-O1X	-2.92	99.82	107.11
3	E	604	311	C13-N22-C19	-2.91	114.32	121.94
2	E	504	NAP	O7N-C7N-N7N	-2.88	118.55	122.59
3	A	601	311	C9-C15-C16	-2.87	116.79	120.54
2	D	503	NAP	C4B-O4B-C1B	-2.65	106.81	109.72
2	E	504	NAP	C4B-O4B-C1B	-2.60	106.86	109.72
3	E	604	311	O23-C19-N22	-2.57	118.34	122.42
2	A	501	NAP	O4D-C4D-C5D	-2.51	100.34	109.32
3	D	603	311	C3-C20-C11	-2.48	106.17	110.02
2	B	502	NAP	C4B-O4B-C1B	-2.47	107.00	109.72
3	B	602	311	C2-C20-C11	-2.44	106.23	110.02
3	B	602	311	C5-C16-N21	-2.43	118.66	122.01
3	A	601	311	C4-C6-C17	-2.37	115.56	118.64
3	B	602	311	C9-C15-C16	-2.32	117.51	120.54
3	B	602	311	C19-C17-N21	-2.29	112.58	117.40
2	A	501	NAP	C4D-O4D-C1D	-2.28	107.22	109.72
3	D	603	311	C8-C7-C14	-2.21	118.94	122.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	E	604	311	C8-C15-C9	-2.19	115.26	118.17
3	B	602	311	C6-C17-N21	-2.18	120.30	122.90
3	A	601	311	C5-C16-N21	-2.16	119.03	122.01
3	E	604	311	C11-C10-C12	-2.09	107.64	110.72
3	E	604	311	C3-C20-C11	-2.08	106.80	110.02
3	E	604	311	C4-C6-C17	-2.06	115.96	118.64
2	D	503	NAP	O3B-C3B-C2B	-2.05	105.22	111.16
3	E	604	311	C1-C14-C7	2.01	124.43	120.33
3	D	603	311	C4-C5-C16	2.01	121.57	118.88
3	E	604	311	C16-N21-C17	2.03	121.30	118.03
2	E	504	NAP	O2N-PN-O1N	2.11	123.97	112.53
2	E	504	NAP	C3N-C7N-N7N	2.12	120.14	117.82
3	B	602	311	C3-C20-C13	2.13	114.31	109.42
3	B	602	311	C1-C14-C7	2.15	124.72	120.33
3	D	603	311	C12-N22-C13	2.18	117.20	113.98
3	A	601	311	C4-C5-C16	2.33	121.99	118.88
3	A	601	311	C5-C16-C15	2.38	126.94	121.84
3	A	601	311	C7-C14-C18	2.42	117.71	115.93
3	D	603	311	C2-C20-C11	2.50	113.91	110.02
3	B	602	311	O23-C19-N22	2.61	126.57	122.42
2	A	501	NAP	O4D-C1D-N1N	2.61	111.00	108.13
3	A	601	311	C1-C14-C7	2.63	125.69	120.33
3	D	603	311	C8-C15-C16	2.64	125.54	121.24
3	D	603	311	C1-C14-C7	2.64	125.72	120.33
3	B	602	311	C7-C14-C18	2.66	117.89	115.93
2	D	503	NAP	O4D-C1D-N1N	2.88	111.29	108.13
3	A	601	311	C7-C8-C15	3.10	125.67	121.14
3	E	604	311	C7-C8-C15	3.31	125.97	121.14
3	E	604	311	C3-C20-C13	3.33	117.09	109.42
3	E	604	311	F24-C18-C14	3.34	120.99	117.83
3	E	604	311	C6-C4-C5	3.43	125.14	120.24
2	E	504	NAP	O4D-C1D-N1N	3.61	112.10	108.13
3	B	602	311	C6-C17-C19	3.79	126.63	119.20
3	D	603	311	C6-C17-C19	4.28	127.60	119.20
3	E	604	311	C7-C14-C18	4.29	119.09	115.93
3	A	601	311	C8-C15-C16	4.91	129.25	121.24
3	E	604	311	C12-N22-C13	5.02	121.39	113.98
2	B	502	NAP	O4D-C1D-N1N	5.41	114.07	108.13
3	E	604	311	C8-C15-C16	6.04	131.09	121.24
3	D	603	311	C11-C20-C13	7.01	111.80	108.12

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

7 monomers are involved in 16 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	501	NAP	1	0
3	A	601	311	1	0
2	B	502	NAP	4	0
3	B	602	311	1	0
2	D	503	NAP	4	0
2	E	504	NAP	3	0
3	E	604	311	2	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	264/286 (92%)	-0.10	10 (3%) 44 58	17, 29, 56, 100	0
1	B	279/286 (97%)	-0.09	9 (3%) 51 64	18, 30, 60, 100	0
1	D	273/286 (95%)	-0.16	9 (3%) 50 63	14, 26, 66, 86	0
1	E	263/286 (91%)	0.07	12 (4%) 36 51	18, 31, 58, 86	0
All	All	1079/1144 (94%)	-0.07	40 (3%) 45 59	14, 29, 60, 100	0

All (40) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	12	SER	5.3
1	D	23	SER	5.2
1	E	263	TRP	5.1
1	E	25	GLU	4.3
1	D	13	MET	4.2
1	D	262	ARG	4.1
1	A	288	ARG	3.8
1	D	24	ASN	3.7
1	E	285	ASN	3.5
1	E	205	ARG	3.4
1	D	22	GLY	3.3
1	B	24	ASN	3.3
1	E	286	MET	3.2
1	B	262	ARG	3.2
1	A	232	HIS	3.1
1	E	203	VAL	3.0
1	A	266	LEU	2.9
1	D	205	ARG	2.9
1	B	168	VAL	2.8
1	B	203	VAL	2.8
1	B	25	GLU	2.8

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Mol	Chain	Res	Type	RSRZ
1	E	287	ASP	2.7
1	B	12	SER	2.6
1	A	234	GLN	2.6
1	B	10	MET	2.6
1	E	279	LEU	2.6
1	B	205	ARG	2.5
1	A	233	MET	2.5
1	E	262	ARG	2.5
1	A	205	ARG	2.4
1	B	190	LEU	2.4
1	A	263	TRP	2.3
1	A	289	PHE	2.2
1	D	21	ARG	2.2
1	A	203	VAL	2.1
1	E	117	ILE	2.1
1	E	228	SER	2.1
1	D	282	THR	2.0
1	A	190	LEU	2.0
1	E	190	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, 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	LLDF	B-factors(Å ²)	Q<0.9
3	311	B	602	24/24	0.95	0.12	-0.39	12,21,26,27	0
3	311	D	603	24/24	0.97	0.10	-0.55	11,18,27,28	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
3	311	A	601	24/24	0.96	0.11	-0.69	18,25,37,38	0
2	NAP	B	502	48/48	0.97	0.10	-0.74	20,23,27,28	0
2	NAP	D	503	48/48	0.98	0.09	-0.77	18,20,24,26	0
2	NAP	E	504	48/48	0.97	0.10	-0.78	24,25,29,30	0
2	NAP	A	501	48/48	0.97	0.09	-0.90	22,23,26,28	0
3	311	E	604	24/24	0.97	0.09	-1.07	16,22,30,43	0

6.5 Other polymers [i](#)

There are no such residues in this entry.