



# Full wwPDB X-ray Structure Validation Report

Feb 28, 2014 – 11:27 PM GMT

PDB ID : 3OQ1  
Title : Crystal Structure of 11beta-HydroxysteroidDehydrogenase-1 (11b-HSD1) in  
Complex with Diarylsulfone Inhibitor  
Authors : Wang, Z.; Sudom, A.; Walker, N.P.  
Deposited on : 2010-09-02  
Resolution : 2.60 Å(reported)

This is a full wwPDB 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/ValidationPDFNotes.html>

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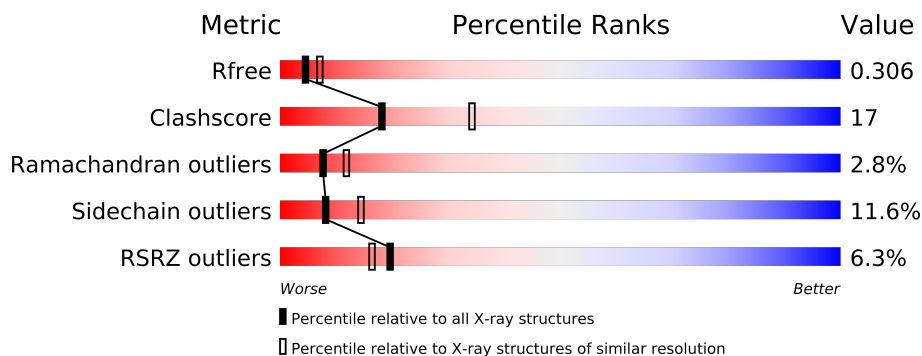
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467  
Mogul : 1.15 2013  
Xtriage (Phenix) : dev-1323  
EDS : stable22639  
Percentile statistics : 21963  
Refmac : 5.8.0049  
CCP4 : 6.3.0 (Settle)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)  
Validation Pipeline (wwPDB-VP) : stable22683

# 1 Overall quality at a glance

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))
$R_{free}$	66092	1718 (2.60-2.60)
Clashscore	79885	2154 (2.60-2.60)
Ramachandran outliers	78287	2113 (2.60-2.60)
Sidechain outliers	78261	2113 (2.60-2.60)
RSRZ outliers	66119	1718 (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. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Mol	Chain	Length	Quality of chain
1	A	286	
1	B	286	
1	C	286	
1	D	286	

## 2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 8469 atoms, of which 0 are hydrogen and 0 are deuterium.

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	261	Total	C	N	O	S	0	0	0
			2001	1277	339	370	15			
1	B	267	Total	C	N	O	S	0	1	0
			2057	1311	348	382	16			
1	C	269	Total	C	N	O	S	0	0	0
			2072	1321	351	384	16			
1	D	261	Total	C	N	O	S	0	1	0
			2008	1282	341	370	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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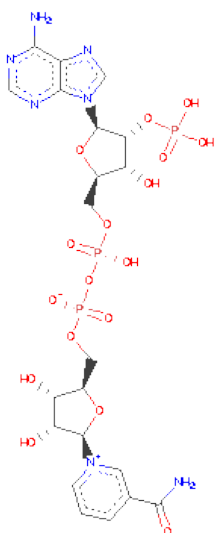
Chain	Residue	Modelled	Actual	Comment	Reference
B	10	GLN	-	EXPRESSION TAG	UNP P28845
B	11	HIS	-	EXPRESSION TAG	UNP P28845
B	12	GLN	-	EXPRESSION TAG	UNP P28845
B	13	HIS	-	EXPRESSION TAG	UNP P28845
B	14	GLN	-	EXPRESSION TAG	UNP P28845
B	15	HIS	-	EXPRESSION TAG	UNP P28845
B	16	GLN	-	EXPRESSION TAG	UNP P28845
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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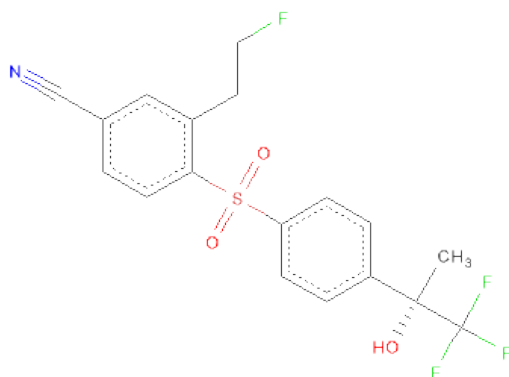
Chain	Residue	Modelled	Actual	Comment	Reference
D	16	GLN	-	EXPRESSION TAG	UNP P28845
D	17	HIS	-	EXPRESSION TAG	UNP P28845
D	18	GLN	-	EXPRESSION TAG	UNP P28845
D	19	HIS	-	EXPRESSION TAG	UNP P28845
D	20	GLN	-	EXPRESSION TAG	UNP P28845
D	21	GLN	-	EXPRESSION TAG	UNP P28845
D	22	PRO	-	EXPRESSION TAG	UNP P28845
D	23	LEU	-	EXPRESSION TAG	UNP P28845
D	272	SER	CYS	ENGINEERED MUTATION	UNP P28845

- Molecule 2 is NADP NICOTINAMIDE-ADENINE-DINUCLEOTIDEPHOSPHATE (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 3-(2-FLUOROETHYL)-4-({4-[(2S)-1,1,1-TRIFLUORO-2-HYDROXYPRO PAN-2-YL]PHENYL}SULFONYL)BENZONITRILE (three-letter code: 3OQ) (formula:  $C_{18}H_{15}F_4NO_3S$ ).

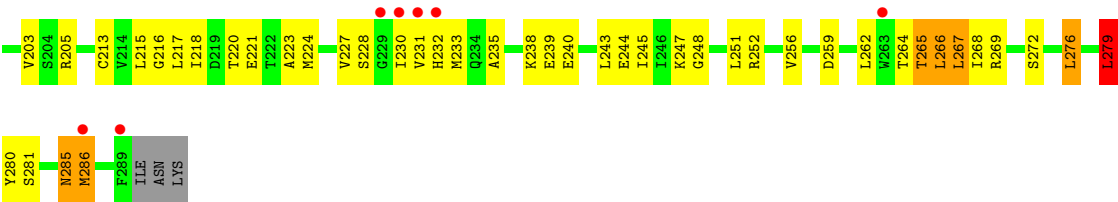


Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
3	C	1	Total	C	F	N	O	S	0	0
			27	18	4	1	3	1		
3	B	1	Total	C	F	N	O	S	0	0
			27	18	4	1	3	1		
3	D	1	Total	C	F	N	O	S	0	0
			27	18	4	1	3	1		
3	A	1	Total	C	F	N	O	S	0	0
			27	18	4	1	3	1		

- Molecule 4 is water.

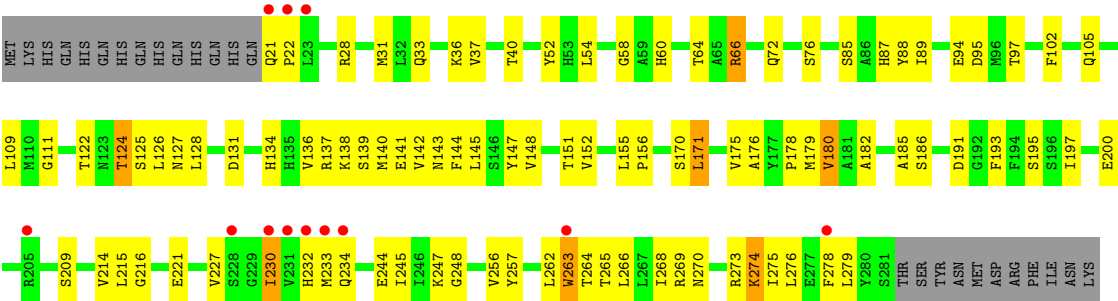
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	C	10	Total	O	0	0
			10	10		
4	B	10	Total	O	0	0
			10	10		
4	D	9	Total	O	0	0
			9	9		
4	A	2	Total	O	0	0
			2	2		





● Molecule 1: Corticosteroid 11-beta-dehydrogenaseisozyme 1

Chain D: 





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	56.30Å 153.40Å 73.59Å 90.00° 92.40° 90.00°	Depositor
Resolution (Å)	38.00 – 2.60 38.04 – 2.60	Depositor EDS
% Data completeness (in resolution range)	96.2 (38.00-2.60) 96.2 (38.04-2.60)	Depositor EDS
$R_{merge}$	0.07	Depositor
$R_{sym}$	0.07	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.88 (at 2.61Å)	Xtriage
Refinement program	REFMAC 5.5.0109	Depositor
R, $R_{free}$	0.220 , 0.308 0.222 , 0.306	Depositor DCC
$R_{free}$ test set	1843 reflections (5.26%)	DCC
Wilson B-factor (Å <sup>2</sup> )	60.2	Xtriage
Anisotropy	0.357	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.34 , 45.3	EDS
Estimated twinning fraction	0.055 for h,-k,-l	Xtriage
L-test for twinning	$\langle  L  \rangle = 0.46$ , $\langle L^2 \rangle = 0.29$	Xtriage
Outliers	0 of 36860 reflections	Xtriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	8469	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	65.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.63% of the height of the origin peak. No significant pseudotranslation is detected.*

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

## 5 Model quality

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: 3OQ, 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	0.65	0/2035	0.76	0/2748
1	B	0.73	0/2096	0.84	1/2831 (0.0%)
1	C	0.69	0/2108	0.78	1/2846 (0.0%)
1	D	0.78	0/2046	0.82	0/2763
All	All	0.71	0/8285	0.80	2/11188 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	66	ARG	NE-CZ-NH1	-6.19	117.21	120.30
1	C	276	LEU	CA-CB-CG	5.38	127.69	115.30

There are no chirality outliers.

There are no planarity outliers.

### 5.2 Close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2001	0	2051	96	0
1	B	2057	0	2098	75	0
1	C	2072	0	2113	75	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	D	2008	0	2058	61	0
2	A	48	0	25	6	0
2	B	48	0	25	5	0
2	C	48	0	25	4	0
2	D	48	0	25	3	0
3	A	27	0	15	0	0
3	B	27	0	15	0	0
3	C	27	0	15	3	0
3	D	27	0	15	3	0
4	A	2	0	0	0	0
4	B	10	0	0	0	0
4	C	10	0	0	2	0
4	D	9	0	0	1	0
All	All	8469	0	8480	288	0

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 17.

All (288) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:62:VAL:HG23	1:A:110:MET:HE3	1.23	1.09
1:C:44:LYS:O	1:C:48:ARG:HB3	1.63	0.99
1:B:126:LEU:O	1:B:127:ASN:ND2	2.00	0.94
1:C:60:HIS:HD1	1:C:85:SER:HG	1.24	0.84
1:A:206:VAL:HG12	1:A:208:VAL:HG23	1.61	0.82
1:A:32:LEU:O	1:A:35:LYS:HG2	1.79	0.82
1:C:43:SER:HB3	2:C:3:NAP:O3B	1.80	0.80
1:B:248:GLY:HA2	1:B:253:GLN:HE21	1.47	0.79
1:D:140:MET:HE1	1:D:186:SER:HA	1.66	0.78
1:A:271:PRO:O	1:A:275:ILE:HD12	1.82	0.78
1:A:273:ARG:HG3	1:D:175:VAL:HG12	1.67	0.77
1:B:259:ASP:OD1	1:B:264:THR:HG21	1.84	0.76
1:A:129:PHE:CD2	1:D:197:ILE:HD11	2.21	0.75
1:C:60:HIS:ND1	1:C:85:SER:OG	2.20	0.75
1:C:179:MET:O	1:C:180:VAL:HG23	1.86	0.74
1:A:269:ARG:HH21	1:A:269:ARG:HB2	1.51	0.74
1:D:233:MET:HG3	3:D:293:3OQ:N6	2.01	0.73
1:B:44:LYS:HG3	2:B:2:NAP:H3B	1.70	0.72
1:B:216:GLY:HA3	1:B:259:ASP:OD2	1.90	0.72
1:B:40:THR:HA	1:B:64:THR:HG22	1.71	0.71
1:B:276:LEU:HD13	1:C:267:LEU:HD12	1.70	0.71
1:D:140:MET:CE	1:D:186:SER:HA	2.20	0.70

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:185:ALA:HB2	1:D:193:PHE:HB2	1.73	0.69
1:B:27:PHE:CD2	1:B:247:LYS:HE2	2.27	0.69
1:D:171:LEU:HD12	1:D:216:GLY:HA2	1.74	0.69
1:A:62:VAL:HG23	1:A:110:MET:CE	2.13	0.68
1:B:66:ARG:HB2	2:B:2:NAP:O2X	1.93	0.68
1:C:279:LEU:HD13	1:D:263:TRP:CZ2	2.29	0.68
1:B:92:THR:OG1	1:B:94:GLU:HB2	1.93	0.68
1:D:275:ILE:O	1:D:279:LEU:HG	1.94	0.67
1:D:270:ASN:ND2	1:D:273:ARG:H	1.93	0.67
1:D:137:ARG:O	1:D:141:GLU:HG3	1.95	0.67
1:B:179:MET:CE	1:C:286:MET:HB3	2.25	0.66
1:B:200:GLU:O	1:B:204:SER:HB2	1.95	0.66
1:A:200:GLU:O	1:A:204:SER:HB2	1.97	0.65
1:D:178:PRO:O	1:D:179:MET:HB2	1.96	0.64
1:D:248:GLY:HA3	1:D:256:VAL:HG21	1.80	0.64
1:D:37:VAL:HG11	1:D:54:LEU:HD13	1.79	0.64
1:B:126:LEU:C	1:B:127:ASN:HD22	2.00	0.63
1:A:35:LYS:O	1:A:59:ALA:HB1	1.98	0.63
1:D:136:VAL:HG22	1:D:182:ALA:HB2	1.79	0.63
1:B:148:VAL:HG22	1:B:193:PHE:CE1	2.33	0.63
2:D:4:NAP:O2N	2:D:4:NAP:N7N	2.32	0.63
1:C:239:GLU:CD	1:C:239:GLU:H	2.00	0.63
1:C:94:GLU:OE2	1:C:138:LYS:HE3	1.99	0.63
1:A:121:ILE:HG13	1:A:143:ASN:ND2	2.14	0.62
3:C:293:3OQ:H15	3:C:293:3OQ:C16	2.29	0.62
3:C:293:3OQ:H11	3:C:293:3OQ:H15	1.82	0.62
1:C:113:LEU:CD2	1:C:158:LEU:HD21	2.30	0.62
1:D:124:THR:HG22	3:D:293:3OQ:F23	1.91	0.61
1:B:262:LEU:H	1:B:263:TRP:HE3	1.47	0.61
1:A:202:SER:O	1:A:204:SER:N	2.33	0.60
1:C:139:SER:O	1:C:143:ASN:HB2	2.00	0.60
1:B:261:SER:HG	1:B:263:TRP:HE3	1.50	0.60
1:D:28:ARG:O	1:D:31:MET:HG3	2.02	0.60
1:B:270:ASN:HD22	1:B:270:ASN:C	2.05	0.60
1:B:151:THR:HG23	1:B:165:ILE:HD12	1.83	0.59
1:D:60:HIS:ND1	1:D:85:SER:HB2	2.17	0.59
1:A:243:LEU:O	1:A:247:LYS:HG3	2.03	0.59
1:A:272:SER:O	1:A:276:LEU:HD23	2.03	0.59
1:C:215:LEU:O	2:C:3:NAP:H5N	2.03	0.59
1:B:193:PHE:HB2	1:C:185:ALA:HB2	1.85	0.59
1:D:66:ARG:HD3	2:D:4:NAP:C6A	2.33	0.59
1:A:170:SER:OG	2:A:1:NAP:H6N	2.04	0.58

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:268:ILE:HG23	1:C:276:LEU:HD21	1.84	0.58
1:B:270:ASN:C	1:B:270:ASN:ND2	2.57	0.58
1:B:133:ILE:HD13	1:C:149:VAL:HG22	1.84	0.58
1:B:261:SER:OG	1:B:264:THR:HG22	2.04	0.58
1:A:263:TRP:C	1:A:263:TRP:HE3	2.07	0.58
1:B:27:PHE:CE2	1:B:247:LYS:HE2	2.39	0.58
1:D:264:THR:O	1:D:268:ILE:HG13	2.02	0.58
1:A:176:ALA:HB2	1:D:195:SER:HB3	1.84	0.57
1:C:215:LEU:HD11	1:C:245:ILE:HD11	1.86	0.57
1:C:220:THR:O	1:C:224:MET:HG2	2.04	0.57
1:A:262:LEU:HA	1:A:265:THR:OG1	2.04	0.56
1:C:227:VAL:CG1	1:C:231:VAL:HG22	2.34	0.56
1:C:25:GLU:HG2	1:C:26:GLU:H	1.71	0.56
1:B:223:ALA:O	1:B:227:VAL:HG22	2.05	0.56
1:C:33:GLN:HB2	1:C:57:MET:O	2.05	0.56
1:A:62:VAL:CG2	1:A:110:MET:HE3	2.15	0.56
1:D:139:SER:O	1:D:143:ASN:HB2	2.06	0.56
1:C:35:LYS:HD2	1:C:114:ASP:OD1	2.05	0.56
1:D:95:ASP:OD1	1:D:97:THR:HB	2.07	0.55
1:C:28:ARG:O	1:C:31:MET:HG3	2.05	0.55
1:A:37:VAL:HG22	1:A:115:MET:HB3	1.88	0.55
1:B:262:LEU:HA	1:B:265:THR:OG1	2.06	0.55
1:B:94:GLU:OE2	1:B:138:LYS:HE2	2.07	0.55
1:A:197:ILE:HA	1:A:200:GLU:HG3	1.88	0.55
1:C:216:GLY:HA3	1:C:259:ASP:OD2	2.07	0.55
1:A:39:VAL:HB	1:A:63:VAL:HG12	1.87	0.55
1:C:227:VAL:HG13	1:C:231:VAL:HG22	1.89	0.55
1:A:276:LEU:O	1:A:280:TYR:HD1	1.90	0.55
1:D:180:VAL:HG13	1:D:180:VAL:O	2.07	0.55
1:B:162:ASN:OD1	1:B:207:ASN:ND2	2.39	0.54
1:A:58:GLY:HA2	1:A:83:ALA:HA	1.89	0.54
1:A:124:THR:HG23	1:A:135:HIS:NE2	2.22	0.54
1:C:248:GLY:HA3	1:C:256:VAL:HG21	1.89	0.54
1:C:33:GLN:HA	1:C:58:GLY:O	2.07	0.54
1:D:33:GLN:HA	1:D:58:GLY:O	2.08	0.54
1:A:198:ARG:NE	1:A:254:GLU:HG2	2.22	0.54
1:A:244:GLU:HG3	1:A:258:TYR:CD2	2.43	0.54
1:C:38:ILE:HD12	1:C:113:LEU:HD11	1.90	0.54
1:D:87:HIS:CG	1:D:109:LEU:HD22	2.43	0.54
1:B:126:LEU:HD13	1:B:179:MET:HG3	1.90	0.54
1:D:214:VAL:HG11	1:D:268:ILE:HG21	1.90	0.54
1:A:240:GLU:O	1:A:244:GLU:HG2	2.08	0.53

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:27:PHE:CD2	1:A:247:LYS:HG2	2.44	0.53
1:C:178:PRO:O	1:C:179:MET:HB2	2.09	0.53
1:D:40:THR:HA	1:D:64:THR:HG22	1.90	0.53
1:A:276:LEU:O	1:A:280:TYR:CD1	2.62	0.53
1:D:145:LEU:O	1:D:148:VAL:HB	2.08	0.53
1:D:270:ASN:HD22	1:D:273:ARG:CB	2.21	0.52
1:B:141:GLU:OE1	1:B:145:LEU:HD23	2.10	0.52
1:D:215:LEU:HD11	1:D:245:ILE:HD11	1.90	0.52
1:A:144:PHE:O	1:A:148:VAL:HG23	2.10	0.52
1:A:180:VAL:O	1:A:183:TYR:HB3	2.09	0.52
1:A:198:ARG:HA	1:A:210:ILE:HD12	1.92	0.52
1:A:263:TRP:C	1:A:263:TRP:CE3	2.83	0.51
1:D:64:THR:HB	1:D:102:PHE:CE1	2.45	0.51
1:B:264:THR:HG23	1:B:265:THR:N	2.25	0.51
1:D:244:GLU:OE1	1:D:247:LYS:HE2	2.10	0.51
1:D:151:THR:O	1:D:152:VAL:C	2.48	0.51
1:B:179:MET:HE1	1:C:286:MET:HB3	1.92	0.51
1:A:192:GLY:O	1:A:196:SER:HB3	2.11	0.51
1:A:212:LEU:HB3	1:A:255:GLU:HG3	1.93	0.51
1:C:203:VAL:HG11	1:C:286:MET:CE	2.41	0.51
1:A:223:ALA:CB	2:A:1:NAP:H72N	2.24	0.51
1:A:193:PHE:HB2	1:D:185:ALA:HB2	1.93	0.50
1:C:113:LEU:HD23	1:C:158:LEU:HD21	1.92	0.50
1:A:62:VAL:HG11	1:A:106:ALA:HB2	1.93	0.50
1:C:36:LYS:HG2	1:C:110:MET:HB3	1.93	0.50
1:C:73:LYS:HE3	4:C:5:HOH:O	2.11	0.50
1:B:219:ASP:OD2	1:B:219:ASP:O	2.30	0.50
1:B:63:VAL:HG23	1:B:71:LEU:HD22	1.94	0.50
1:A:257:TYR:O	1:A:258:TYR:HB2	2.12	0.50
1:A:95:ASP:HB3	1:A:98:PHE:HB3	1.94	0.50
1:A:128:LEU:HA	1:D:200:GLU:OE2	2.11	0.50
1:D:215:LEU:O	2:D:4:NAP:H5N	2.12	0.49
1:C:171:LEU:HD23	1:C:268:ILE:HD11	1.94	0.49
1:C:49:GLU:HG3	1:C:238:LYS:HG3	1.95	0.49
1:D:88:TYR:O	1:D:89:ILE:HG13	2.12	0.49
1:B:185:ALA:HB2	1:C:193:PHE:HB2	1.94	0.49
1:A:218:ILE:C	1:A:235:ALA:HB1	2.33	0.49
1:A:64:THR:O	1:A:65:ALA:HB2	2.13	0.49
1:D:227:VAL:HB	1:D:230:ILE:HG21	1.94	0.49
1:B:131:ASP:O	1:B:131:ASP:CG	2.50	0.49
1:A:29:PRO:HB3	1:A:57:MET:HG2	1.95	0.49
1:C:227:VAL:HG12	1:C:228:SER:N	2.28	0.48

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:C:180:VAL:O	1:C:180:VAL:CG1	2.60	0.48
1:C:259:ASP:HB3	1:C:265:THR:HG23	1.95	0.48
1:D:274:LYS:NZ	4:D:300:HOH:O	2.38	0.48
1:B:39:VAL:HG22	1:B:117:ILE:HD12	1.94	0.48
1:A:201:TYR:O	1:A:204:SER:CB	2.62	0.48
1:C:43:SER:HB2	1:C:65:ALA:CB	2.44	0.48
1:A:64:THR:HG22	1:A:65:ALA:H	1.79	0.48
1:A:61:VAL:HG23	1:A:61:VAL:O	2.13	0.48
1:B:261:SER:OG	1:B:263:TRP:HE3	1.97	0.48
1:B:62:VAL:HG23	1:B:110:MET:SD	2.53	0.48
1:A:220:THR:OG1	1:A:223:ALA:HB3	2.14	0.48
1:A:121:ILE:HG23	1:A:122:THR:N	2.29	0.47
1:B:44:LYS:HD2	2:B:2:NAP:H51A	1.95	0.47
1:A:219:ASP:OD2	1:A:237:PRO:HA	2.14	0.47
1:D:37:VAL:HG11	1:D:54:LEU:CD1	2.43	0.47
1:A:248:GLY:HA2	1:A:251:LEU:HB2	1.96	0.47
1:B:126:LEU:HD22	1:B:180:VAL:HG13	1.96	0.47
1:C:217:LEU:HD23	1:C:235:ALA:HB2	1.96	0.47
1:C:230:ILE:HG22	1:C:231:VAL:HG12	1.97	0.47
1:A:75:VAL:HG21	1:A:88:TYR:HB3	1.96	0.47
1:A:275:ILE:O	1:A:279:LEU:HG	2.15	0.47
1:B:263:TRP:HE3	1:B:263:TRP:H	1.57	0.47
1:B:192:GLY:O	1:B:196:SER:HB3	2.15	0.47
1:A:37:VAL:HG11	1:A:54:LEU:HD13	1.97	0.47
1:A:88:TYR:C	1:A:88:TYR:CD1	2.88	0.46
1:A:27:PHE:HB2	1:A:251:LEU:HD21	1.97	0.46
1:A:70:THR:O	1:A:73:LYS:HB2	2.15	0.46
1:B:157:MET:O	1:B:160:GLN:HG2	2.15	0.46
1:D:178:PRO:O	1:D:179:MET:CB	2.62	0.46
1:D:88:TYR:C	1:D:89:ILE:HG13	2.35	0.46
1:A:89:ILE:HD12	1:A:102:PHE:HD1	1.81	0.46
1:C:279:LEU:C	1:C:279:LEU:HD12	2.36	0.46
1:A:267:LEU:HD13	1:B:275:ILE:CD1	2.46	0.46
1:C:26:GLU:HG2	1:C:27:PHE:N	2.31	0.45
1:C:155:LEU:HB3	1:C:156:PRO:HD3	1.98	0.45
1:C:38:ILE:CD1	1:C:113:LEU:HD11	2.46	0.45
1:D:36:LYS:HE3	1:D:111:GLY:O	2.16	0.45
1:B:37:VAL:HG22	1:B:115:MET:HB3	1.97	0.45
1:C:66:ARG:HB2	2:C:3:NAP:O2X	2.16	0.45
1:A:264:THR:O	1:A:266:LEU:N	2.49	0.45
1:A:243:LEU:HD12	1:A:243:LEU:HA	1.76	0.45
1:B:199:LYS:O	1:B:200:GLU:C	2.54	0.45

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:D:94:GLU:HG3	1:D:142:VAL:HG22	1.99	0.45
1:B:45:GLY:HA2	1:B:220:THR:HG23	1.99	0.45
1:C:223:ALA:HB2	2:C:3:NAP:H72N	1.82	0.45
1:D:270:ASN:ND2	1:D:273:ARG:HB2	2.32	0.45
1:A:175:VAL:HG12	1:D:273:ARG:HG3	1.96	0.45
1:D:88:TYR:CD1	1:D:88:TYR:C	2.90	0.45
1:B:220:THR:O	1:B:221:GLU:C	2.54	0.45
1:B:66:ARG:N	2:B:2:NAP:O2X	2.48	0.45
1:A:196:SER:O	1:A:200:GLU:HG3	2.17	0.45
1:C:27:PHE:HB2	1:C:251:LEU:HD11	1.97	0.45
1:A:118:LEU:HB3	1:A:147:TYR:CD2	2.52	0.45
1:D:21:GLN:N	1:D:22:PRO:HD3	2.32	0.45
1:B:179:MET:HE2	1:B:230:ILE:HG21	1.98	0.44
1:A:212:LEU:HD23	1:A:255:GLU:OE1	2.18	0.44
1:D:227:VAL:O	1:D:230:ILE:HG22	2.16	0.44
1:B:197:ILE:HD11	1:C:129:PHE:HB3	1.99	0.44
1:B:220:THR:HG22	1:B:222:THR:H	1.83	0.44
1:D:140:MET:HE3	1:D:186:SER:HA	1.99	0.44
1:C:77:HIS:ND1	1:C:81:LEU:HD11	2.33	0.44
1:A:191:ASP:O	1:A:192:GLY:C	2.55	0.44
1:A:201:TYR:O	1:A:202:SER:C	2.54	0.44
1:A:200:GLU:HB3	1:D:128:LEU:HD22	1.98	0.44
1:B:179:MET:HE3	1:C:286:MET:HB3	2.00	0.44
1:A:198:ARG:NH2	1:A:254:GLU:O	2.50	0.44
1:B:270:ASN:HA	1:B:271:PRO:HD3	1.79	0.44
1:C:25:GLU:HG2	1:C:26:GLU:N	2.32	0.44
1:C:41:GLY:O	1:C:47:GLY:HA3	2.18	0.44
1:B:259:ASP:CG	1:B:264:THR:HG21	2.39	0.44
1:A:89:ILE:HD12	1:A:102:PHE:CD1	2.53	0.44
1:B:268:ILE:HG12	1:B:268:ILE:H	1.57	0.44
1:A:267:LEU:HD13	1:B:275:ILE:HD11	1.99	0.44
1:C:95:ASP:OD1	1:C:95:ASP:C	2.56	0.44
1:D:193:PHE:CZ	1:D:197:ILE:HD12	2.53	0.43
1:B:96:MET:HG3	1:C:137:ARG:HH22	1.83	0.43
1:C:264:THR:C	1:C:266:LEU:H	2.22	0.43
1:A:49:GLU:HG3	1:A:238:LYS:HB2	1.99	0.43
1:B:106:ALA:HA	1:B:109:LEU:HD12	1.99	0.43
1:A:201:TYR:O	1:A:204:SER:HB2	2.18	0.43
1:C:26:GLU:HG2	1:C:27:PHE:H	1.83	0.43
1:C:197:ILE:O	1:C:200:GLU:HB2	2.19	0.43
3:C:293:3OQ:H4	3:C:293:3OQ:F25	2.08	0.43
1:B:190:LEU:CD2	1:B:194:PHE:HE1	2.31	0.43

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:273:ARG:HH21	1:D:176:ALA:HB2	1.83	0.43
1:A:129:PHE:CD2	1:D:197:ILE:CD1	2.98	0.43
1:A:32:LEU:O	1:A:35:LYS:CG	2.58	0.42
1:A:53:HIS:CG	1:A:243:LEU:HD13	2.53	0.42
1:A:43:SER:HG	2:A:1:NAP:P2B	2.42	0.42
1:A:72:GLN:O	1:A:73:LYS:C	2.58	0.42
1:C:243:LEU:O	1:C:247:LYS:HG3	2.20	0.42
1:C:197:ILE:HD13	1:C:197:ILE:HA	1.83	0.42
1:D:257:TYR:CE1	1:D:269:ARG:HG2	2.54	0.42
1:C:180:VAL:HG12	1:C:184:SER:HB2	2.02	0.42
1:C:42:ALA:HA	1:C:47:GLY:HA3	2.02	0.42
1:C:74:VAL:O	1:C:78:CYS:SG	2.71	0.42
1:B:44:LYS:CG	2:B:2:NAP:H3B	2.44	0.42
1:C:77:HIS:CE1	1:C:81:LEU:HD11	2.54	0.42
1:D:191:ASP:O	1:D:195:SER:HB2	2.19	0.42
1:A:217:LEU:HG	1:A:235:ALA:HB2	2.01	0.42
1:B:261:SER:CB	1:B:264:THR:HG22	2.50	0.42
1:D:144:PHE:O	1:D:147:TYR:HB2	2.20	0.42
1:C:28:ARG:HA	1:C:29:PRO:HD2	1.83	0.42
1:C:73:LYS:CE	4:C:5:HOH:O	2.66	0.42
1:C:217:LEU:O	1:C:218:ILE:HD13	2.20	0.42
1:C:133:ILE:H	1:C:133:ILE:HG13	1.60	0.42
1:C:252:ARG:NH1	1:C:252:ARG:HG2	2.35	0.42
1:D:40:THR:HA	1:D:64:THR:CG2	2.50	0.41
1:B:264:THR:HG23	1:B:265:THR:H	1.85	0.41
1:A:83:ALA:C	1:A:85:SER:H	2.23	0.41
1:C:169:SER:N	1:C:213:CYS:O	2.51	0.41
1:A:197:ILE:O	1:A:198:ARG:C	2.59	0.41
1:A:121:ILE:HG23	1:A:122:THR:H	1.86	0.41
1:A:46:ILE:HD12	2:A:1:NAP:PN	2.61	0.41
1:B:21:GLN:N	1:B:22:PRO:HD3	2.36	0.41
1:D:233:MET:CG	3:D:293:3OQ:N6	2.79	0.41
1:A:272:SER:O	1:A:276:LEU:CD2	2.67	0.41
1:B:53:HIS:HD2	1:B:243:LEU:HD13	1.86	0.41
1:B:261:SER:OG	1:B:262:LEU:N	2.53	0.41
1:B:134:HIS:O	1:B:138:LYS:HB2	2.21	0.41
1:A:223:ALA:HB2	2:A:1:NAP:H72N	1.86	0.41
1:A:217:LEU:HD22	1:A:232:HIS:HB2	2.02	0.41
1:C:252:ARG:HG2	1:C:252:ARG:HH11	1.86	0.41
1:B:91:GLY:HA3	1:B:98:PHE:CZ	2.56	0.41
1:C:285:ASN:ND2	1:C:285:ASN:O	2.54	0.41
1:B:75:VAL:HG21	1:B:88:TYR:HD2	1.85	0.41

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:171:LEU:HD23	1:A:268:ILE:HD13	2.03	0.41
1:A:202:SER:OG	1:A:203:VAL:N	2.54	0.40
1:A:44:LYS:HB2	2:A:1:NAP:H3B	2.03	0.40
1:A:119:ASN:HD22	1:A:168:VAL:HG21	1.86	0.40
1:A:115:MET:HE3	1:A:115:MET:HB2	2.00	0.40
1:B:221:GLU:HG3	1:B:221:GLU:H	1.63	0.40
1:B:105:GLN:HB2	1:B:105:GLN:HE21	1.64	0.40
1:A:84:ALA:O	1:A:85:SER:CB	2.68	0.40
1:C:168:VAL:O	1:C:187:LYS:NZ	2.55	0.40
1:B:121:ILE:HG13	1:B:121:ILE:O	2.21	0.40
1:B:124:THR:HG23	1:B:135:HIS:CE1	2.57	0.40
1:A:37:VAL:HA	1:A:115:MET:O	2.21	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles

### 5.3.1 Protein backbone ⓘ

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution. The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	259/286 (91%)	205 (79%)	40 (15%)	14 (5%)	3	3
1	B	266/286 (93%)	232 (87%)	29 (11%)	5 (2%)	12	23
1	C	267/286 (93%)	229 (86%)	31 (12%)	7 (3%)	8	13
1	D	260/286 (91%)	225 (86%)	32 (12%)	3 (1%)	19	39
All	All	1052/1144 (92%)	891 (85%)	132 (12%)	29 (3%)	8	12

All (29) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	85	SER
1	A	228	SER
1	A	265	THR
1	C	180	VAL
1	A	33	GLN
1	A	45	GLY

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Mol	Chain	Res	Type
1	A	65	ALA
1	A	203	VAL
1	A	204	SER
1	A	258	TYR
1	B	69	GLU
1	C	45	GLY
1	D	52	TYR
1	D	180	VAL
1	A	109	LEU
1	A	263	TRP
1	C	65	ALA
1	C	279	LEU
1	B	22	PRO
1	B	65	ALA
1	B	70	THR
1	C	29	PRO
1	A	80	GLU
1	C	280	TYR
1	A	202	SER
1	B	279	LEU
1	C	265	THR
1	D	156	PRO
1	A	121	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	218/243 (90%)	197 (90%)	21 (10%)	12	22
1	B	225/243 (93%)	202 (90%)	23 (10%)	11	19
1	C	226/243 (93%)	193 (85%)	33 (15%)	5	8
1	D	219/243 (90%)	193 (88%)	26 (12%)	8	14
All	All	888/972 (91%)	785 (88%)	103 (12%)	8	14

All (103) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	21	GLN
1	A	33	GLN
1	A	36	LYS
1	A	56	LYS
1	A	64	THR
1	A	67	SER
1	A	70	THR
1	A	80	GLU
1	A	124	THR
1	A	126	LEU
1	A	145	LEU
1	A	152	VAL
1	A	180	VAL
1	A	204	SER
1	A	221	GLU
1	A	238	LYS
1	A	251	LEU
1	A	262	LEU
1	A	263	TRP
1	A	269	ARG
1	A	277	GLU
1	B	25	GLU
1	B	26	GLU
1	B	28	ARG
1	B	35	LYS
1	B	44	LYS
1	B	68	LYS
1	B	73	LYS
1	B	131	ASP
1	B	165	ILE
1	B	171	LEU
1	B	180	VAL
1	B	184	SER
1	B	203	VAL
1	B	204	SER
1	B	221	GLU
1	B	222	THR
1	B	228	SER
1	B	263	TRP
1	B	268	ILE
1	B	270	ASN
1	B	276	LEU
1	B	283	SER

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Mol	Chain	Res	Type
1	B	285	ASN
1	C	21	GLN
1	C	26	GLU
1	C	28	ARG
1	C	36	LYS
1	C	48	ARG
1	C	56	LYS
1	C	68	LYS
1	C	73	LYS
1	C	85	SER
1	C	109	LEU
1	C	119	ASN
1	C	126	LEU
1	C	127	ASN
1	C	132	ASP
1	C	157	MET
1	C	170	SER
1	C	179	MET
1	C	196	SER
1	C	205	ARG
1	C	221	GLU
1	C	232	HIS
1	C	233	MET
1	C	240	GLU
1	C	244	GLU
1	C	262	LEU
1	C	266	LEU
1	C	267	LEU
1	C	269	ARG
1	C	272	SER
1	C	279	LEU
1	C	281	SER
1	C	285	ASN
1	C	286	MET
1	D	66	ARG
1	D	72	GLN
1	D	76	SER
1	D	105	GLN
1	D	122	THR
1	D	124	THR
1	D	125	SER
1	D	126	LEU

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Mol	Chain	Res	Type
1	D	127	ASN
1	D	134	HIS
1	D	138	LYS
1	D	155	LEU
1	D	170	SER
1	D	171	LEU
1	D	209	SER
1	D	221	GLU
1	D	230	ILE
1	D	232	HIS
1	D	234	GLN
1	D	262	LEU
1	D	263	TRP
1	D	265	THR
1	D	266	LEU
1	D	274	LYS
1	D	276	LEU
1	D	278	PHE

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (20) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	77	HIS
1	A	119	ASN
1	A	130	HIS
1	A	160	GLN
1	A	162	ASN
1	A	253	GLN
1	B	33	GLN
1	B	105	GLN
1	B	135	HIS
1	B	253	GLN
1	B	270	ASN
1	C	53	HIS
1	C	127	ASN
1	C	232	HIS
1	D	72	GLN
1	D	101	GLN
1	D	105	GLN
1	D	160	GLN
1	D	232	HIS
1	D	270	ASN

### 5.3.3 RNA ⓘ

There are no RNA chains 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	-	52,52,52	1.36	3 (5%)	80,80,80	1.79	12 (15%)
3	3OQ	A	293	-	28,28,28	1.65	4 (14%)	43,43,43	2.12	8 (18%)
2	NAP	B	2	-	52,52,52	1.38	4 (7%)	80,80,80	2.13	11 (13%)
3	3OQ	B	293	-	28,28,28	1.59	5 (17%)	43,43,43	2.17	9 (20%)
3	3OQ	C	293	-	28,28,28	1.29	3 (10%)	43,43,43	2.38	13 (30%)
2	NAP	C	3	-	52,52,52	1.47	4 (7%)	80,80,80	1.75	8 (10%)
3	3OQ	D	293	-	28,28,28	2.39	4 (14%)	43,43,43	2.52	9 (20%)
2	NAP	D	4	-	52,52,52	1.42	4 (7%)	80,80,80	1.81	12 (15%)

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	-	-	0/35/67/67	0/3/5/5
3	3OQ	A	293	-	-	0/32/32/32	0/2/2/2
2	NAP	B	2	-	-	0/35/67/67	0/3/5/5
3	3OQ	B	293	-	-	0/32/32/32	0/2/2/2
3	3OQ	C	293	-	-	0/32/32/32	0/2/2/2
2	NAP	C	3	-	-	0/35/67/67	0/3/5/5
3	3OQ	D	293	-	-	0/32/32/32	0/2/2/2
2	NAP	D	4	-	-	0/35/67/67	0/3/5/5

All (31) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	D	293	3OQ	C1-S12	-8.99	1.66	1.78
2	C	3	NAP	O7N-C7N	7.56	1.41	1.24
2	A	1	NAP	O7N-C7N	7.32	1.41	1.24
2	B	2	NAP	O7N-C7N	7.19	1.41	1.24
2	D	4	NAP	O7N-C7N	6.96	1.40	1.24
3	D	293	3OQ	C15-S12	-5.11	1.69	1.76
3	B	293	3OQ	O14-S12	4.90	1.51	1.44
3	A	293	3OQ	O14-S12	4.84	1.51	1.44
3	D	293	3OQ	O13-S12	4.80	1.51	1.44
3	A	293	3OQ	C1-S12	-4.67	1.72	1.78
3	D	293	3OQ	O14-S12	4.47	1.50	1.44
3	B	293	3OQ	O13-S12	4.45	1.50	1.44
2	D	4	NAP	C2N-N1N	3.89	1.40	1.35
3	C	293	3OQ	O14-S12	3.83	1.49	1.44
3	A	293	3OQ	O13-S12	3.69	1.49	1.44
3	C	293	3OQ	O13-S12	3.46	1.49	1.44
2	C	3	NAP	C2N-N1N	3.26	1.39	1.35
2	C	3	NAP	C2A-N3A	3.19	1.38	1.32
3	A	293	3OQ	C15-S12	-3.09	1.72	1.76
2	A	1	NAP	C2A-N3A	3.06	1.38	1.32
2	B	2	NAP	C2A-N3A	3.01	1.38	1.32
3	C	293	3OQ	C1-S12	-2.86	1.74	1.78
3	B	293	3OQ	C1-S12	-2.83	1.74	1.78
3	B	293	3OQ	O20-C19	-2.80	1.39	1.43
2	C	3	NAP	C2A-N1A	2.34	1.38	1.33
2	B	2	NAP	C2A-N1A	2.24	1.38	1.33
2	D	4	NAP	C3N-C7N	2.12	1.54	1.50
2	D	4	NAP	C2A-N1A	2.08	1.38	1.33
3	B	293	3OQ	C15-S12	-2.08	1.73	1.76
2	A	1	NAP	C2A-N1A	2.06	1.38	1.33
2	B	2	NAP	C2N-N1N	2.04	1.37	1.35



All (82) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	2	NAP	N3A-C2A-N1A	-13.00	117.84	128.71
2	A	1	NAP	N3A-C2A-N1A	-11.12	119.41	128.71
3	C	293	3OQ	O13-S12-O14	-9.99	105.84	119.03
3	B	293	3OQ	O13-S12-O14	-9.79	106.10	119.03
2	C	3	NAP	N3A-C2A-N1A	-9.48	120.78	128.71
3	A	293	3OQ	O13-S12-O14	-8.84	107.35	119.03
3	D	293	3OQ	C15-S12-C1	8.77	117.06	105.31
3	D	293	3OQ	O13-S12-O14	-8.41	107.93	119.03
2	D	4	NAP	N3A-C2A-N1A	-7.56	122.38	128.71
2	B	2	NAP	O4B-C1B-N9A	6.56	114.54	108.44
2	C	3	NAP	O4B-C1B-N9A	6.39	114.38	108.44
3	D	293	3OQ	O13-S12-C15	5.99	113.85	107.95
2	D	4	NAP	C3N-C7N-N7N	5.85	124.42	117.77
2	B	2	NAP	O4D-C1D-N1N	5.49	113.57	107.95
3	A	293	3OQ	F24-C22-C19	-4.91	106.24	112.49
3	B	293	3OQ	F24-C22-C19	-4.58	106.66	112.49
3	B	293	3OQ	O13-S12-C15	4.29	112.18	107.95
2	D	4	NAP	O4D-C1D-C2D	-4.28	100.22	106.77
2	A	1	NAP	O4D-C1D-N1N	4.10	112.15	107.95
2	D	4	NAP	C4A-C5A-N7A	-4.00	106.10	109.52
3	C	293	3OQ	F23-C22-C19	-3.96	107.45	112.49
3	D	293	3OQ	F23-C22-C19	-3.92	107.50	112.49
2	D	4	NAP	O7N-C7N-N7N	-3.91	116.94	122.59
3	C	293	3OQ	C26-C18-C19	-3.91	117.00	121.53
3	D	293	3OQ	O14-S12-C15	-3.60	104.41	107.95
3	A	293	3OQ	C15-S12-C1	3.58	110.10	105.31
3	C	293	3OQ	F24-C22-C19	-3.55	107.97	112.49
3	A	293	3OQ	O13-S12-C15	3.50	111.40	107.95
2	B	2	NAP	C4A-C5A-N7A	-3.50	106.52	109.52
2	A	1	NAP	N3A-C4A-N9A	3.42	131.60	125.43
2	B	2	NAP	N3A-C4A-N9A	3.38	131.54	125.43
3	C	293	3OQ	C8-C1-S12	-3.38	119.52	123.01
3	C	293	3OQ	C22-C19-C18	3.36	115.28	109.54
2	C	3	NAP	N3A-C4A-N9A	3.31	131.40	125.43
2	B	2	NAP	C2A-N3A-C4A	3.28	123.34	114.01
2	C	3	NAP	C3N-C7N-N7N	3.25	121.47	117.77
3	C	293	3OQ	C15-S12-C1	3.22	109.62	105.31
3	C	293	3OQ	O13-S12-C15	3.21	111.11	107.95
2	A	1	NAP	O4B-C1B-N9A	3.12	111.34	108.44
2	B	2	NAP	O4B-C1B-C2B	-3.08	104.07	106.95
2	D	4	NAP	N3A-C4A-N9A	3.03	130.90	125.43
3	B	293	3OQ	O14-S12-C15	2.95	110.86	107.95

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	293	3OQ	C2-C1-S12	2.95	119.44	116.23
2	A	1	NAP	C8A-N9A-C4A	2.93	109.14	106.90
3	D	293	3OQ	C7-C4-C5	2.87	123.28	119.50
3	D	293	3OQ	C22-C19-C18	2.87	114.43	109.54
2	D	4	NAP	C4D-O4D-C1D	2.85	112.84	109.75
3	A	293	3OQ	C17-C18-C19	-2.81	118.28	121.53
2	B	2	NAP	C5A-C4A-N3A	-2.79	119.62	125.70
3	A	293	3OQ	C7-C4-C5	2.78	123.16	119.50
3	C	293	3OQ	C16-C15-S12	2.75	123.30	119.61
2	A	1	NAP	C1B-N9A-C4A	-2.74	121.91	126.64
3	A	293	3OQ	C3-C4-C5	-2.72	115.13	120.00
3	C	293	3OQ	C17-C18-C19	2.69	124.64	121.53
2	C	3	NAP	C4D-O4D-C1D	2.68	112.66	109.75
2	A	1	NAP	O7N-C7N-C3N	-2.65	116.59	119.58
3	D	293	3OQ	C2-C1-S12	-2.61	113.41	116.23
2	A	1	NAP	N7A-C8A-N9A	-2.61	106.99	114.36
3	D	293	3OQ	C3-C4-C5	-2.59	115.36	120.00
2	A	1	NAP	O2A-PA-O3	2.56	117.27	105.14
2	B	2	NAP	C3N-C7N-N7N	2.53	120.65	117.77
3	A	293	3OQ	F23-C22-C19	-2.53	109.27	112.49
2	B	2	NAP	N7A-C8A-N9A	-2.47	107.37	114.36
3	B	293	3OQ	C21-C19-C22	2.46	112.53	109.10
2	D	4	NAP	C5A-C4A-N3A	-2.43	120.40	125.70
3	C	293	3OQ	C7-C8-C1	2.42	118.83	117.22
3	C	293	3OQ	O14-S12-C15	2.36	110.27	107.95
3	B	293	3OQ	O20-C19-C22	2.33	109.22	106.34
2	D	4	NAP	O2B-C2B-C1B	2.30	118.86	110.36
2	D	4	NAP	O2D-C2D-C1D	2.30	118.17	111.23
2	C	3	NAP	C1B-N9A-C4A	-2.26	122.73	126.64
2	A	1	NAP	O3X-P2B-O2B	2.26	113.59	107.09
2	A	1	NAP	C4A-C5A-N7A	-2.26	107.59	109.52
3	B	293	3OQ	C9-C8-C7	-2.24	114.70	119.36
2	C	3	NAP	O4B-C4B-C3B	2.20	109.63	105.17
2	A	1	NAP	C2A-N3A-C4A	2.13	120.08	114.01
2	D	4	NAP	C5B-C4B-C3B	-2.11	106.78	115.21
3	B	293	3OQ	O13-S12-C1	2.09	111.28	107.92
2	B	2	NAP	O7N-C7N-C3N	-2.09	117.22	119.58
3	B	293	3OQ	O20-C19-C18	-2.08	103.17	107.79
2	D	4	NAP	C8A-N7A-C5A	2.05	109.94	103.58
2	C	3	NAP	O2A-PA-O3	2.00	114.63	105.14

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

## 5.7 Other polymers ⓘ

There are no such residues in this entry.

## 5.8 Polymer linkage issues

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	261/286 (91%)	0.73	29 (11%) 6 4	33, 74, 100, 115	0
1	B	267/286 (93%)	0.18	11 (4%) 35 32	37, 58, 91, 109	0
1	C	269/286 (94%)	0.35	15 (5%) 24 20	42, 63, 96, 112	0
1	D	261/286 (91%)	0.13	12 (4%) 31 27	34, 57, 89, 103	0
All	All	1058/1144 (92%)	0.35	67 (6%) 19 16	33, 62, 97, 115	0

All (67) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	23	LEU	6.8
1	A	22	PRO	6.3
1	A	231	VAL	5.8
1	A	24	ASN	5.8
1	C	22	PRO	5.6
1	B	23	LEU	5.5
1	D	21	GLN	5.3
1	C	23	LEU	5.3
1	D	232	HIS	5.2
1	C	289	PHE	5.1
1	D	22	PRO	4.8
1	D	23	LEU	4.7
1	C	25	GLU	4.7
1	B	285	ASN	4.7
1	A	263	TRP	4.6
1	C	263	TRP	4.2
1	A	75	VAL	4.2
1	A	232	HIS	4.1
1	A	233	MET	4.0
1	A	237	PRO	3.9
1	C	229	GLY	3.9

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Mol	Chain	Res	Type	RSRZ
1	C	231	VAL	3.8
1	D	233	MET	3.6
1	B	25	GLU	3.6
1	A	71	LEU	3.5
1	C	286	MET	3.5
1	B	24	ASN	3.4
1	D	231	VAL	3.4
1	D	263	TRP	3.4
1	A	166	VAL	3.2
1	C	27	PHE	3.2
1	A	262	LEU	3.2
1	C	192	GLY	3.0
1	A	21	GLN	3.0
1	A	230	ILE	2.9
1	A	76	SER	2.9
1	A	31	MET	2.8
1	B	263	TRP	2.8
1	D	205	ARG	2.7
1	A	107	GLY	2.7
1	A	278	PHE	2.7
1	A	211	THR	2.7
1	C	189	ALA	2.7
1	D	228	SER	2.6
1	A	167	VAL	2.6
1	A	117	ILE	2.6
1	A	234	GLN	2.6
1	A	27	PHE	2.6
1	D	278	PHE	2.5
1	D	234	GLN	2.5
1	B	173	GLY	2.5
1	A	74	VAL	2.5
1	C	230	ILE	2.4
1	C	21	GLN	2.4
1	B	134	HIS	2.4
1	A	40	THR	2.3
1	D	230	ILE	2.2
1	A	79	LEU	2.2
1	A	203	VAL	2.2
1	B	28	ARG	2.2
1	B	188	PHE	2.1
1	B	27	PHE	2.1
1	C	191	ASP	2.1

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Mol	Chain	Res	Type	RSRZ
1	A	68	LYS	2.0
1	A	72	GLN	2.0
1	B	286	MET	2.0
1	C	232	HIS	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	RSR	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
3	3OQ	B	293	27/27	0.26	1.04	62,70,78,83	0
3	3OQ	D	293	27/27	0.23	0.44	80,84,91,95	0
3	3OQ	C	293	27/27	0.20	0.02	63,66,72,74	0
3	3OQ	A	293	27/27	0.16	-0.59	69,72,75,78	0
2	NAP	D	4	48/48	0.13	-0.71	36,47,51,55	0
2	NAP	B	2	48/48	0.14	-0.72	40,52,59,60	0
2	NAP	A	1	48/48	0.14	-0.96	64,70,74,76	0
2	NAP	C	3	48/48	0.12	-1.47	44,53,63,65	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.