Full wwPDB X-ray Structure Validation Report (i)

Feb 10, 2024 – 03:46 PM EST

PDB ID	:	2R2D
Title	:	Structure of a quorum-quenching lactonase (AiiB) from Agrobacterium tumefaciens
Authors	:	Liu, D.; Thomas, P.W.; Momb, J.; Hoang, Q.; Petsko, G.A.; Ringe, D.; Fast, W.
Deposited on	:	2007-08-24
Resolution	:	1.75 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
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

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

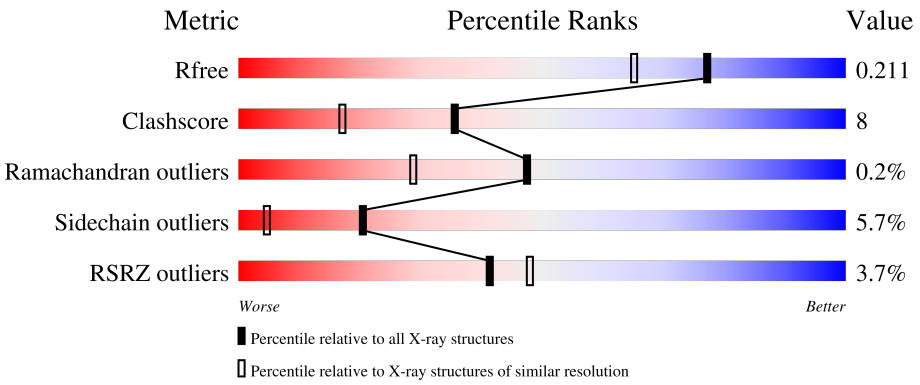
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 1.75 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}	130704	2340 (1.76-1.76)
Clashscore	141614	2466 (1.76-1.76)
Ramachandran outliers	138981	2437 (1.76-1.76)
Sidechain outliers	138945	2437 (1.76-1.76)
RSRZ outliers	127900	2298 (1.76-1.76)

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 of the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. 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 <=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	276	2%, 87%, 12%, •
1	B	276	3%, 84%, 14%, •
1	C	276	%, 87%, 12%, •
1	D	276	5%, 83%, 12%, 5%
1	E	276	6%, 79%, 18%, •

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Mol	Chain	Length	Quality of chain
1	F	276	5% 82% 16%

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	PO4	B	280	-	-	X	-
4	GOL	B	282	-	-	X	-

2 Entry composition (i)

There are 5 unique types of molecules in this entry. The entry contains 15215 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.

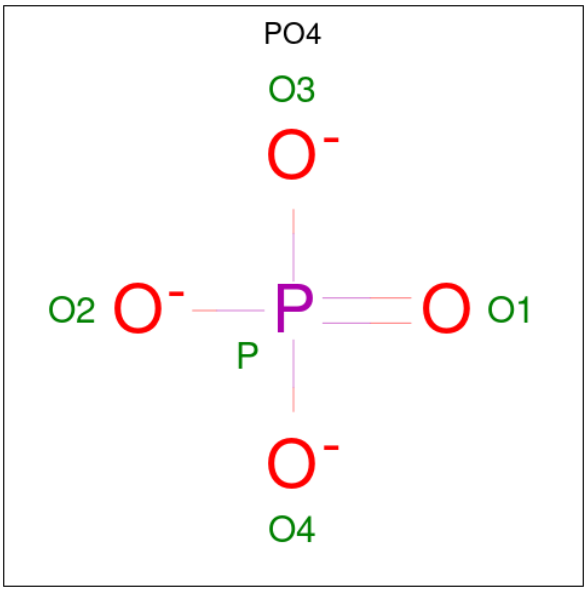
- Molecule 1 is a protein called Zn-dependent hydrolases.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	276	2278	1433	408	428	9	0	17	0
1	B	276	2264	1430	404	421	9	0	17	0
1	C	276	2271	1427	404	431	9	0	18	0
1	D	276	2244	1409	400	426	9	0	14	0
1	E	276	2311	1454	407	440	10	0	23	0
1	F	276	2200	1383	392	416	9	0	6	0

- Molecule 2 is ZINC ION (three-letter code: ZN) (formula: Zn).

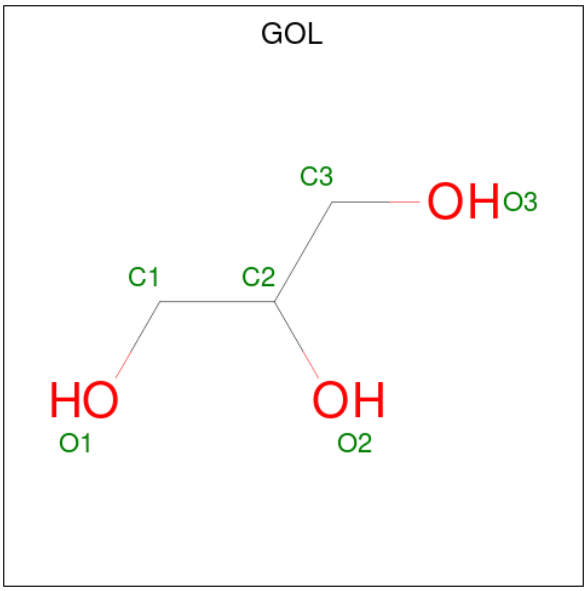
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Zn		
2	A	2	2	2	0	0
2	B	2	2	2	0	0
2	C	2	2	2	0	0
2	D	2	2	2	0	0
2	E	2	2	2	0	0
2	F	2	2	2	0	0

- Molecule 3 is PHOSPHATE ION (three-letter code: PO4) (formula: O_4P).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	O	P		
3	A	1	5	4	1	0	0
3	B	1	5	4	1	0	0
3	B	1	5	4	1	0	0
3	C	1	5	4	1	0	0
3	C	1	10	8	2	0	1
3	D	1	5	4	1	0	0
3	E	1	5	4	1	0	0
3	E	1	5	4	1	0	0
3	F	1	5	4	1	0	0

- Molecule 4 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	C	O		
4	A	1	6	3	3	0	0
			Total	C	O		
4	A	1	6	3	3	0	0
			Total	C	O		
4	A	1	6	3	3	0	0
			Total	C	O		
4	B	1	6	3	3	0	0
			Total	C	O		
4	B	1	6	3	3	0	0
			Total	C	O		
4	C	1	6	3	3	0	0
			Total	C	O		
4	C	1	6	3	3	0	0
			Total	C	O		
4	D	1	6	3	3	0	0
			Total	C	O		
4	E	1	6	3	3	0	0
			Total	C	O		
4	F	1	6	3	3	0	0

- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
5	A	301	301	301	0	0
			Total	O		
5	B	277	277	277	0	0

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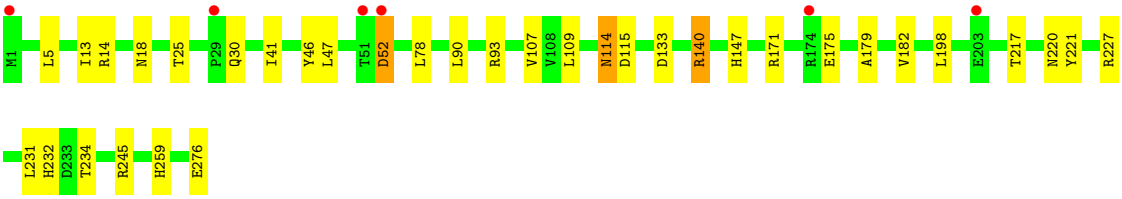
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
5	C	303	305	305	0	2
			Total	O		
5	D	201	201	201	0	0
			Total	O		
5	E	239	239	239	0	0
			Total	O		
5	F	200	202	202	0	2

3 Residue-property plots (i)

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

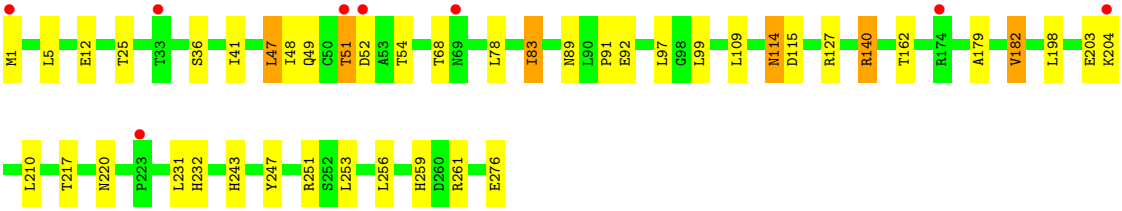
• Molecule 1: Zn-dependent hydrolases

Chain A:



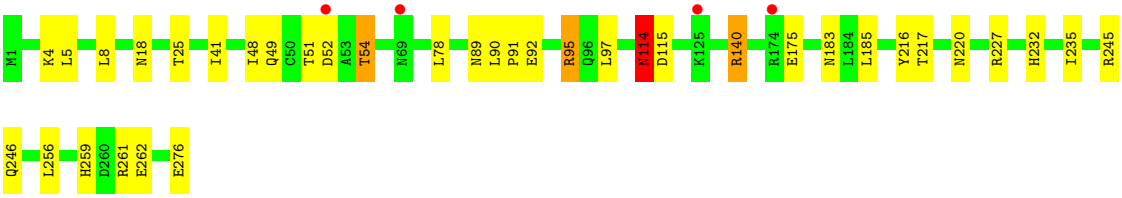
• Molecule 1: Zn-dependent hydrolases

Chain B:



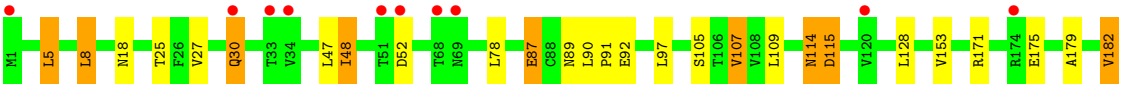
• Molecule 1: Zn-dependent hydrolases

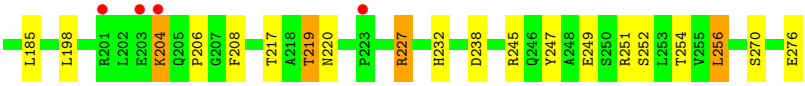
Chain C:



• Molecule 1: Zn-dependent hydrolases

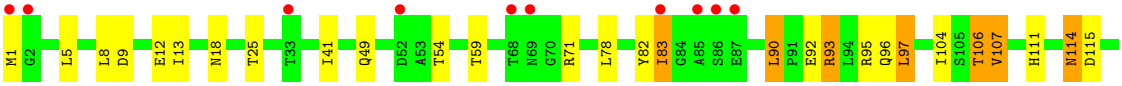
Chain D:

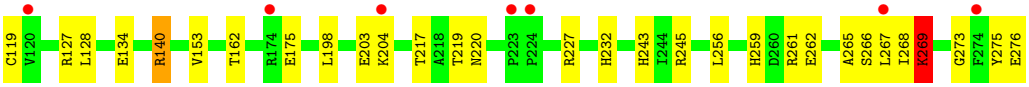




• Molecule 1: Zn-dependent hydrolases

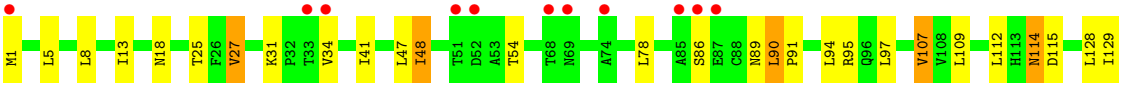
Chain E:

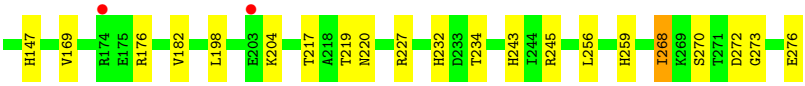




• Molecule 1: Zn-dependent hydrolases

Chain F:





4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	79.15Å 158.03Å 80.44Å 90.00° 104.48° 90.00°	Depositor
Resolution (Å)	18.10 – 1.75 18.09 – 1.75	Depositor EDS
% Data completeness (in resolution range)	96.5 (18.10-1.75) 96.6 (18.09-1.75)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.45 (at 1.75Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.159 , 0.213 0.159 , 0.211	Depositor DCC
R_{free} test set	9324 reflections (5.04%)	wwPDB-VP
Wilson B-factor (Å^2)	30.5	Xtriage
Anisotropy	0.064	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.39 , 60.4	EDS
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.34$	Xtriage
Estimated twinning fraction	0.012 for l,-k,h	Xtriage
F_o,F_c correlation	0.97	EDS
Total number of atoms	15215	wwPDB-VP
Average B, all atoms (Å^2)	35.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.21% of the height of the origin peak. No significant pseudotranslation is detected.*

[1]Intensities estimated from amplitudes.

[2]Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 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: ZN, PO4, GOL

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	0.73	0/2362	0.81	4/3207 (0.1%)
1	B	0.67	0/2360	0.73	2/3204 (0.1%)
1	C	0.71	0/2359	0.82	6/3204 (0.2%)
1	D	0.64	0/2321	0.77	7/3153 (0.2%)
1	E	0.67	0/2397	0.80	3/3255 (0.1%)
1	F	0.62	0/2272	0.77	2/3087 (0.1%)
All	All	0.68	0/14071	0.78	24/19110 (0.1%)

There are no bond length outliers.

All (24) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	245	ARG	NE-CZ-NH2	-10.81	114.89	120.30
1	E	245	ARG	NE-CZ-NH2	-8.14	116.23	120.30
1	F	245	ARG	NE-CZ-NH2	-7.68	116.46	120.30
1	C	245	ARG	NE-CZ-NH1	7.45	124.02	120.30
1	B	140	ARG	NE-CZ-NH2	-6.18	117.21	120.30
1	D	109	LEU	CA-CB-CG	-6.10	101.27	115.30
1	D	245	ARG	NE-CZ-NH1	6.09	123.35	120.30
1	B	109	LEU	CA-CB-CG	-6.08	101.31	115.30
1	D	227	ARG	NE-CZ-NH1	5.94	123.27	120.30
1	A	109	LEU	CB-CG-CD1	5.78	120.82	111.00
1	A	109	LEU	CA-CB-CG	-5.77	102.04	115.30
1	D	245	ARG	NE-CZ-NH2	-5.72	117.44	120.30
1	A	93	ARG	NE-CZ-NH2	-5.58	117.51	120.30
1	D	5	LEU	CA-CB-CG	5.57	128.11	115.30
1	F	245	ARG	NE-CZ-NH1	5.47	123.04	120.30
1	E	140	ARG	NE-CZ-NH2	-5.23	117.69	120.30
1	A	140	ARG	NE-CZ-NH2	-5.19	117.70	120.30
1	C	140[A]	ARG	NE-CZ-NH1	5.16	122.88	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	140[B]	ARG	NE-CZ-NH1	5.16	122.88	120.30
1	C	140[A]	ARG	NE-CZ-NH2	-5.05	117.77	120.30
1	C	140[B]	ARG	NE-CZ-NH2	-5.05	117.77	120.30
1	E	245	ARG	NE-CZ-NH1	5.05	122.82	120.30
1	D	227	ARG	NE-CZ-NH2	-5.04	117.78	120.30
1	D	115	ASP	CB-CG-OD2	5.02	122.81	118.30

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	2278	0	2246	24	1
1	B	2264	0	2250	49	0
1	C	2271	0	2224	35	0
1	D	2244	0	2197	26	0
1	E	2311	0	2268	59	2
1	F	2200	0	2146	29	0
2	A	2	0	0	0	0
2	B	2	0	0	0	0
2	C	2	0	0	0	0
2	D	2	0	0	0	0
2	E	2	0	0	0	0
2	F	2	0	0	0	0
3	A	5	0	0	0	0
3	B	10	0	0	3	0
3	C	15	0	0	1	0
3	D	5	0	0	0	0
3	E	10	0	0	0	0
3	F	5	0	0	0	0
4	A	18	0	24	3	0
4	B	12	0	16	10	0
4	C	12	0	16	2	0
4	D	6	0	8	0	0
4	E	6	0	8	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	F	6	0	8	1	0
5	A	301	0	0	8	0
5	B	277	0	0	10	0
5	C	305	0	0	3	0
5	D	201	0	0	3	1
5	E	239	0	0	7	0
5	F	202	0	0	5	0
All	All	15215	0	13411	219	2

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 8.

All (219) 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:E:93[A]:ARG:NH1	1:E:269[A]:LYS:HD2	1.46	1.28
1:C:261[B]:ARG:CZ	1:C:262[B]:GLU:OE2	1.86	1.23
1:E:267[A]:LEU:O	1:E:268[A]:ILE:HG13	1.35	1.21
1:C:261[B]:ARG:NH2	1:C:262[B]:GLU:OE2	1.74	1.20
1:E:93[A]:ARG:HH11	1:E:269[A]:LYS:CD	1.57	1.18
1:E:93[A]:ARG:NH1	1:E:269[A]:LYS:CD	2.10	1.15
1:B:140:ARG:CD	4:B:282:GOL:H11	1.77	1.14
1:E:265[A]:ALA:O	1:E:266[A]:SER:CB	1.96	1.09
1:E:268[B]:ILE:O	1:E:269[B]:LYS:O	1.75	1.03
1:B:68[A]:THR:HG21	1:F:204:LYS:HB3	1.39	1.02
1:D:30:GLN:HG3	5:D:410:HOH:O	1.58	1.02
1:B:140:ARG:HD2	4:B:282:GOL:H11	1.39	0.99
1:E:267[A]:LEU:O	1:E:268[A]:ILE:CG1	2.12	0.98
1:E:92[A]:GLU:HA	1:E:95[A]:ARG:NE	1.79	0.98
1:E:265[A]:ALA:O	1:E:266[A]:SER:HB3	1.15	0.96
1:F:204:LYS:HD2	1:F:276:GLU:HG3	1.49	0.95
1:B:140:ARG:HD3	4:B:282:GOL:H11	1.48	0.94
1:C:175:GLU:HG2	1:C:183[B]:ASN:ND2	1.80	0.94
1:E:93[A]:ARG:HH12	1:E:269[A]:LYS:HD2	1.28	0.93
1:E:92[A]:GLU:HA	1:E:95[A]:ARG:HE	1.32	0.92
1:E:93[A]:ARG:HH11	1:E:269[A]:LYS:HD3	1.36	0.90
1:C:261[B]:ARG:NH1	1:C:262[B]:GLU:OE2	2.05	0.89
1:C:261[B]:ARG:NH2	1:C:262[B]:GLU:CD	2.27	0.88
1:F:89:ASN:HD22	1:F:91:PRO:HD2	1.38	0.85
1:E:92[B]:GLU:OE2	1:E:95[B]:ARG:NH2	2.13	0.82
1:E:92[A]:GLU:HB2	1:E:95[A]:ARG:HH21	1.45	0.81

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:221:TYR:OH	1:A:245[A]:ARG:HG3	1.81	0.81
1:B:243:HIS:HE1	5:B:548:HOH:O	1.64	0.80
1:C:175:GLU:HG2	1:C:183[B]:ASN:HD21	1.47	0.78
1:B:89:ASN:HD22	1:B:91:PRO:HD2	1.49	0.77
1:E:93[B]:ARG:NH1	1:E:269[B]:LYS:NZ	2.31	0.77
1:B:25[B]:THR:HG21	1:B:36:SER:HA	1.67	0.75
1:E:140:ARG:HD3	5:E:398:HOH:O	1.87	0.75
1:F:18:ASN:HD21	1:F:25:THR:H	1.31	0.75
1:C:89:ASN:HD22	1:C:91:PRO:HD2	1.50	0.74
1:C:51[A]:THR:O	1:C:52[A]:ASP:CB	2.36	0.73
1:C:51[A]:THR:O	1:C:52[A]:ASP:HB3	1.89	0.72
1:B:251[A]:ARG:NH2	3:B:280:PO4:O4	2.22	0.72
1:A:18:ASN:HD21	1:A:25:THR:H	1.38	0.70
1:C:5:LEU:HD23	1:C:48[B]:ILE:CD1	2.22	0.70
1:B:179:ALA:HB3	1:B:182:VAL:HG13	1.73	0.70
1:C:18:ASN:HD21	1:C:25:THR:H	1.37	0.69
1:D:89:ASN:HD22	1:D:91:PRO:HD2	1.57	0.69
1:F:5:LEU:HD23	1:F:48:ILE:HD12	1.74	0.69
1:D:18:ASN:HD21	1:D:25:THR:H	1.40	0.68
1:E:9:ASP:HB3	1:E:93[B]:ARG:NH1	2.10	0.66
1:E:93[A]:ARG:NH1	1:E:269[A]:LYS:HD3	1.98	0.66
1:A:14[B]:ARG:NH2	5:A:319:HOH:O	2.28	0.66
1:B:127[B]:ARG:HG3	1:B:127[B]:ARG:HH11	1.60	0.66
1:B:140:ARG:HD3	4:B:282:GOL:H32	1.78	0.65
1:B:261[A]:ARG:NH2	5:B:321:HOH:O	2.27	0.65
1:B:25[B]:THR:HG21	1:B:36:SER:CA	2.25	0.65
1:F:268:ILE:HD11	1:F:273:GLY:CA	2.27	0.64
1:B:243:HIS:CE1	5:B:548:HOH:O	2.45	0.63
1:E:93[B]:ARG:NH1	1:E:269[B]:LYS:HZ3	1.96	0.63
1:B:232:HIS:HE1	5:B:526:HOH:O	1.81	0.63
1:E:93[B]:ARG:HH12	1:E:269[B]:LYS:NZ	1.97	0.61
1:D:204[A]:LYS:HD2	1:D:276:GLU:HG3	1.83	0.61
1:E:267[A]:LEU:O	1:E:268[A]:ILE:CB	2.49	0.60
1:D:249:GLU:O	1:D:251[B]:ARG:O	2.19	0.60
1:B:140:ARG:HD2	4:B:282:GOL:C1	2.25	0.59
1:F:31:LYS:HG3	1:F:34[B]:VAL:HG13	1.84	0.59
1:A:179:ALA:HB3	1:A:182[A]:VAL:CG1	2.33	0.59
1:E:92[A]:GLU:CA	1:E:95[A]:ARG:HE	2.09	0.59
1:C:261[B]:ARG:NH2	1:C:262[B]:GLU:OE1	2.36	0.59
1:E:243:HIS:HD2	5:E:340:HOH:O	1.85	0.58
1:E:107[A]:VAL:HG13	1:E:128:LEU:HD23	1.86	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:140:ARG:HD3	5:A:481:HOH:O	2.02	0.58
1:F:41:ILE:HB	1:F:259:HIS:HB3	1.86	0.58
1:C:175:GLU:CG	1:C:183[B]:ASN:ND2	2.61	0.57
1:D:175:GLU:HG3	1:D:185:LEU:HD23	1.85	0.57
1:E:268[B]:ILE:HG13	1:E:275:TYR:HH	1.70	0.57
1:E:92[A]:GLU:HA	1:E:95[A]:ARG:HG2	1.87	0.57
1:E:49:GLN:OE1	1:E:54:THR:HG22	2.05	0.57
1:B:140:ARG:CB	4:B:282:GOL:H32	2.35	0.56
1:C:114:ASN:ND2	1:C:115:ASP:H	2.02	0.56
5:B:397:HOH:O	1:C:232:HIS:HD2	1.89	0.56
1:A:5[B]:LEU:HD21	1:A:46:TYR:HB3	1.88	0.56
1:C:5:LEU:HD23	1:C:48[B]:ILE:HD12	1.88	0.55
1:C:92:GLU:OE2	1:C:95[A]:ARG:NE	2.39	0.55
1:D:227:ARG:HD3	1:D:238:ASP:OD2	2.07	0.55
1:E:204:LYS:HD2	1:E:276:GLU:HB3	1.89	0.55
1:E:18:ASN:HD21	1:E:25:THR:H	1.54	0.54
1:A:133:ASP:OD2	1:A:171[A]:ARG:HD3	2.05	0.54
1:F:31:LYS:HG3	1:F:34[A]:VAL:CG2	2.38	0.54
1:C:261[B]:ARG:CZ	1:C:262[B]:GLU:CD	2.69	0.54
1:A:52[A]:ASP:OD1	1:A:52[A]:ASP:N	2.37	0.53
1:F:232:HIS:HE1	5:F:301:HOH:O	1.90	0.53
1:E:114:ASN:ND2	1:E:115:ASP:H	2.07	0.53
1:E:203:GLU:OE2	1:E:203:GLU:HA	2.08	0.53
1:D:217:THR:H	1:D:220:ASN:HD22	1.57	0.53
1:B:140:ARG:HB2	4:B:282:GOL:H32	1.90	0.53
1:E:93[B]:ARG:NH1	1:E:269[B]:LYS:HZ1	2.05	0.53
1:B:232:HIS:HD2	5:C:494:HOH:O	1.90	0.53
1:E:217:THR:H	1:E:220:ASN:HD22	1.56	0.52
1:F:243:HIS:HE1	5:F:383:HOH:O	1.93	0.52
1:B:231:LEU:O	1:C:227[A]:ARG:NH2	2.42	0.52
1:A:114:ASN:HD22	1:A:114:ASN:N	2.07	0.52
1:C:175:GLU:HG3	1:C:185:LEU:HD23	1.92	0.52
1:E:267[A]:LEU:O	1:E:275:TYR:OH	2.23	0.52
1:B:51:THR:HG22	5:B:415:HOH:O	2.09	0.51
1:D:114:ASN:HD22	1:D:114:ASN:N	2.09	0.51
1:E:268[B]:ILE:HG22	1:E:273:GLY:HA3	1.92	0.51
1:B:1:MET:N	5:B:460:HOH:O	2.42	0.51
1:D:107:VAL:HG13	1:D:128:LEU:HD23	1.93	0.51
1:E:106:THR:HG22	5:E:314:HOH:O	2.10	0.51
1:E:232:HIS:HD2	5:E:388:HOH:O	1.93	0.51
1:E:175:GLU:OE2	5:E:449:HOH:O	2.18	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:114:ASN:ND2	1:F:115:ASP:H	2.10	0.50
1:B:89:ASN:ND2	1:B:92:GLU:H	2.09	0.50
1:D:219:THR:HG23	5:D:460:HOH:O	2.11	0.50
1:B:204:LYS:HD3	1:B:276:GLU:HG3	1.93	0.50
1:D:89:ASN:ND2	1:D:92:GLU:H	2.09	0.49
1:A:30[B]:GLN:NE2	1:A:30[B]:GLN:H	2.10	0.49
1:A:232:HIS:HE1	5:A:420:HOH:O	1.95	0.49
1:F:268:ILE:HD11	1:F:273:GLY:C	2.33	0.49
1:B:49[A]:GLN:NE2	1:B:54:THR:HG21	2.27	0.49
1:D:5:LEU:HD23	1:D:48:ILE:CD1	2.42	0.49
1:E:268[B]:ILE:O	1:E:269[B]:LYS:C	2.50	0.49
1:A:30[B]:GLN:H	1:A:30[B]:GLN:CD	2.16	0.49
1:A:41:ILE:HB	1:A:259:HIS:HB3	1.95	0.49
1:A:221:TYR:CZ	1:A:245[A]:ARG:HG3	2.48	0.48
1:B:140:ARG:NH2	5:B:473:HOH:O	2.45	0.48
1:B:251[A]:ARG:HG3	1:B:253:LEU:HG	1.93	0.48
1:E:92[A]:GLU:CA	1:E:95[A]:ARG:NE	2.63	0.48
1:C:114:ASN:HD22	1:C:115:ASP:H	1.61	0.48
1:E:92[B]:GLU:OE2	1:E:96:GLN:HG3	2.13	0.48
1:F:27:VAL:HG23	1:F:34[B]:VAL:HG22	1.96	0.48
1:F:147:HIS:HE1	5:F:392:HOH:O	1.96	0.48
1:B:114:ASN:HD22	1:B:114:ASN:N	2.11	0.48
1:E:232:HIS:HE1	5:E:503:HOH:O	1.96	0.48
1:D:87:GLU:H	1:D:87:GLU:CD	2.17	0.48
1:D:247:TYR:O	1:D:251[B]:ARG:HD2	2.13	0.48
1:D:206:PRO:HB2	1:D:252[A]:SER:O	2.14	0.47
1:B:210:LEU:CD2	1:B:256[B]:LEU:HD12	2.44	0.47
1:C:232:HIS:HE1	5:C:328:HOH:O	1.97	0.47
1:F:227[B]:ARG:CZ	1:F:234:THR:HB	2.44	0.47
1:E:13:ILE:HD13	1:E:82:TYR:HA	1.96	0.47
1:A:245[A]:ARG:NH1	5:A:392:HOH:O	2.47	0.47
1:B:25[B]:THR:HG21	1:B:36:SER:CB	2.44	0.47
1:B:251[A]:ARG:HH22	3:B:280:PO4:P	2.38	0.47
1:D:204[B]:LYS:HB2	1:D:276:GLU:OXT	2.15	0.47
1:E:71:ARG:HD3	5:E:497:HOH:O	2.14	0.47
1:F:243:HIS:HD2	5:F:363:HOH:O	1.98	0.47
1:F:13:ILE:HD13	4:F:280:GOL:H32	1.97	0.47
1:B:5:LEU:HD23	1:B:48:ILE:HG13	1.97	0.47
1:C:41:ILE:HD11	4:C:281:GOL:H11	1.97	0.47
1:E:41:ILE:HB	1:E:259:HIS:HB3	1.96	0.47
1:E:114:ASN:HD22	1:E:115:ASP:H	1.63	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:217:THR:H	1:A:220:ASN:HD22	1.63	0.46
1:B:217:THR:H	1:B:220:ASN:HD22	1.63	0.46
1:C:235:ILE:HB	4:C:282:GOL:H2	1.97	0.46
1:E:93[B]:ARG:HH12	1:E:269[B]:LYS:CE	2.28	0.46
1:E:106:THR:HB	1:E:127:ARG:HB3	1.96	0.46
1:A:13:ILE:HG21	4:A:280:GOL:H32	1.97	0.46
1:A:227[B]:ARG:CZ	1:A:234:THR:HB	2.46	0.45
1:F:90:LEU:HD22	1:F:94:LEU:HG	1.98	0.45
1:B:247:TYR:O	1:B:251[A]:ARG:HG2	2.16	0.45
1:D:232:HIS:HE1	5:D:373:HOH:O	1.98	0.45
1:F:78:LEU:HD13	5:F:471:HOH:O	2.15	0.45
1:B:41:ILE:HB	1:B:259:HIS:HB3	1.97	0.45
1:C:49:GLN:OE1	1:C:54:THR:HB	2.17	0.45
1:C:51[B]:THR:O	1:C:52[B]:ASP:HB2	2.16	0.44
1:F:89:ASN:HD22	1:F:91:PRO:CD	2.19	0.44
1:A:232:HIS:HD2	5:A:576:HOH:O	2.01	0.44
1:B:78[A]:LEU:HD23	1:F:272:ASP:HB3	2.00	0.44
1:C:140[B]:ARG:NH2	5:C:326:HOH:O	2.50	0.44
1:E:8[A]:LEU:CD2	1:E:90:LEU:HD23	2.47	0.44
1:C:216:TYR:HB2	1:C:220:ASN:ND2	2.33	0.44
1:F:107:VAL:HG13	1:F:128:LEU:HD23	2.00	0.44
1:F:109:LEU:HD13	1:F:112:LEU:HD21	2.00	0.44
1:B:203:GLU:HG3	5:B:319:HOH:O	2.17	0.43
1:A:114:ASN:ND2	1:A:115:ASP:H	2.17	0.43
1:C:92:GLU:OE2	1:C:95[A]:ARG:NH2	2.51	0.43
1:D:179:ALA:HB3	1:D:182:VAL:HG13	2.01	0.43
1:B:179:ALA:HB3	1:B:182:VAL:CG1	2.45	0.43
1:B:47:LEU:HD11	1:B:99:LEU:CD1	2.49	0.43
1:A:147:HIS:HE1	5:A:403:HOH:O	2.02	0.43
1:B:114:ASN:ND2	1:B:115:ASP:H	2.16	0.43
1:B:49[A]:GLN:NE2	1:B:54:THR:CG2	2.82	0.43
1:B:127[B]:ARG:HG3	1:B:127[B]:ARG:NH1	2.33	0.42
1:E:92[A]:GLU:HA	1:E:95[A]:ARG:CG	2.49	0.42
1:E:111:HIS:HA	1:E:134:GLU:HG2	2.00	0.42
1:C:41:ILE:HB	1:C:259:HIS:HB3	2.00	0.42
1:F:97:LEU:HD11	1:F:270:SER:HB2	2.01	0.42
1:F:129:ILE:HD11	1:F:176[C]:ARG:HH11	1.84	0.42
1:F:217:THR:H	1:F:220:ASN:HD22	1.66	0.42
1:E:12:GLU:HB2	1:E:83:ILE:HG22	2.02	0.42
1:E:217:THR:N	1:E:220:ASN:HD22	2.17	0.42
1:A:18:ASN:HD22	1:A:18:ASN:HA	1.70	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:140:ARG:HD3	4:B:282:GOL:C1	2.35	0.42
1:C:246:GLN:HE22	3:C:280[A]:PO4:P	2.42	0.42
1:D:18:ASN:HD22	1:D:18:ASN:HA	1.72	0.42
1:D:217:THR:N	1:D:220:ASN:HD22	2.17	0.42
1:C:92:GLU:OE2	1:C:95[A]:ARG:CZ	2.67	0.42
1:E:59:THR:HB	1:E:119:CYS:HB2	2.02	0.42
1:B:251[A]:ARG:NH2	3:B:280:PO4:P	2.93	0.42
1:D:114:ASN:ND2	1:D:115:ASP:H	2.17	0.42
1:D:208:PHE:CD2	1:D:254:THR:HB	2.55	0.42
1:B:68[A]:THR:HG22	5:B:304:HOH:O	2.19	0.41
1:E:267[A]:LEU:HD23	1:E:267[A]:LEU:HA	1.91	0.41
1:A:140:ARG:HB2	5:A:536:HOH:O	2.20	0.41
1:B:12:GLU:HB2	1:B:83[A]:ILE:HG22	2.01	0.41
1:C:4:LYS:HG2	1:C:276:GLU:HG3	2.02	0.41
1:E:54:THR:OG1	1:E:104:ILE:HA	2.21	0.41
1:B:232:HIS:HA	1:C:227[A]:ARG:HH22	1.86	0.41
1:D:8:LEU:HD12	1:D:270:SER:HB3	2.02	0.41
4:A:282:GOL:H32	5:A:570:HOH:O	2.20	0.41
1:B:140:ARG:CD	4:B:282:GOL:C1	2.71	0.41
1:B:140:ARG:HB2	4:B:282:GOL:C3	2.51	0.41
1:E:18:ASN:HD22	1:E:18:ASN:HA	1.76	0.41
1:E:5:LEU:HB3	1:E:275:TYR:HB2	2.03	0.41
1:A:41:ILE:HD11	4:A:280:GOL:H11	2.01	0.41
1:E:268[B]:ILE:HG13	1:E:275:TYR:CZ	2.55	0.41
1:C:217:THR:H	1:C:220:ASN:HD22	1.68	0.41
1:D:251[A]:ARG:O	1:D:252[A]:SER:HB2	2.21	0.41
1:D:208:PHE:HB3	1:D:256:LEU:HD22	2.03	0.40
1:F:268:ILE:HD11	1:F:273:GLY:N	2.35	0.40
1:F:114:ASN:N	1:F:114:ASN:HD22	2.18	0.40

All (2) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:97:LEU:O	5:D:446:HOH:O[1_556]	2.13	0.07
1:A:231:LEU:O	1:E:227[A]:ARG:NH2[1_455]	2.18	0.02

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	292/276 (106%)	281 (96%)	11 (4%)	0	100	100
1	B	291/276 (105%)	277 (95%)	14 (5%)	0	100	100
1	C	292/276 (106%)	282 (97%)	9 (3%)	1 (0%)	41	22
1	D	288/276 (104%)	275 (96%)	11 (4%)	2 (1%)	22	8
1	E	296/276 (107%)	280 (95%)	14 (5%)	2 (1%)	22	8
1	F	281/276 (102%)	269 (96%)	12 (4%)	0	100	100
All	All	1740/1656 (105%)	1664 (96%)	71 (4%)	5 (0%)	47	22

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	E	269[A]	LYS
1	E	269[B]	LYS
1	D	204[A]	LYS
1	D	204[B]	LYS
1	C	114	ASN

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	249/232 (107%)	239 (96%)	10 (4%)	31	10
1	B	249/232 (107%)	239 (96%)	10 (4%)	31	10
1	C	250/232 (108%)	241 (96%)	9 (4%)	35	13

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	D	246/232 (106%)	226 (92%)	20 (8%)	11 1
1	E	253/232 (109%)	230 (91%)	23 (9%)	9 1
1	F	239/232 (103%)	222 (93%)	17 (7%)	14 2
All	All	1486/1392 (107%)	1397 (94%)	89 (6%)	20 4

All (89) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	47	LEU
1	A	52[A]	ASP
1	A	52[B]	ASP
1	A	78	LEU
1	A	90	LEU
1	A	107	VAL
1	A	114	ASN
1	A	175	GLU
1	A	198	LEU
1	A	276	GLU
1	B	47	LEU
1	B	51	THR
1	B	52	ASP
1	B	83[A]	ILE
1	B	83[B]	ILE
1	B	97	LEU
1	B	114	ASN
1	B	162	THR
1	B	182	VAL
1	B	198	LEU
1	C	8	LEU
1	C	54	THR
1	C	78	LEU
1	C	90	LEU
1	C	95[A]	ARG
1	C	95[B]	ARG
1	C	97	LEU
1	C	114	ASN
1	C	256	LEU
1	D	8	LEU
1	D	27	VAL
1	D	30	GLN
1	D	47	LEU

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Mol	Chain	Res	Type
1	D	48	ILE
1	D	52	ASP
1	D	78	LEU
1	D	87	GLU
1	D	90	LEU
1	D	97	LEU
1	D	105[A]	SER
1	D	105[B]	SER
1	D	107	VAL
1	D	114	ASN
1	D	153	VAL
1	D	171	ARG
1	D	182	VAL
1	D	198	LEU
1	D	219	THR
1	D	256	LEU
1	E	1[A]	MET
1	E	1[B]	MET
1	E	78	LEU
1	E	83	ILE
1	E	90	LEU
1	E	93[A]	ARG
1	E	93[B]	ARG
1	E	97	LEU
1	E	106	THR
1	E	107[A]	VAL
1	E	107[B]	VAL
1	E	114	ASN
1	E	153	VAL
1	E	162[A]	THR
1	E	162[B]	THR
1	E	198	LEU
1	E	219	THR
1	E	256	LEU
1	E	261[A]	ARG
1	E	261[B]	ARG
1	E	262	GLU
1	E	269[A]	LYS
1	E	269[B]	LYS
1	F	1	MET
1	F	8	LEU
1	F	27	VAL

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Mol	Chain	Res	Type
1	F	47	LEU
1	F	48	ILE
1	F	54	THR
1	F	86	SER
1	F	90	LEU
1	F	95	ARG
1	F	107	VAL
1	F	114	ASN
1	F	169	VAL
1	F	182	VAL
1	F	198	LEU
1	F	219	THR
1	F	256	LEU
1	F	268	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (31) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	18	ASN
1	A	114	ASN
1	A	220	ASN
1	A	232	HIS
1	B	89	ASN
1	B	114	ASN
1	B	220	ASN
1	B	232	HIS
1	C	18	ASN
1	C	75	GLN
1	C	89	ASN
1	C	114	ASN
1	C	220	ASN
1	C	232	HIS
1	C	246	GLN
1	D	18	ASN
1	D	89	ASN
1	D	114	ASN
1	D	220	ASN
1	E	18	ASN
1	E	75	GLN
1	E	114	ASN
1	E	220	ASN
1	E	232	HIS

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Mol	Chain	Res	Type
1	E	246	GLN
1	F	18	ASN
1	F	49	GLN
1	F	75	GLN
1	F	89	ASN
1	F	114	ASN
1	F	220	ASN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 32 ligands modelled in this entry, 12 are monoatomic - leaving 20 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	$\#\|Z\| > 2$
3	PO4	B	280	-	4,4,4	0.91	0	6,6,6	0.58	0
4	GOL	C	282	-	5,5,5	0.28	0	5,5,5	0.43	0
4	GOL	F	280	-	5,5,5	0.43	0	5,5,5	0.58	0
3	PO4	C	280[A]	-	4,4,4	0.95	0	6,6,6	0.62	0
4	GOL	B	281	-	5,5,5	0.38	0	5,5,5	0.72	0
3	PO4	E	279	2	4,4,4	0.84	0	6,6,6	0.87	0
4	GOL	E	281	-	5,5,5	0.43	0	5,5,5	0.70	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
3	PO4	B	279	2	4,4,4	0.97	0	6,6,6	0.93	0
4	GOL	B	282	-	5,5,5	0.40	0	5,5,5	0.87	0
4	GOL	C	281	-	5,5,5	0.29	0	5,5,5	0.84	0
4	GOL	D	280	-	5,5,5	0.48	0	5,5,5	0.76	0
3	PO4	E	280	-	4,4,4	0.92	0	6,6,6	0.46	0
3	PO4	C	279	2	4,4,4	1.12	0	6,6,6	0.58	0
4	GOL	A	280	-	5,5,5	0.42	0	5,5,5	0.85	0
3	PO4	C	280[B]	-	4,4,4	1.05	0	6,6,6	0.45	0
4	GOL	A	281	-	5,5,5	0.45	0	5,5,5	0.60	0
3	PO4	F	279	2	4,4,4	0.68	0	6,6,6	0.57	0
4	GOL	A	282	-	5,5,5	0.43	0	5,5,5	0.47	0
3	PO4	D	279	2	4,4,4	0.66	0	6,6,6	0.40	0
3	PO4	A	279	2	4,4,4	0.94	0	6,6,6	0.63	0

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
4	GOL	A	280	-	-	4/4/4/4	-
4	GOL	C	282	-	-	2/4/4/4	-
4	GOL	A	281	-	-	2/4/4/4	-
4	GOL	F	280	-	-	2/4/4/4	-
4	GOL	B	282	-	-	2/4/4/4	-
4	GOL	C	281	-	-	0/4/4/4	-
4	GOL	D	280	-	-	3/4/4/4	-
4	GOL	B	281	-	-	2/4/4/4	-
4	GOL	A	282	-	-	2/4/4/4	-
4	GOL	E	281	-	-	3/4/4/4	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (22) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	280	GOL	C1-C2-C3-O3
4	A	282	GOL	C1-C2-C3-O3

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Mol	Chain	Res	Type	Atoms
4	A	282	GOL	O2-C2-C3-O3
4	C	282	GOL	O1-C1-C2-C3
4	D	280	GOL	C1-C2-C3-O3
4	E	281	GOL	C1-C2-C3-O3
4	F	280	GOL	C1-C2-C3-O3
4	A	281	GOL	O1-C1-C2-O2
4	A	280	GOL	O1-C1-C2-C3
4	A	281	GOL	O1-C1-C2-C3
4	B	281	GOL	C1-C2-C3-O3
4	B	282	GOL	C1-C2-C3-O3
4	D	280	GOL	O1-C1-C2-C3
4	E	281	GOL	O1-C1-C2-C3
4	A	280	GOL	O2-C2-C3-O3
4	C	282	GOL	O1-C1-C2-O2
4	D	280	GOL	O2-C2-C3-O3
4	E	281	GOL	O2-C2-C3-O3
4	F	280	GOL	O2-C2-C3-O3
4	B	281	GOL	O2-C2-C3-O3
4	A	280	GOL	O1-C1-C2-O2
4	B	282	GOL	O2-C2-C3-O3

There are no ring outliers.

8 monomers are involved in 20 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	280	PO4	3	0
4	C	282	GOL	1	0
4	F	280	GOL	1	0
3	C	280[A]	PO4	1	0
4	B	282	GOL	10	0
4	C	281	GOL	1	0
4	A	280	GOL	2	0
4	A	282	GOL	1	0

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data (i)

6.1 Protein, DNA and RNA chains (i)

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	276/276 (100%)	-0.16	6 (2%)	62	69	21, 28, 42, 56	0
1	B	276/276 (100%)	-0.05	8 (2%)	51	57	23, 32, 44, 63	0
1	C	276/276 (100%)	-0.20	4 (1%)	75	82	22, 29, 40, 53	0
1	D	276/276 (100%)	0.11	14 (5%)	28	34	25, 35, 54, 65	0
1	E	276/276 (100%)	0.14	17 (6%)	20	26	23, 36, 51, 58	0
1	F	276/276 (100%)	0.09	13 (4%)	31	37	29, 38, 51, 69	0
All	All	1656/1656 (100%)	-0.01	62 (3%)	41	48	21, 33, 49, 69	0

All (62) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	1	MET	9.5
1	E	267[A]	LEU	8.2
1	A	1	MET	7.1
1	F	1	MET	6.7
1	D	51	THR	6.4
1	B	1	MET	5.8
1	F	52[A]	ASP	5.4
1	E	85	ALA	5.1
1	B	51	THR	5.1
1	B	52	ASP	5.1
1	F	69[A]	ASN	4.9
1	E	69	ASN	4.8
1	F	51	THR	4.6
1	F	33	THR	4.5
1	D	33	THR	4.2
1	B	69	ASN	4.0
1	F	68	THR	3.8
1	F	86	SER	3.6
1	E	68	THR	3.6

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Mol	Chain	Res	Type	RSRZ
1	D	30	GLN	3.6
1	E	86	SER	3.5
1	D	204[A]	LYS	3.5
1	D	174	ARG	3.3
1	C	69	ASN	3.3
1	F	34[A]	VAL	3.3
1	E	1[A]	MET	3.2
1	D	52	ASP	3.2
1	E	204	LYS	3.2
1	E	83	ILE	3.1
1	B	33	THR	3.0
1	F	174	ARG	3.0
1	E	174	ARG	2.9
1	E	2[A]	GLY	2.8
1	A	51	THR	2.8
1	D	203	GLU	2.7
1	D	34	VAL	2.7
1	A	174	ARG	2.7
1	E	274	PHE	2.7
1	B	174[A]	ARG	2.6
1	D	120	VAL	2.6
1	C	125[A]	LYS	2.6
1	F	203	GLU	2.5
1	C	52[A]	ASP	2.5
1	E	87[A]	GLU	2.5
1	E	33	THR	2.5
1	D	201[A]	ARG	2.5
1	A	52[A]	ASP	2.5
1	E	223	PRO	2.4
1	E	52	ASP	2.4
1	C	174	ARG	2.4
1	D	69[A]	ASN	2.4
1	D	68	THR	2.4
1	F	87	GLU	2.3
1	A	29	PRO	2.3
1	B	223	PRO	2.2
1	A	203	GLU	2.2
1	F	74	ALA	2.2
1	E	120	VAL	2.2
1	D	223	PRO	2.2
1	B	204	LYS	2.2
1	F	85	ALA	2.2

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Mol	Chain	Res	Type	RSRZ
1	E	224	PRO	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 monosaccharides 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. 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	B-factors(Å^2)	Q<0.9
4	GOL	A	281	6/6	0.67	0.28	47,55,56,57	0
4	GOL	B	281	6/6	0.70	0.14	51,53,55,55	0
4	GOL	A	282	6/6	0.73	0.14	52,52,53,53	0
4	GOL	B	282	6/6	0.88	0.24	43,50,53,57	0
3	PO4	B	280	5/5	0.90	0.15	46,48,49,49	5
4	GOL	E	281	6/6	0.90	0.11	49,51,52,52	0
4	GOL	F	280	6/6	0.90	0.10	51,53,53,55	0
4	GOL	C	281	6/6	0.91	0.12	40,43,44,50	0
3	PO4	C	280[A]	5/5	0.91	0.15	42,44,44,44	5
3	PO4	C	280[B]	5/5	0.91	0.15	43,44,46,46	5
4	GOL	D	280	6/6	0.92	0.10	46,47,49,51	0
3	PO4	E	280	5/5	0.92	0.13	47,48,49,50	5
4	GOL	C	282	6/6	0.92	0.20	46,53,54,56	0
4	GOL	A	280	6/6	0.94	0.09	40,42,43,43	0
3	PO4	E	279	5/5	0.99	0.03	32,33,35,36	0
3	PO4	D	279	5/5	0.99	0.04	29,29,30,31	0
2	ZN	A	278	1/1	1.00	0.06	23,23,23,23	0
2	ZN	B	277	1/1	1.00	0.05	27,27,27,27	0
2	ZN	B	278	1/1	1.00	0.07	26,26,26,26	0
2	ZN	C	277	1/1	1.00	0.04	24,24,24,24	0
2	ZN	C	278	1/1	1.00	0.05	23,23,23,23	0
3	PO4	F	279	5/5	1.00	0.03	30,31,35,35	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	ZN	D	277	1/1	1.00	0.05	30,30,30,30	0
2	ZN	D	278	1/1	1.00	0.06	28,28,28,28	0
2	ZN	E	277	1/1	1.00	0.05	32,32,32,32	0
2	ZN	E	278	1/1	1.00	0.04	29,29,29,29	0
2	ZN	F	277	1/1	1.00	0.03	33,33,33,33	0
2	ZN	F	278	1/1	1.00	0.04	32,32,32,32	0
3	PO4	A	279	5/5	1.00	0.04	22,23,25,28	0
3	PO4	B	279	5/5	1.00	0.04	26,26,28,29	0
2	ZN	A	277	1/1	1.00	0.06	24,24,24,24	0
3	PO4	C	279	5/5	1.00	0.04	21,23,25,25	0

6.5 Other polymers (i)

There are no such residues in this entry.