



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 03:40 PM GMT

PDB ID : 4D06  
Title : Bacterial chalcone isomerase complexed with naringenin  
Authors : Thomsen, M.; Palm, G.J.; Hinrichs, W.  
Deposited on : 2014-04-24  
Resolution : 2.00 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.

---

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

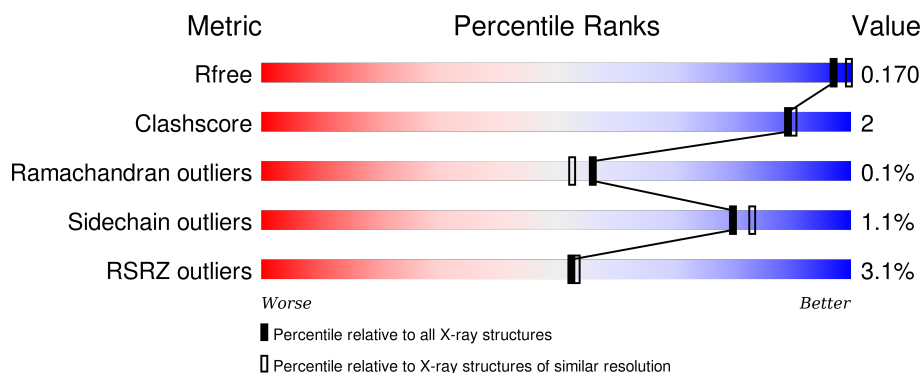
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.00 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	6249 (2.00-2.00)
Clashscore	102246	7340 (2.00-2.00)
Ramachandran outliers	100387	7248 (2.00-2.00)
Sidechain outliers	100360	7247 (2.00-2.00)
RSRZ outliers	91569	6262 (2.00-2.00)

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	283	<div> <div>6%</div> <div> <div></div> <div>93%</div> <div>6%</div> </div> </div>
1	B	283	<div> <div>%</div> <div> <div></div> <div>84%</div> <div>7%</div> <div>8%</div> </div> </div>
1	C	283	<div> <div>4%</div> <div> <div></div> <div>93%</div> <div>6%</div> </div> </div>
1	D	283	<div> <div></div> <div> <div></div> <div>83%</div> <div>8%</div> <div>8%</div> </div> </div>
1	E	283	<div> <div>7%</div> <div> <div></div> <div>93%</div> <div>7%</div> </div> </div>

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Length	Quality of chain
1	F	283	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	NAR	D	301	-	-	-	X
2	NAR	F	301	-	-	-	X
2	NAR	F	302[A]	-	-	-	X
2	NAR	F	302[B]	-	-	-	X
4	X8W	B	301	-	-	-	X
4	X8W	D	303[A]	-	-	-	X
5	GOL	B	302	-	-	-	X
5	GOL	F	303	-	-	-	X

## 2 Entry composition [i](#)

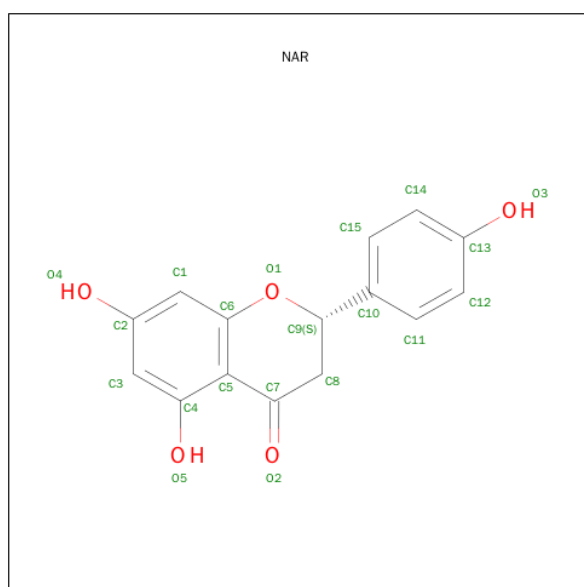
There are 6 unique types of molecules in this entry. The entry contains 15609 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 CHALCONE ISOMERASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	282	Total	C	N	O	S	0	5	0
			2312	1495	380	423	14			
1	B	259	Total	C	N	O	S	0	8	0
			2172	1421	349	387	15			
1	C	282	Total	C	N	O	S	0	7	0
			2326	1509	380	423	14			
1	D	259	Total	C	N	O	S	0	8	0
			2170	1422	349	384	15			
1	E	282	Total	C	N	O	S	0	8	0
			2331	1509	381	426	15			
1	F	259	Total	C	N	O	S	0	6	0
			2161	1417	348	382	14			

- Molecule 2 is NARINGENIN (three-letter code: NAR) (formula: C<sub>15</sub>H<sub>12</sub>O<sub>5</sub>).

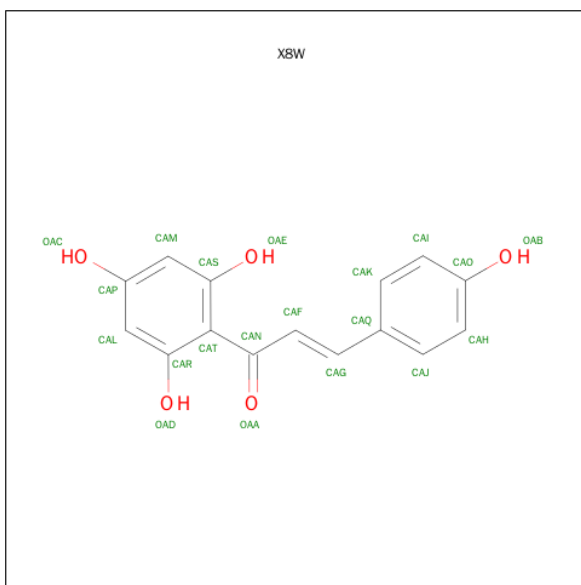


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	C	O	0	0
			20	15	5		
2	C	1	Total	C	O	0	0
			20	15	5		
2	D	1	Total	C	O	0	0
			20	15	5		
2	D	1	Total	C	O	0	0
			20	15	5		
2	E	1	Total	C	O	0	0
			20	15	5		
2	F	1	Total	C	O	0	0
			20	15	5		
2	F	1	Total	C	O	0	1
			19	12	7		

- Molecule 3 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

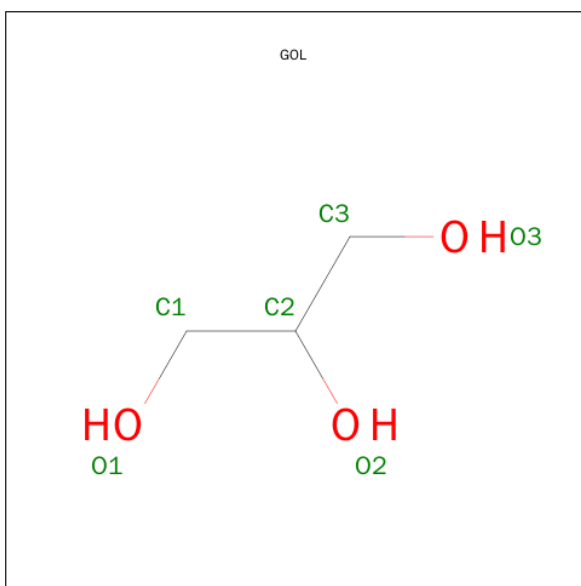
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	D	3	Total	Cl	0	0
			3	3		
3	E	4	Total	Cl	0	0
			4	4		
3	B	2	Total	Cl	0	0
			2	2		
3	C	3	Total	Cl	0	0
			3	3		
3	A	2	Total	Cl	0	0
			2	2		
3	F	3	Total	Cl	0	0
			3	3		

- Molecule 4 is (2E)-3-(4-HYDROXYPHENYL)-1-(2,4,6-TRIHIDROXYPHENYL)PROP-2-EN-1-ONE (three-letter code: X8W) (formula: C<sub>15</sub>H<sub>12</sub>O<sub>5</sub>).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	B	1	Total 20	C 15	O 5	0	0
4	D	1	Total 36	C 26	O 10	0	1

- Molecule 5 is GLYCEROL (three-letter code: GOL) (formula:  $C_3H_8O_3$ ).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	B	1	Total C O 6 3 3	0	0
5	F	1	Total C O 6 3 3	0	0

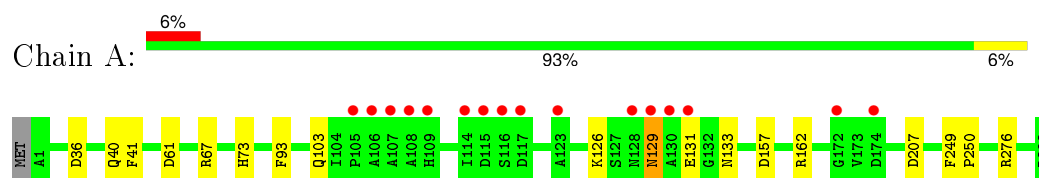
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	357	Total 361	O 361	0	4
6	B	325	Total 329	O 329	0	4
6	C	345	Total 347	O 347	0	2
6	D	294	Total 297	O 297	0	3
6	E	310	Total 312	O 312	0	2
6	F	264	Total 267	O 267	0	3

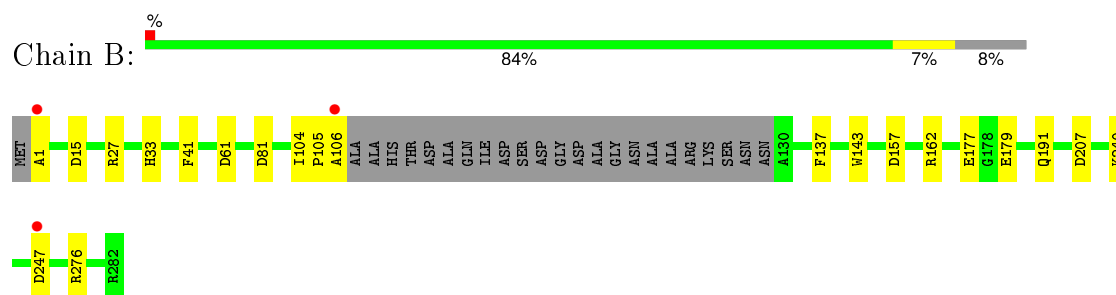
### 3 Residue-property plots

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.

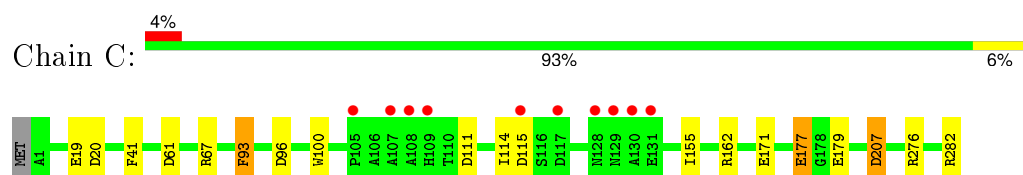
- Molecule 1: CHALCONE ISOMERASE



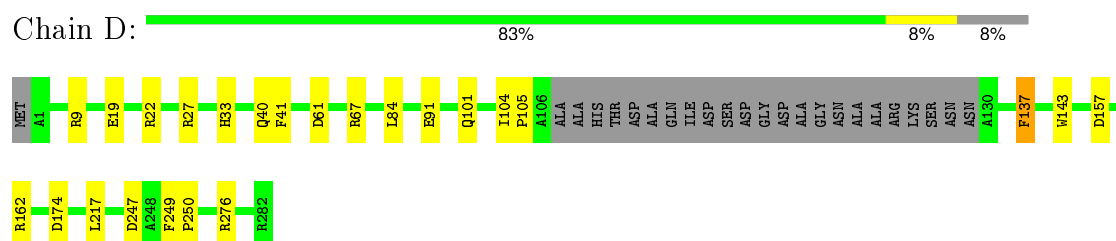
- Molecule 1: CHALCONE ISOMERASE



- Molecule 1: CHALCONE ISOMERASE



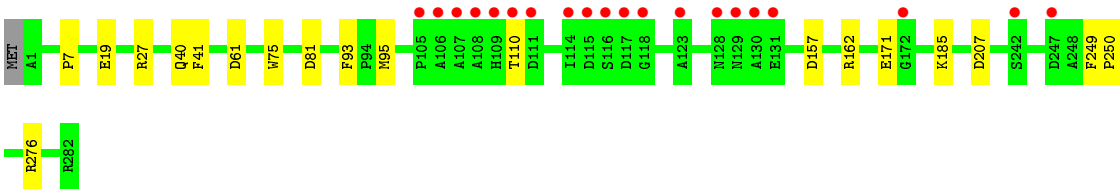
- Molecule 1: CHALCONE ISOMERASE



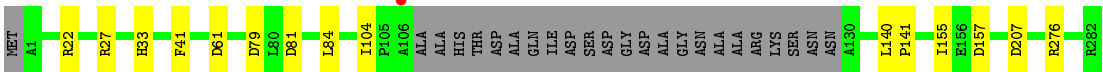
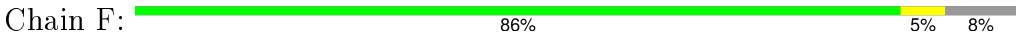
- Molecule 1: CHALCONE ISOMERASE







● Molecule 1: CHALCONE ISOMERASE



## 4 Data and refinement statistics

Property	Value	Source
Space group	I 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	181.16Å 187.99Å 196.22Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.18 – 2.00 49.18 – 2.00	Depositor EDS
% Data completeness (in resolution range)	99.8 (49.18-2.00) 99.8 (49.18-2.00)	Depositor EDS
$R_{merge}$	0.12	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.95 (at 2.00Å)	Xtriage
Refinement program	REFMAC 5.8.0049	Depositor
R, $R_{free}$	0.140 , 0.163 0.151 , 0.170	Depositor DCC
$R_{free}$ test set	11199 reflections (5.26%)	DCC
Wilson B-factor (Å <sup>2</sup> )	24.3	Xtriage
Anisotropy	0.095	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.37 , 48.4	EDS
Estimated twinning fraction	0.012 for -k,-h,-l	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtriage
Outliers	0 of 224291 reflections	Xtriage
$F_o, F_c$ correlation	0.97	EDS
Total number of atoms	15609	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	25.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.06% 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 ⓘ

### 5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: NAR, GOL, X8W, CL

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	0.92	1/2400 (0.0%)	0.96	6/3262 (0.2%)
1	B	0.95	3/2265 (0.1%)	1.00	7/3078 (0.2%)
1	C	1.04	4/2421 (0.2%)	0.97	7/3291 (0.2%)
1	D	1.01	1/2266 (0.0%)	1.05	14/3077 (0.5%)
1	E	0.96	1/2425 (0.0%)	1.00	8/3295 (0.2%)
1	F	0.99	2/2254 (0.1%)	0.98	5/3064 (0.2%)
All	All	0.98	12/14031 (0.1%)	0.99	47/19067 (0.2%)

All (12) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	207	ASP	CB-CG	8.12	1.68	1.51
1	C	177	GLU	CD-OE2	7.09	1.33	1.25
1	C	179	GLU	CD-OE1	-7.07	1.17	1.25
1	B	207	ASP	CB-CG	7.04	1.66	1.51
1	C	19	GLU	CD-OE2	5.83	1.32	1.25
1	A	207	ASP	CB-CG	5.74	1.63	1.51
1	E	19	GLU	CD-OE2	5.72	1.31	1.25
1	D	19	GLU	CD-OE2	5.49	1.31	1.25
1	F	22	ARG	CZ-NH1	-5.30	1.26	1.33
1	B	179	GLU	CD-OE1	-5.18	1.20	1.25
1	F	207	ASP	CB-CG	5.09	1.62	1.51
1	B	106	ALA	N-CA	5.06	1.56	1.46

All (47) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	207	ASP	CB-CG-OD1	9.96	127.27	118.30
1	D	9	ARG	NE-CZ-NH1	9.35	124.97	120.30
1	D	162	ARG	NE-CZ-NH1	9.25	124.92	120.30

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	162	ARG	NE-CZ-NH2	-9.07	115.76	120.30
1	A	162	ARG	NE-CZ-NH1	8.82	124.71	120.30
1	E	157	ASP	CB-CG-OD2	8.47	125.92	118.30
1	D	61	ASP	CB-CG-OD1	8.42	125.87	118.30
1	E	27	ARG	NE-CZ-NH1	8.36	124.48	120.30
1	E	27	ARG	NE-CZ-NH2	-8.18	116.21	120.30
1	C	61	ASP	CB-CG-OD1	7.71	125.24	118.30
1	F	61	ASP	CB-CG-OD1	7.50	125.05	118.30
1	A	61	ASP	CB-CG-OD1	6.97	124.57	118.30
1	F	27	ARG	NE-CZ-NH1	6.91	123.75	120.30
1	D	27	ARG	NE-CZ-NH1	6.80	123.70	120.30
1	E	61	ASP	CB-CG-OD1	6.68	124.31	118.30
1	D	247	ASP	CB-CG-OD1	6.55	124.20	118.30
1	F	157	ASP	CB-CG-OD2	6.55	124.19	118.30
1	C	282	ARG	NE-CZ-NH2	-6.52	117.04	120.30
1	B	27	ARG	NE-CZ-NH1	6.43	123.52	120.30
1	D	247	ASP	CB-CG-OD2	-6.38	112.56	118.30
1	B	61	ASP	CB-CG-OD1	6.33	123.99	118.30
1	D	217	LEU	CB-CG-CD1	-6.27	100.34	111.00
1	D	137	PHE	CB-CG-CD1	6.24	125.17	120.80
1	D	22	ARG	NE-CZ-NH1	6.22	123.41	120.30
1	B	27	ARG	NE-CZ-NH2	-6.15	117.23	120.30
1	C	162	ARG	NE-CZ-NH2	-6.06	117.27	120.30
1	B	157	ASP	CB-CG-OD2	6.00	123.70	118.30
1	B	162	ARG	NE-CZ-NH1	5.99	123.30	120.30
1	C	162	ARG	NE-CZ-NH1	5.96	123.28	120.30
1	F	81	ASP	CB-CG-OD1	5.92	123.62	118.30
1	D	9	ARG	NE-CZ-NH2	-5.71	117.44	120.30
1	C	67	ARG	NE-CZ-NH2	5.66	123.13	120.30
1	E	81	ASP	CB-CG-OD1	5.65	123.39	118.30
1	D	67	ARG	NE-CZ-NH1	-5.61	117.49	120.30
1	B	81	ASP	CB-CG-OD1	5.57	123.31	118.30
1	C	20	ASP	CB-CG-OD1	5.47	123.22	118.30
1	A	157	ASP	CB-CG-OD2	5.43	123.19	118.30
1	E	162	ARG	NE-CZ-NH1	5.43	123.01	120.30
1	E	207	ASP	CB-CG-OD1	5.37	123.13	118.30
1	C	111	ASP	CB-CG-OD1	5.36	123.12	118.30
1	D	174	ASP	CB-CG-OD2	5.30	123.07	118.30
1	F	79	ASP	CB-CG-OD1	5.29	123.07	118.30
1	B	15	ASP	CB-CG-OD1	5.28	123.05	118.30
1	E	185	LYS	CD-CE-NZ	-5.27	99.59	111.70
1	D	162	ARG	NE-CZ-NH2	-5.05	117.78	120.30

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	67	ARG	NE-CZ-NH1	-5.04	117.78	120.30
1	D	157	ASP	CB-CG-OD2	5.03	122.83	118.30

There are no chirality outliers.

There are no planarity outliers.

## 5.2 Too-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 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	2312	0	2229	8	0
1	B	2172	0	2113	11	0
1	C	2326	0	2251	5	0
1	D	2170	0	2123	11	0
1	E	2331	0	2254	7	0
1	F	2161	0	2113	8	0
2	A	20	0	9	3	0
2	C	20	0	9	1	0
2	D	40	0	22	5	0
2	E	20	0	9	1	0
2	F	39	0	15	2	0
3	A	2	0	0	0	0
3	B	2	0	0	0	0
3	C	3	0	0	0	0
3	D	3	0	0	0	0
3	E	4	0	0	0	0
3	F	3	0	0	0	0
4	B	20	0	9	5	0
4	D	36	0	18	8	0
5	B	6	0	8	2	0
5	F	6	0	8	0	0
6	A	361	0	0	4	0
6	B	329	0	0	12	0
6	C	347	0	0	1	0
6	D	297	0	0	7	0
6	E	312	0	0	4	0
6	F	267	0	0	1	0

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
All	All	15609	0	13190	65	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 2.

All (65) 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)
4:D:303[B]:X8W:OAB	6:D:2240:HOH:O	1.73	1.04
1:B:33[A]:HIS:NE2	6:B:2070[A]:HOH:O	1.58	0.93
4:B:301:X8W:HAM	5:B:302:GOL:O1	1.70	0.91
4:B:301:X8W:OAD	6:B:2161:HOH:O	1.92	0.88
2:A:301:NAR:C15	6:A:2090:HOH:O	2.27	0.82
4:B:301:X8W:HAH	6:B:2182:HOH:O	1.83	0.77
1:C:93[B]:PHE:CD1	1:C:114:ILE:HD12	2.19	0.77
1:E:95[A]:MET:HE3	1:E:110:THR:HG22	1.70	0.72
2:C:301:NAR:C15	6:C:2083:HOH:O	2.40	0.69
1:B:177[A]:GLU:HG3	6:B:2230:HOH:O	1.91	0.69
2:D:301:NAR:H81	6:D:2070:HOH:O	1.93	0.68
1:F:33[B]:HIS:ND1	6:F:2055:HOH:O	2.29	0.65
1:B:33[A]:HIS:CE1	6:B:2070[A]:HOH:O	2.19	0.65
1:D:33[B]:HIS:ND1	6:D:2064:HOH:O	2.30	0.64
1:C:171[A]:GLU:H	1:C:171[A]:GLU:CD	2.00	0.63
2:A:301:NAR:H151	6:A:2090:HOH:O	1.93	0.60
1:A:129:ASN:ND2	1:A:131:GLU:H	2.04	0.55
4:B:301:X8W:CAR	6:B:2161:HOH:O	2.50	0.55
1:E:171[A]:GLU:H	1:E:171[A]:GLU:CD	2.08	0.55
1:A:129:ASN:HD22	1:A:131:GLU:H	1.55	0.54
2:D:301:NAR:C15	4:D:303[A]:X8W:HAJ	2.38	0.54
1:F:104:ILE:HG12	2:F:301:NAR:C3	2.37	0.54
4:D:303[B]:X8W:OAB	6:D:2239:HOH:O	2.18	0.53
1:B:240:LYS:NZ	1:B:247[A]:ASP:OD1	2.41	0.53
1:B:104[A]:ILE:HG22	1:B:105:PRO:O	2.08	0.53
6:A:2339:HOH:O	1:B:276:ARG:HD3	2.09	0.52
1:A:276:ARG:HD2	1:D:276:ARG:HD2	1.92	0.51
2:E:301:NAR:C15	6:E:2078:HOH:O	2.37	0.51
1:E:40[A]:GLN:NE2	6:E:2077:HOH:O	2.22	0.51
1:D:104:ILE:HG22	1:D:105:PRO:O	2.11	0.51
4:D:303[B]:X8W:CAH	6:D:2240:HOH:O	2.58	0.50
4:D:303[A]:X8W:CAT	4:D:303[A]:X8W:CAQ	2.90	0.50
4:D:303[B]:X8W:CAO	6:D:2240:HOH:O	2.46	0.50

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1:ALA:HB2	6:B:2002:HOH:O	2.12	0.50
5:B:302:GOL:O2	6:B:2327:HOH:O	1.85	0.49
1:D:104:ILE:HG12	2:D:302:NAR:C3	2.42	0.49
1:D:249:PHE:CD1	1:D:250:PRO:HA	2.46	0.49
4:B:301:X8W:CAL	6:B:2161:HOH:O	2.60	0.49
1:A:126:LYS:HE2	6:A:2197:HOH:O	2.12	0.49
1:C:276:ARG:HD2	1:F:276:ARG:HD2	1.96	0.48
1:B:1:ALA:CB	6:B:2004:HOH:O	2.61	0.48
4:D:303[B]:X8W:HAH	6:D:2240:HOH:O	2.13	0.48
1:F:104:ILE:HG12	2:F:301:NAR:C4	2.44	0.47
1:D:143:TRP:CE2	1:F:84:LEU:HG	2.49	0.47
1:D:101:GLN:OE1	2:D:301:NAR:O4	2.33	0.47
1:D:40:GLN:NE2	1:D:91[B]:GLU:HG3	2.30	0.46
1:E:276:ARG:HD3	6:E:2299:HOH:O	2.16	0.46
1:E:7:PRO:HA	1:E:75:TRP:O	2.15	0.46
1:A:103:GLN:HA	1:A:133:ASN:O	2.17	0.44
1:E:95[A]:MET:CE	1:E:110:THR:HA	2.48	0.43
1:D:33[B]:HIS:CE1	2:D:301:NAR:C7	3.02	0.43
1:A:36:ASP:O	1:A:40[A]:GLN:HG3	2.19	0.43
1:C:96:ASP:HB3	1:C:100:TRP:CZ2	2.54	0.43
1:B:177[A]:GLU:CG	6:B:2230:HOH:O	2.58	0.42
1:F:155:ILE:HD12	1:F:155:ILE:HA	1.95	0.42
1:D:40:GLN:HE22	1:D:91[B]:GLU:HG3	1.85	0.42
1:E:249:PHE:CD1	1:E:250:PRO:HA	2.55	0.42
1:A:73:HIS:CE1	2:A:301:NAR:H82	2.55	0.41
1:F:140:LEU:HB3	1:F:141:PRO:HD2	2.03	0.41
1:A:249:PHE:CD1	1:A:250:PRO:HA	2.55	0.41
1:C:155:ILE:HD12	1:C:155:ILE:HA	1.95	0.41
1:B:143:TRP:CE2	1:D:84:LEU:HG	2.56	0.41
4:D:303[A]:X8W:CAQ	4:D:303[A]:X8W:CAN	2.98	0.41
1:B:1:ALA:HB3	6:B:2004:HOH:O	2.20	0.41
6:E:2298:HOH:O	1:F:276:ARG:HD3	2.20	0.41

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	285/283 (101%)	280 (98%)	5 (2%)	0	100	100
1	B	263/283 (93%)	259 (98%)	4 (2%)	0	100	100
1	C	287/283 (101%)	281 (98%)	5 (2%)	1 (0%)	46	41
1	D	263/283 (93%)	260 (99%)	3 (1%)	0	100	100
1	E	288/283 (102%)	283 (98%)	5 (2%)	0	100	100
1	F	262/283 (93%)	259 (99%)	3 (1%)	0	100	100
All	All	1648/1698 (97%)	1622 (98%)	25 (2%)	1 (0%)	56	53

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	207	ASP

### 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	245/241 (102%)	242 (99%)	3 (1%)	78	81
1	B	233/241 (97%)	230 (99%)	3 (1%)	76	79
1	C	247/241 (102%)	242 (98%)	5 (2%)	63	65
1	D	233/241 (97%)	231 (99%)	2 (1%)	84	88
1	E	248/241 (103%)	246 (99%)	2 (1%)	86	89
1	F	232/241 (96%)	231 (100%)	1 (0%)	93	95
All	All	1438/1446 (99%)	1422 (99%)	16 (1%)	80	83

All (16) residues with a non-rotameric sidechain are listed below:



Mol	Chain	Res	Type
1	A	41	PHE
1	A	93	PHE
1	A	129	ASN
1	B	41	PHE
1	B	137	PHE
1	B	191	GLN
1	C	41	PHE
1	C	93[A]	PHE
1	C	93[B]	PHE
1	C	115	ASP
1	C	177	GLU
1	D	41	PHE
1	D	137	PHE
1	E	41	PHE
1	E	93	PHE
1	F	41	PHE

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (10) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	101	GLN
1	A	129	ASN
1	A	133	ASN
1	B	191	GLN
1	C	101	GLN
1	C	133	ASN
1	D	101	GLN
1	D	133	ASN
1	E	101	GLN
1	F	133	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 ⓘ

Of 30 ligands modelled in this entry, 17 are monoatomic - leaving 13 for Mogul analysis.

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	NAR	A	301	-	22,22,22	1.57	3 (13%)	32,32,32	1.96	9 (28%)
4	X8W	B	301	-	21,21,21	2.40	6 (28%)	29,29,29	1.49	7 (24%)
5	GOL	B	302	-	5,5,5	0.57	0	5,5,5	1.73	1 (20%)
2	NAR	C	301	-	22,22,22	1.92	4 (18%)	32,32,32	2.24	11 (34%)
2	NAR	D	301	-	22,22,22	2.76	8 (36%)	32,32,32	2.53	10 (31%)
2	NAR	D	302	-	22,22,22	3.27	6 (27%)	32,32,32	5.92	15 (46%)
4	X8W	D	303[A]	-	18,18,21	1.18	2 (11%)	23,23,29	1.77	4 (17%)
4	X8W	D	303[B]	-	18,18,21	1.16	2 (11%)	23,23,29	1.73	2 (8%)
2	NAR	E	301	-	22,22,22	1.66	4 (18%)	32,32,32	2.50	14 (43%)
2	NAR	F	301	-	22,22,22	1.21	2 (9%)	32,32,32	2.24	7 (21%)
2	NAR	F	302[A]	-	9,9,22	2.69	2 (22%)	12,12,32	1.11	1 (8%)
2	NAR	F	302[B]	-	9,9,22	3.20	2 (22%)	12,12,32	1.02	1 (8%)
5	GOL	F	303	-	5,5,5	1.04	0	5,5,5	1.80	2 (40%)

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	NAR	A	301	-	-	0/4/16/16	0/3/3/3
4	X8W	B	301	-	-	0/9/9/9	0/2/2/2
5	GOL	B	302	-	-	0/4/4/4	0/0/0/0
2	NAR	C	301	-	-	0/4/16/16	0/3/3/3

*Continued on next page...*

*Continued from previous page...*

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	NAR	D	301	-	-	0/4/16/16	0/3/3/3
2	NAR	D	302	-	-	0/4/16/16	0/3/3/3
4	X8W	D	303[A]	-	-	0/2/2/9	0/2/2/2
4	X8W	D	303[B]	-	-	0/2/2/9	0/2/2/2
2	NAR	E	301	-	-	0/4/16/16	0/3/3/3
2	NAR	F	301	-	-	0/4/16/16	0/3/3/3
2	NAR	F	302[A]	-	-	0/0/0/16	0/1/1/3
2	NAR	F	302[B]	-	-	0/0/0/16	0/1/1/3
5	GOL	F	303	-	-	0/4/4/4	0/0/0/0

All (41) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	302	NAR	C14-C13	-10.63	1.17	1.38
4	D	303[A]	X8W	CAT-CAN	-3.83	1.37	1.46
4	B	301	X8W	CAQ-CAG	-3.09	1.38	1.47
4	B	301	X8W	CAT-CAN	-3.00	1.42	1.49
4	D	303[B]	X8W	CAT-CAS	-2.51	1.38	1.41
4	B	301	X8W	OAC-CAP	-2.25	1.31	1.37
4	D	303[A]	X8W	CAT-CAS	-2.13	1.39	1.41
2	E	301	NAR	C5-C7	2.05	1.51	1.46
2	D	301	NAR	C1-C2	2.14	1.42	1.39
4	B	301	X8W	CAH-CAJ	2.19	1.42	1.38
2	D	301	NAR	C3-C4	2.25	1.42	1.38
4	D	303[B]	X8W	CAL-CAR	2.41	1.42	1.38
2	D	301	NAR	O2-C7	2.46	1.26	1.22
2	D	302	NAR	C5-C4	2.57	1.46	1.41
2	D	302	NAR	C11-C10	2.77	1.43	1.39
2	F	301	NAR	C5-C4	2.80	1.46	1.41
2	A	301	NAR	O1-C9	2.88	1.51	1.44
2	E	301	NAR	O1-C9	2.93	1.51	1.44
2	A	301	NAR	C5-C4	3.06	1.46	1.41
2	F	301	NAR	C5-C6	3.11	1.45	1.40
2	D	302	NAR	C12-C11	3.25	1.44	1.38
2	C	301	NAR	O1-C6	3.39	1.42	1.37
2	C	301	NAR	O1-C9	3.46	1.53	1.44
2	D	301	NAR	C5-C7	3.79	1.55	1.46
2	D	301	NAR	O5-C4	3.82	1.44	1.36
2	D	301	NAR	O1-C6	3.88	1.43	1.37
2	D	302	NAR	C5-C6	4.11	1.47	1.40
2	E	301	NAR	C5-C6	4.12	1.47	1.40
2	E	301	NAR	C5-C4	4.19	1.48	1.41

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	301	NAR	C5-C6	4.38	1.48	1.40
2	C	301	NAR	C5-C4	4.77	1.49	1.41
2	C	301	NAR	C5-C6	4.96	1.49	1.40
2	F	302[A]	NAR	C1-C2	5.33	1.47	1.39
2	F	302[A]	NAR	C1-C6	5.49	1.47	1.39
4	B	301	X8W	CAF-CAN	5.82	1.58	1.47
2	F	302[B]	NAR	C1-C6	6.17	1.48	1.39
2	F	302[B]	NAR	C1-C2	6.81	1.49	1.39
2	D	301	NAR	C5-C4	6.90	1.53	1.41
2	D	301	NAR	C5-C6	6.94	1.52	1.40
4	B	301	X8W	CAF-CAG	7.19	1.52	1.32
2	D	302	NAR	C12-C13	8.24	1.55	1.38

All (84) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	302	NAR	C15-C10-C11	-15.42	98.65	118.31
2	D	302	NAR	O1-C6-C5	-6.79	113.80	121.55
2	D	302	NAR	C14-C13-C12	-6.56	110.45	119.79
2	F	301	NAR	O1-C6-C5	-6.34	114.32	121.55
2	D	301	NAR	C6-C5-C7	-6.09	114.79	120.34
2	D	302	NAR	C11-C10-C9	-5.25	110.40	120.62
2	E	301	NAR	O1-C6-C5	-5.07	115.76	121.55
2	A	301	NAR	O1-C6-C5	-4.93	115.92	121.55
2	D	301	NAR	C3-C4-C5	-4.89	114.89	121.00
2	C	301	NAR	O1-C6-C5	-4.85	116.02	121.55
4	D	303[B]	X8W	CAS-CAT-CAN	-4.44	117.39	120.35
4	D	303[A]	X8W	OAA-CAN-CAT	-3.91	117.21	125.11
2	D	301	NAR	C1-C6-C5	-3.70	115.34	121.92
2	D	302	NAR	O1-C9-C10	-3.68	100.79	107.64
2	F	301	NAR	C15-C10-C9	-3.62	113.58	120.62
2	E	301	NAR	C1-C6-C5	-3.48	115.72	121.92
2	E	301	NAR	O2-C7-C8	-3.26	115.87	120.76
5	F	303	GOL	C3-C2-C1	-3.14	98.80	111.12
2	C	301	NAR	O2-C7-C8	-3.14	116.06	120.76
5	B	302	GOL	O1-C1-C2	-3.12	95.07	110.18
4	D	303[A]	X8W	CAS-CAT-CAN	-3.06	118.31	120.35
2	C	301	NAR	C1-C6-C5	-3.03	116.52	121.92
2	A	301	NAR	O5-C4-C5	-2.87	115.55	121.10
2	F	301	NAR	O5-C4-C5	-2.77	115.74	121.10
2	A	301	NAR	C1-C6-C5	-2.59	117.31	121.92
2	E	301	NAR	C3-C4-C5	-2.58	117.78	121.00

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	E	301	NAR	C6-C5-C7	-2.53	118.03	120.34
2	C	301	NAR	C3-C4-C5	-2.51	117.86	121.00
4	B	301	X8W	CAI-CAO-CAH	-2.48	116.26	119.79
4	B	301	X8W	CAG-CAF-CAN	-2.46	117.36	121.47
4	D	303[A]	X8W	CAM-CAS-CAT	-2.44	118.24	120.90
2	E	301	NAR	O2-C7-C5	-2.42	118.19	122.28
2	E	301	NAR	C11-C10-C9	-2.30	116.14	120.62
2	C	301	NAR	C6-C5-C7	-2.30	118.25	120.34
4	B	301	X8W	CAR-CAL-CAP	-2.29	117.47	119.67
4	B	301	X8W	OAA-CAN-CAF	-2.26	117.07	120.88
2	D	301	NAR	O4-C2-C1	-2.23	113.94	119.79
2	E	301	NAR	O4-C2-C3	-2.19	114.04	119.79
2	A	301	NAR	O2-C7-C5	-2.18	118.59	122.28
2	D	302	NAR	C9-C8-C7	-2.17	106.32	113.16
2	D	301	NAR	O2-C7-C5	-2.04	118.82	122.28
4	B	301	X8W	CAK-CAQ-CAG	-2.03	114.13	121.28
2	C	301	NAR	O4-C2-C3	-2.01	114.52	119.79
2	E	301	NAR	C15-C10-C9	2.02	124.56	120.62
2	D	302	NAR	C6-O1-C9	2.03	119.03	115.62
2	F	302[B]	NAR	C4-C3-C2	2.04	122.09	119.17
2	A	301	NAR	C4-C5-C6	2.09	119.20	117.19
2	A	301	NAR	C3-C2-C1	2.10	123.48	120.39
4	B	301	X8W	OAB-CAO-CAH	2.10	126.00	120.05
5	F	303	GOL	O2-C2-C3	2.13	118.43	108.65
2	A	301	NAR	O1-C9-C10	2.24	111.79	107.64
2	E	301	NAR	C6-O1-C9	2.25	119.42	115.62
2	D	302	NAR	C15-C14-C13	2.33	122.56	119.87
2	C	301	NAR	O1-C9-C10	2.34	111.97	107.64
2	A	301	NAR	C8-C7-C5	2.34	121.26	117.31
2	D	302	NAR	C6-C5-C7	2.44	122.56	120.34
2	D	301	NAR	C6-O1-C9	2.48	119.80	115.62
2	D	302	NAR	C4-C3-C2	2.52	122.08	119.67
2	F	302[A]	NAR	C5-C4-C3	2.54	124.13	120.39
4	B	301	X8W	CAJ-CAH-CAO	2.57	122.84	119.87
2	F	301	NAR	O1-C9-C10	2.67	112.59	107.64
2	D	302	NAR	O3-C13-C12	2.95	128.41	120.05
2	D	302	NAR	C12-C11-C10	3.16	124.45	121.20
2	F	301	NAR	C11-C10-C9	3.34	127.13	120.62
2	C	301	NAR	C8-C7-C5	3.38	123.01	117.31
2	E	301	NAR	C8-C7-C5	3.70	123.54	117.31
2	C	301	NAR	C4-C5-C6	3.71	120.75	117.19
2	C	301	NAR	C3-C2-C1	3.74	125.90	120.39

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	301	NAR	O1-C6-C1	3.97	123.32	116.37
2	E	301	NAR	C4-C5-C6	4.16	121.17	117.19
2	F	301	NAR	C6-O1-C9	4.17	122.64	115.62
2	E	301	NAR	C3-C2-C1	4.19	126.55	120.39
2	D	301	NAR	O1-C9-C10	4.75	116.46	107.64
2	D	301	NAR	C3-C2-C1	5.21	128.06	120.39
4	D	303[A]	X8W	CAS-CAT-CAR	5.72	121.90	117.76
2	A	301	NAR	O1-C6-C1	5.92	126.73	116.37
2	F	301	NAR	O1-C6-C1	5.93	126.75	116.37
2	D	302	NAR	O1-C6-C1	5.99	126.85	116.37
2	D	301	NAR	C4-C5-C6	6.04	122.98	117.19
4	D	303[B]	X8W	CAR-CAT-CAN	6.22	124.50	120.35
2	C	301	NAR	O1-C6-C1	6.33	127.45	116.37
2	E	301	NAR	O1-C6-C1	6.94	128.51	116.37
2	D	302	NAR	C15-C10-C9	15.47	150.78	120.62
2	D	302	NAR	C14-C15-C10	20.25	142.02	121.20

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

10 monomers are involved in 25 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	301	NAR	3	0
4	B	301	X8W	5	0
5	B	302	GOL	2	0
2	C	301	NAR	1	0
2	D	301	NAR	4	0
2	D	302	NAR	1	0
4	D	303[A]	X8W	3	0
4	D	303[B]	X8W	5	0
2	E	301	NAR	1	0
2	F	301	NAR	2	0

## 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	282/283 (99%)	-0.30	16 (5%) 27 29	18, 24, 46, 70	0
1	B	259/283 (91%)	-0.76	3 (1%) 81 81	17, 21, 32, 77	0
1	C	282/283 (99%)	-0.34	10 (3%) 48 49	17, 22, 40, 64	0
1	D	259/283 (91%)	-0.75	0 100 100	18, 20, 29, 59	0
1	E	282/283 (99%)	-0.18	20 (7%) 19 20	18, 22, 46, 69	0
1	F	259/283 (91%)	-0.68	1 (0%) 93 93	18, 20, 33, 62	0
All	All	1623/1698 (95%)	-0.49	50 (3%) 52 53	17, 22, 41, 77	0

All (50) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	130	ALA	5.9
1	E	107	ALA	5.5
1	E	130	ALA	5.2
1	E	115	ASP	4.8
1	F	106	ALA	4.7
1	E	108	ALA	4.6
1	E	109	HIS	4.0
1	E	128	ASN	3.9
1	E	117	ASP	3.9
1	A	109	HIS	3.9
1	C	130	ALA	3.8
1	A	107	ALA	3.8
1	A	108	ALA	3.6
1	A	129	ASN	3.4
1	A	117	ASP	3.4
1	E	131	GLU	3.3
1	E	106	ALA	3.2
1	C	129	ASN	3.1
1	E	116	SER	3.0

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
1	A	115	ASP	3.0
1	A	172	GLY	3.0
1	A	131	GLU	2.9
1	E	114	ILE	2.9
1	A	128	ASN	2.9
1	C	115	ASP	2.9
1	C	131	GLU	2.8
1	E	129	ASN	2.8
1	C	108	ALA	2.7
1	A	105	PRO	2.7
1	A	116	SER	2.7
1	E	118	GLY	2.7
1	E	172	GLY	2.6
1	B	247[A]	ASP	2.5
1	C	117	ASP	2.5
1	A	114	ILE	2.5
1	E	242	SER	2.4
1	B	1	ALA	2.4
1	A	174	ASP	2.4
1	A	106	ALA	2.3
1	C	128	ASN	2.3
1	C	109	HIS	2.3
1	E	110	THR	2.2
1	A	123	ALA	2.2
1	E	111	ASP	2.2
1	E	105	PRO	2.2
1	C	105	PRO	2.2
1	E	123	ALA	2.1
1	E	247[A]	ASP	2.1
1	B	106	ALA	2.0
1	C	107	ALA	2.0

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

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

## 6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

## 6.4 Ligands ⓘ

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
2	NAR	D	301	20/20	0.74	0.23	8.34	35,49,61,62	11
2	NAR	F	302[B]	10/20	0.86	0.20	6.54	44,54,59,74	9
5	GOL	B	302	6/6	0.96	0.17	5.63	26,27,27,27	6
2	NAR	F	302[A]	10/20	0.86	0.20	5.52	47,57,59,74	9
4	X8W	D	303[A]	18/20	0.92	0.16	4.52	36,62,67,70	18
5	GOL	F	303	6/6	0.90	0.14	2.81	34,36,39,44	0
4	X8W	B	301	20/20	0.80	0.20	2.54	49,58,69,78	8
2	NAR	F	301	20/20	0.94	0.11	2.00	28,30,32,32	20
4	X8W	D	303[B]	18/20	0.92	0.16	1.60	37,39,76,77	18
2	NAR	C	301	20/20	0.93	0.14	1.37	26,30,32,32	20
2	NAR	A	301	20/20	0.92	0.13	1.27	26,30,33,33	20
2	NAR	E	301	20/20	0.93	0.14	1.22	27,32,36,36	20
2	NAR	D	302	20/20	0.95	0.10	1.07	26,28,35,44	20
3	CL	E	403	1/1	0.96	0.03	-	63,63,63,63	1
3	CL	D	403	1/1	0.97	0.05	-	49,49,49,49	0
3	CL	B	402	1/1	0.89	0.09	-	54,54,54,54	0
3	CL	E	404	1/1	0.74	0.15	-	60,60,60,60	0
3	CL	D	402	1/1	0.95	0.05	-	56,56,56,56	0
3	CL	F	402	1/1	0.97	0.05	-	51,51,51,51	0
3	CL	E	401	1/1	0.97	0.07	-	50,50,50,50	0
3	CL	D	401	1/1	0.97	0.04	-	48,48,48,48	0
3	CL	C	402	1/1	0.92	0.20	-	60,60,60,60	0
3	CL	A	402	1/1	0.95	0.10	-	53,53,53,53	0
3	CL	C	403	1/1	0.89	0.12	-	54,54,54,54	0
3	CL	F	401	1/1	0.90	0.09	-	48,48,48,48	0
3	CL	F	403	1/1	0.98	0.08	-	45,45,45,45	0
3	CL	C	401	1/1	0.92	0.08	-	52,52,52,52	0
3	CL	E	402	1/1	0.93	0.08	-	59,59,59,59	0
3	CL	B	401	1/1	0.97	0.09	-	53,53,53,53	0
3	CL	A	401	1/1	0.94	0.07	-	59,59,59,59	0

## 6.5 Other polymers ⓘ

There are no such residues in this entry.