Full wwPDB X-ray Structure Validation Report (i)

Jan 31, 2016 – 09:20 PM GMT

PDB ID	:	1OFG
Title	:	GLUCOSE-FRUCTOSE OXIDOREDUCTASE
Authors	:	Kingston, R.L.; Scopes, R.K.; Baker, E.N.
Deposited on	:	1996-10-17
Resolution	:	2.70 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.
We welcome your comments at validation@mail.wwpdb.org
A user guide is available at
http://wwpdb.org/validation/2016/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The following versions of software and data (see references (1)) were used in the production of this report:

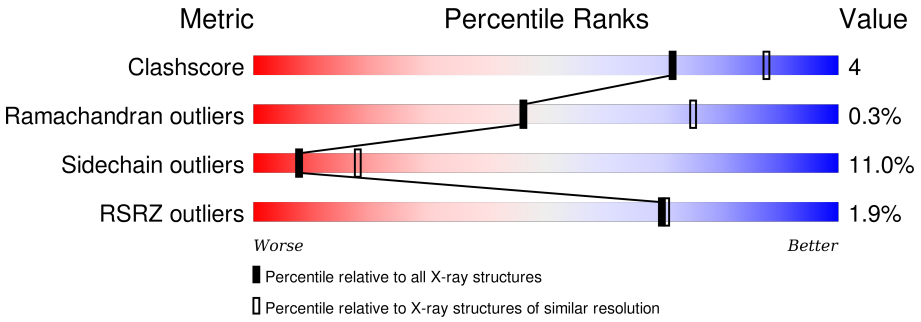
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	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 2.70 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))
Clashscore	102246	2422 (2.70-2.70)
Ramachandran outliers	100387	2382 (2.70-2.70)
Sidechain outliers	100360	2382 (2.70-2.70)
RSRZ outliers	91569	2107 (2.70-2.70)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=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	381	81% 15%
1	B	381	2% 82% 15%
1	C	381	8% 81% 15%
1	D	381	82% 15%
1	E	381	% 83% 14%
1	F	381	% 82% 15%

2 Entry composition

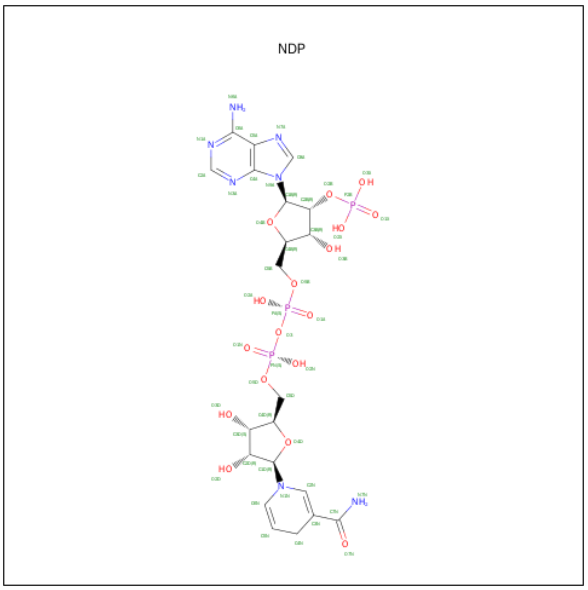
There are 3 unique types of molecules in this entry. The entry contains 18498 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 GLUCOSE-FRUCTOSE OXIDOREDUCTASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	381	Total	C	N	O	S	0	0	0
			2895	1823	504	548	20			
1	B	381	Total	C	N	O	S	0	0	0
			2895	1823	504	548	20			
1	C	381	Total	C	N	O	S	0	0	0
			2895	1823	504	548	20			
1	D	381	Total	C	N	O	S	0	0	0
			2895	1823	504	548	20			
1	E	381	Total	C	N	O	S	0	0	0
			2895	1823	504	548	20			
1	F	381	Total	C	N	O	S	0	0	0
			2895	1823	504	548	20			

- Molecule 2 is NADPH DIHYDRO-NICOTINAMIDE-ADENINE-DINUCLEOTIDE PHOSPHATE (three-letter code: NDP) (formula: $C_{21}H_{30}N_7O_{17}P_3$).



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		
2	E	1	Total	C	N	O	P	0	0
			48	21	7	17	3		
2	F	1	Total	C	N	O	P	0	0
			48	21	7	17	3		

- Molecule 3 is water.

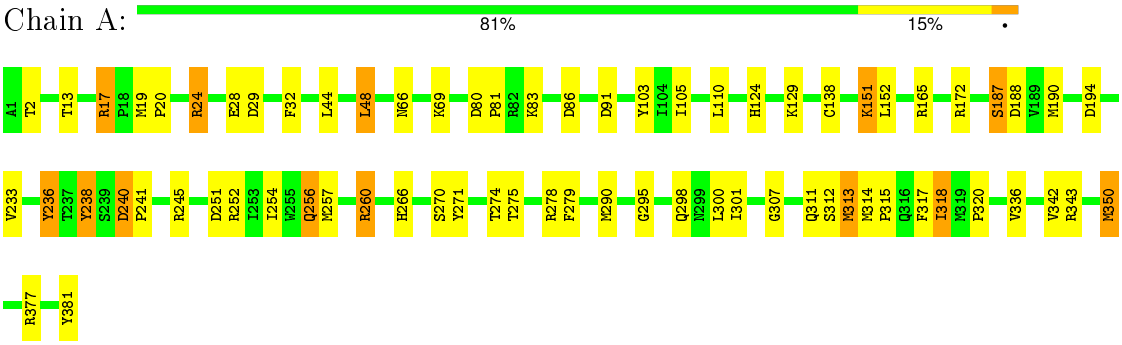
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	142	Total	O	0	0
			142	142		
3	B	140	Total	O	0	0
			140	140		
3	C	139	Total	O	0	0
			139	139		
3	D	139	Total	O	0	0
			139	139		
3	E	139	Total	O	0	0
			139	139		
3	F	141	Total	O	0	0
			141	141		

3 Residue-property plots (i)

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.

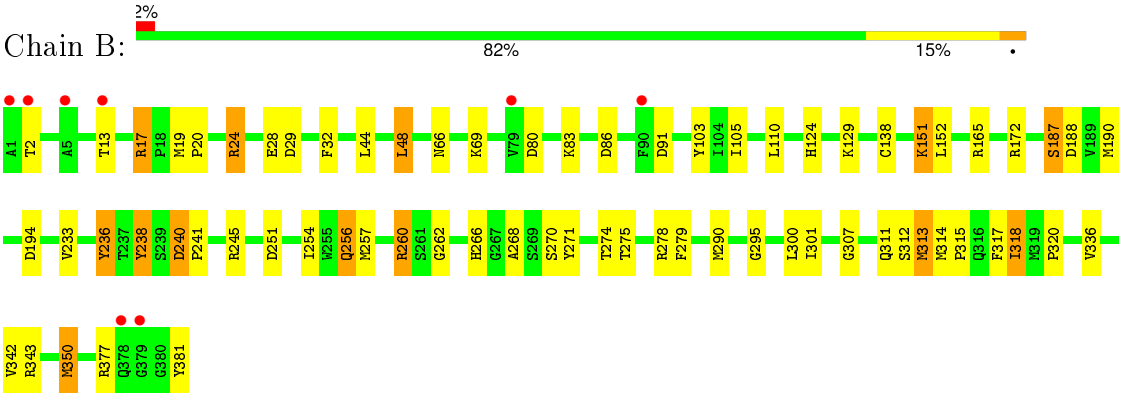
- Molecule 1: GLUCOSE-FRUCTOSE OXIDOREDUCTASE

Chain A:



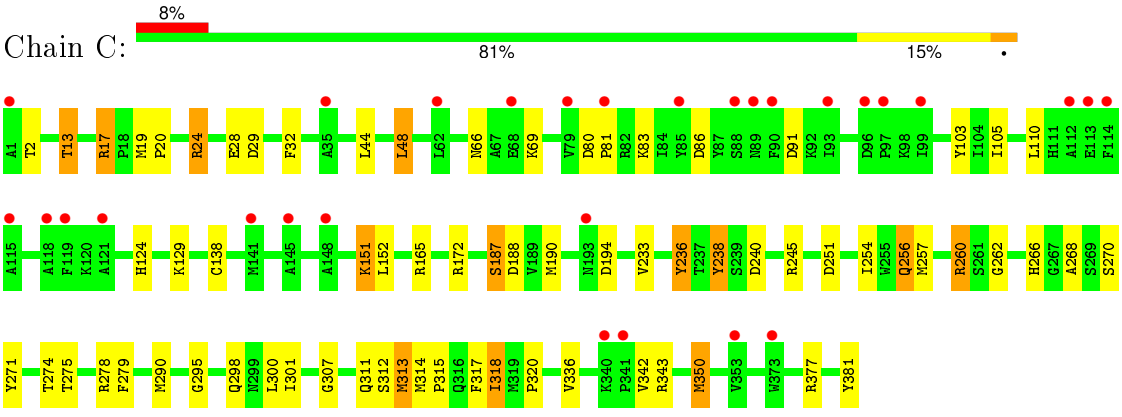
- Molecule 1: GLUCOSE-FRUCTOSE OXIDOREDUCTASE

Chain B:



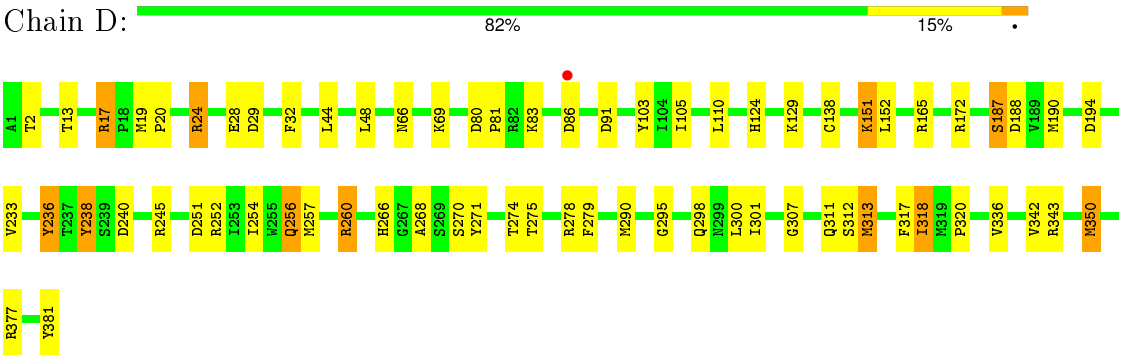
- Molecule 1: GLUCOSE-FRUCTOSE OXIDOREDUCTASE

Chain C:



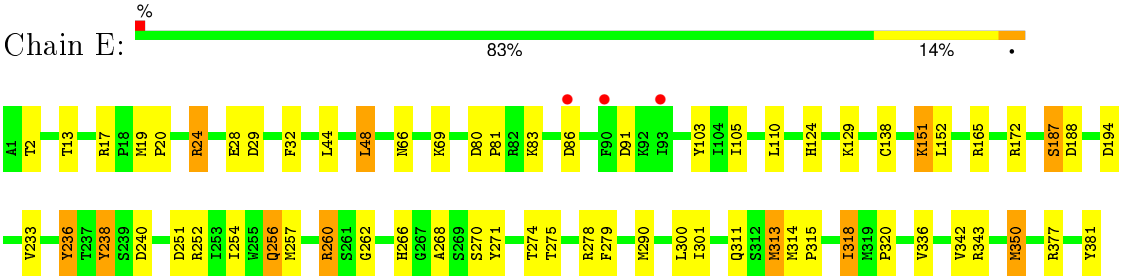
• Molecule 1: GLUCOSE-FRUCTOSE OXIDOREDUCTASE

Chain D:



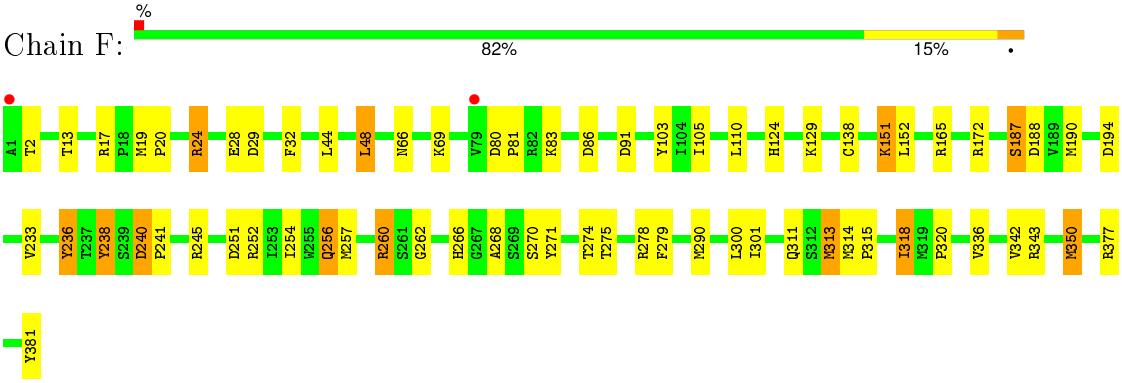
• Molecule 1: GLUCOSE-FRUCTOSE OXIDOREDUCTASE

Chain E:



• Molecule 1: GLUCOSE-FRUCTOSE OXIDOREDUCTASE

Chain F:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, α, β, γ	84.49Å 283.69Å 116.99Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	50.00 – 2.70 49.27 – 2.70	Depositor EDS
% Data completeness (in resolution range)	91.0 (50.00-2.70) 91.5 (49.27-2.70)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	4.40 (at 2.69Å)	Xtriage
Refinement program	TNT	Depositor
R, R_{free}	0.203 , (Not available) 0.184 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	DCC
Wilson B-factor (Å^2)	31.7	Xtriage
Anisotropy	0.253	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.32 , 75.7	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.34$	Xtriage
Outliers	4 of 71500 reflections (0.006%)	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	18498	wwPDB-VP
Average B, all atoms (Å^2)	43.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 36.59 % of the origin peak, indicating pseudo translational symmetry.The chance of finding a peak of this or larger height randomly in a structure without pseudo translational symmetry is equal to 4.8857e-04.The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ 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: NDP

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	0.77	5/2959 (0.2%)	0.98	7/4019 (0.2%)
1	B	0.77	5/2959 (0.2%)	0.98	8/4019 (0.2%)
1	C	0.77	5/2959 (0.2%)	0.98	7/4019 (0.2%)
1	D	0.77	5/2959 (0.2%)	0.98	7/4019 (0.2%)
1	E	0.77	5/2959 (0.2%)	0.98	7/4019 (0.2%)
1	F	0.77	5/2959 (0.2%)	0.98	7/4019 (0.2%)
All	All	0.77	30/17754 (0.2%)	0.98	43/24114 (0.2%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1
1	B	0	1
1	C	0	1
1	D	0	1
1	E	0	1
1	F	0	1
All	All	0	6

All (30) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	F	381	TYR	C-O	7.65	1.37	1.23
1	E	381	TYR	C-O	7.64	1.37	1.23
1	D	381	TYR	C-O	7.63	1.37	1.23
1	A	381	TYR	C-O	7.61	1.37	1.23
1	B	381	TYR	C-O	7.58	1.37	1.23
1	C	381	TYR	C-O	7.56	1.37	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	F	236	TYR	CG-CD2	7.14	1.48	1.39
1	D	236	TYR	CG-CD2	7.13	1.48	1.39
1	A	236	TYR	CG-CD2	7.11	1.48	1.39
1	B	236	TYR	CG-CD2	7.11	1.48	1.39
1	C	236	TYR	CG-CD2	7.09	1.48	1.39
1	E	236	TYR	CG-CD2	7.05	1.48	1.39
1	F	238	TYR	CB-CG	6.37	1.61	1.51
1	D	238	TYR	CB-CG	6.35	1.61	1.51
1	C	238	TYR	CB-CG	6.34	1.61	1.51
1	E	238	TYR	CB-CG	6.33	1.61	1.51
1	B	238	TYR	CB-CG	6.32	1.61	1.51
1	A	238	TYR	CB-CG	6.31	1.61	1.51
1	B	381	TYR	C-OXT	-5.46	1.12	1.23
1	C	381	TYR	C-OXT	-5.45	1.12	1.23
1	A	381	TYR	C-OXT	-5.45	1.12	1.23
1	E	381	TYR	C-OXT	-5.44	1.13	1.23
1	D	381	TYR	C-OXT	-5.43	1.13	1.23
1	E	24	ARG	CB-CG	-5.42	1.38	1.52
1	F	24	ARG	CB-CG	-5.42	1.38	1.52
1	D	24	ARG	CB-CG	-5.41	1.38	1.52
1	F	381	TYR	C-OXT	-5.41	1.13	1.23
1	A	24	ARG	CB-CG	-5.40	1.38	1.52
1	B	24	ARG	CB-CG	-5.40	1.38	1.52
1	C	24	ARG	CB-CG	-5.38	1.38	1.52

All (43) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	236	TYR	CD1-CE1-CZ	7.00	126.10	119.80
1	A	236	TYR	CD1-CE1-CZ	6.98	126.08	119.80
1	E	236	TYR	CD1-CE1-CZ	6.96	126.06	119.80
1	F	236	TYR	CD1-CE1-CZ	6.96	126.06	119.80
1	D	236	TYR	CD1-CE1-CZ	6.95	126.06	119.80
1	C	236	TYR	CD1-CE1-CZ	6.95	126.05	119.80
1	B	260	ARG	NE-CZ-NH1	6.24	123.42	120.30
1	D	260	ARG	NE-CZ-NH1	6.24	123.42	120.30
1	A	260	ARG	NE-CZ-NH1	6.23	123.42	120.30
1	C	260	ARG	NE-CZ-NH1	6.23	123.41	120.30
1	F	260	ARG	NE-CZ-NH1	6.18	123.39	120.30
1	E	260	ARG	NE-CZ-NH1	6.17	123.39	120.30
1	E	251	ASP	CB-CG-OD1	6.09	123.78	118.30
1	C	251	ASP	CB-CG-OD1	6.06	123.75	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	F	251	ASP	CB-CG-OD1	6.05	123.75	118.30
1	D	251	ASP	CB-CG-OD1	6.04	123.74	118.30
1	B	251	ASP	CB-CG-OD1	6.03	123.73	118.30
1	A	251	ASP	CB-CG-OD1	6.00	123.70	118.30
1	D	238	TYR	CD1-CE1-CZ	-5.70	114.67	119.80
1	C	238	TYR	CD1-CE1-CZ	-5.68	114.68	119.80
1	E	238	TYR	CD1-CE1-CZ	-5.68	114.69	119.80
1	F	238	TYR	CD1-CE1-CZ	-5.68	114.69	119.80
1	A	238	TYR	CD1-CE1-CZ	-5.67	114.70	119.80
1	B	238	TYR	CD1-CE1-CZ	-5.66	114.71	119.80
1	B	194	ASP	CB-CG-OD1	5.51	123.26	118.30
1	C	194	ASP	CB-CG-OD1	5.51	123.26	118.30
1	E	194	ASP	CB-CG-OD1	5.49	123.25	118.30
1	A	194	ASP	CB-CG-OD1	5.46	123.22	118.30
1	D	194	ASP	CB-CG-OD1	5.46	123.21	118.30
1	F	194	ASP	CB-CG-OD1	5.45	123.20	118.30
1	A	24	ARG	N-CA-CB	-5.08	101.45	110.60
1	B	260	ARG	NE-CZ-NH2	-5.08	117.76	120.30
1	D	24	ARG	N-CA-CB	-5.08	101.46	110.60
1	C	24	ARG	N-CA-CB	-5.07	101.47	110.60
1	F	238	TYR	CZ-CE2-CD2	-5.07	115.24	119.80
1	D	238	TYR	CZ-CE2-CD2	-5.06	115.24	119.80
1	B	238	TYR	CZ-CE2-CD2	-5.06	115.25	119.80
1	B	24	ARG	N-CA-CB	-5.04	101.52	110.60
1	F	24	ARG	N-CA-CB	-5.04	101.52	110.60
1	A	238	TYR	CZ-CE2-CD2	-5.04	115.27	119.80
1	C	238	TYR	CZ-CE2-CD2	-5.04	115.27	119.80
1	E	24	ARG	N-CA-CB	-5.03	101.55	110.60
1	E	238	TYR	CZ-CE2-CD2	-5.00	115.30	119.80

There are no chirality outliers.

All (6) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	238	TYR	Sidechain
1	B	238	TYR	Sidechain
1	C	238	TYR	Sidechain
1	D	238	TYR	Sidechain
1	E	238	TYR	Sidechain
1	F	238	TYR	Sidechain

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	2895	0	2783	31	0
1	B	2895	0	2783	31	0
1	C	2895	0	2783	34	0
1	D	2895	0	2783	30	0
1	E	2895	0	2783	23	0
1	F	2895	0	2783	25	0
2	A	48	0	26	2	0
2	B	48	0	26	2	0
2	C	48	0	26	1	0
2	D	48	0	26	2	0
2	E	48	0	26	0	0
2	F	48	0	26	0	0
3	A	142	0	0	3	0
3	B	140	0	0	2	0
3	C	139	0	0	3	0
3	D	139	0	0	3	0
3	E	139	0	0	1	0
3	F	141	0	0	1	0
All	All	18498	0	16854	147	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 4.

All (147) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:19:MET:HE3	1:A:20:PRO:HD2	1.68	0.74
1:E:19:MET:HE3	1:E:20:PRO:HD2	1.67	0.74
1:D:19:MET:HE3	1:D:20:PRO:HD2	1.73	0.71
1:F:187:SER:HB3	1:F:270:SER:HB3	1.75	0.69
1:B:187:SER:HB3	1:B:270:SER:HB3	1.75	0.69
1:C:187:SER:HB3	1:C:270:SER:HB3	1.75	0.69
1:A:187:SER:HB3	1:A:270:SER:HB3	1.75	0.69
1:D:187:SER:HB3	1:D:270:SER:HB3	1.75	0.69
1:E:187:SER:HB3	1:E:270:SER:HB3	1.75	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:19:MET:HE3	1:B:20:PRO:HD2	1.73	0.68
1:F:19:MET:HE3	1:F:20:PRO:HD2	1.73	0.68
1:A:124:HIS:HD2	1:A:151:LYS:H	1.43	0.67
1:E:124:HIS:HD2	1:E:151:LYS:H	1.43	0.67
1:D:124:HIS:HD2	1:D:151:LYS:H	1.43	0.67
1:C:124:HIS:HD2	1:C:151:LYS:H	1.43	0.67
1:B:124:HIS:HD2	1:B:151:LYS:H	1.43	0.67
1:F:124:HIS:HD2	1:F:151:LYS:H	1.43	0.66
1:A:256:GLN:HE22	1:B:236:TYR:HB3	1.61	0.65
1:A:236:TYR:HB3	1:B:256:GLN:HE22	1.63	0.64
1:C:19:MET:HE3	1:C:20:PRO:HD2	1.80	0.63
1:E:236:TYR:HB3	1:F:256:GLN:HE22	1.65	0.62
1:E:256:GLN:HE22	1:F:236:TYR:HB3	1.65	0.61
3:B:554:HOH:O	1:C:17:ARG:HD3	2.01	0.60
1:B:307:GLY:O	1:D:312:SER:HA	2.02	0.59
1:C:256:GLN:HE22	1:D:236:TYR:HB3	1.68	0.59
1:A:254:ILE:HD13	1:B:266:HIS:HB3	1.85	0.59
1:A:266:HIS:HB3	1:B:254:ILE:HD13	1.84	0.59
1:E:254:ILE:HD13	1:F:266:HIS:HB3	1.87	0.57
1:C:236:TYR:HB3	1:D:256:GLN:HE22	1.70	0.57
1:E:266:HIS:HB3	1:F:254:ILE:HD13	1.87	0.56
1:A:17:ARG:HD2	2:D:500:NDP:C2A	2.36	0.55
3:A:546:HOH:O	1:D:17:ARG:HD3	2.06	0.55
1:C:266:HIS:HB3	1:D:254:ILE:HD13	1.89	0.54
1:B:17:ARG:HD3	3:C:564:HOH:O	2.08	0.53
1:A:312:SER:HA	1:C:307:GLY:O	2.08	0.53
2:A:500:NDP:C2A	1:D:17:ARG:HD2	2.39	0.53
1:D:66:ASN:HB3	1:D:69:LYS:HE2	1.91	0.53
1:F:66:ASN:HB3	1:F:69:LYS:HE2	1.91	0.53
1:A:66:ASN:HB3	1:A:69:LYS:HE2	1.91	0.52
1:B:66:ASN:HB3	1:B:69:LYS:HE2	1.91	0.52
1:B:312:SER:HA	1:D:307:GLY:O	2.09	0.52
1:C:254:ILE:HD13	1:D:266:HIS:HB3	1.91	0.52
1:C:66:ASN:HB3	1:C:69:LYS:HE2	1.91	0.52
1:E:66:ASN:HB3	1:E:69:LYS:HE2	1.91	0.52
1:A:17:ARG:HD3	3:D:571:HOH:O	2.08	0.52
1:A:307:GLY:O	1:C:312:SER:HA	2.10	0.52
1:C:298:GLN:HB3	3:C:509:HOH:O	2.12	0.49
1:B:295:GLY:HA2	1:C:317:PHE:CE1	2.47	0.48
1:E:80:ASP:HA	1:E:81:PRO:HD2	1.63	0.48
1:E:300:LEU:HD12	1:E:313:MET:HB3	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:278:ARG:HD2	3:C:636:HOH:O	2.14	0.47
1:A:80:ASP:HA	1:A:81:PRO:HD2	1.63	0.47
1:B:17:ARG:HD2	2:C:500:NDP:C2A	2.44	0.47
1:A:300:LEU:HD12	1:A:313:MET:HB3	1.96	0.47
1:A:252:ARG:NH2	1:B:262:GLY:O	2.40	0.47
1:C:300:LEU:HD12	1:C:313:MET:HB3	1.97	0.46
1:F:300:LEU:HD12	1:F:313:MET:HB3	1.96	0.46
2:B:500:NDP:C2A	1:C:17:ARG:HD2	2.46	0.46
1:E:278:ARG:HD2	3:E:782:HOH:O	2.15	0.46
1:C:80:ASP:HA	1:C:81:PRO:HD2	1.63	0.46
1:C:314:MET:HA	1:C:315:PRO:HD3	1.75	0.46
1:A:278:ARG:HD2	3:A:618:HOH:O	2.14	0.46
1:B:317:PHE:CE1	1:C:295:GLY:HA2	2.51	0.46
1:B:300:LEU:HD12	1:B:313:MET:HB3	1.97	0.46
1:D:300:LEU:HD12	1:D:313:MET:HB3	1.96	0.46
1:D:298:GLN:HB3	3:D:508:HOH:O	2.15	0.46
1:C:266:HIS:ND1	1:D:266:HIS:ND1	2.58	0.45
1:E:48:LEU:HD12	1:E:48:LEU:HA	1.81	0.45
1:E:233:VAL:HG22	1:E:257:MET:HG2	1.99	0.45
1:D:80:ASP:HA	1:D:81:PRO:HD2	1.63	0.45
1:C:233:VAL:HG22	1:C:257:MET:HG2	1.98	0.45
1:A:233:VAL:HG22	1:A:257:MET:HG2	1.99	0.44
1:F:240:ASP:HA	1:F:241:PRO:HD2	1.73	0.44
1:A:32:PHE:HE1	1:A:336:VAL:HG11	1.83	0.44
1:B:240:ASP:HA	1:B:241:PRO:HD2	1.73	0.44
1:C:32:PHE:HE1	1:C:336:VAL:HG11	1.83	0.44
1:F:233:VAL:HG22	1:F:257:MET:HG2	1.98	0.44
1:E:32:PHE:HE1	1:E:336:VAL:HG11	1.83	0.44
1:B:233:VAL:HG22	1:B:257:MET:HG2	1.98	0.44
1:D:32:PHE:HE1	1:D:336:VAL:HG11	1.83	0.44
1:D:233:VAL:HG22	1:D:257:MET:HG2	1.99	0.44
1:A:295:GLY:HA2	1:D:317:PHE:CE1	2.53	0.44
1:E:279:PHE:HB2	1:E:290:MET:HB2	2.00	0.44
1:C:138:CYS:HB3	1:C:350:MET:HG3	2.00	0.43
1:F:290:MET:HG2	1:F:301:ILE:HG22	2.00	0.43
1:B:290:MET:HG2	1:B:301:ILE:HG22	2.00	0.43
1:F:278:ARG:HD2	3:F:642:HOH:O	2.16	0.43
1:E:252:ARG:NH2	1:F:262:GLY:O	2.44	0.43
1:A:138:CYS:HB3	1:A:350:MET:HG3	2.00	0.43
1:C:279:PHE:HB2	1:C:290:MET:HB2	2.00	0.43
1:A:279:PHE:HB2	1:A:290:MET:HB2	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:138:CYS:HB3	1:E:350:MET:HG3	2.00	0.43
1:C:290:MET:HG2	1:C:301:ILE:HG22	2.00	0.43
1:D:278:ARG:HD2	3:D:522:HOH:O	2.18	0.43
1:D:138:CYS:HB3	1:D:350:MET:HG3	2.00	0.43
1:F:318:ILE:HG13	1:F:320:PRO:HG3	2.01	0.43
1:B:138:CYS:HB3	1:B:350:MET:HG3	2.00	0.43
1:B:32:PHE:HE1	1:B:336:VAL:HG11	1.83	0.43
1:B:279:PHE:HB2	1:B:290:MET:HB2	2.00	0.43
1:A:48:LEU:HA	1:A:48:LEU:HD12	1.81	0.43
1:A:317:PHE:CE1	1:D:295:GLY:HA2	2.54	0.43
1:B:318:ILE:HG13	1:B:320:PRO:HG3	2.01	0.43
1:C:318:ILE:HG13	1:C:320:PRO:HG3	2.01	0.43
1:D:318:ILE:HG13	1:D:320:PRO:HG3	2.01	0.43
1:A:314:MET:HA	1:A:315:PRO:HD3	1.75	0.43
1:A:318:ILE:HG13	1:A:320:PRO:HG3	2.01	0.43
1:F:279:PHE:HB2	1:F:290:MET:HB2	2.00	0.42
1:F:32:PHE:HE1	1:F:336:VAL:HG11	1.83	0.42
1:D:279:PHE:HB2	1:D:290:MET:HB2	2.00	0.42
1:E:318:ILE:HG13	1:E:320:PRO:HG3	2.01	0.42
1:F:138:CYS:HB3	1:F:350:MET:HG3	2.00	0.42
1:B:317:PHE:CZ	1:C:295:GLY:HA2	2.54	0.42
1:E:290:MET:HG2	1:E:301:ILE:HG22	2.00	0.42
1:D:290:MET:HG2	1:D:301:ILE:HG22	2.00	0.42
1:E:314:MET:HA	1:E:315:PRO:HD3	1.75	0.42
1:A:290:MET:HG2	1:A:301:ILE:HG22	2.00	0.42
1:B:295:GLY:HA2	1:C:317:PHE:CZ	2.55	0.42
1:F:314:MET:HA	1:F:315:PRO:HD3	1.75	0.41
1:F:48:LEU:HD12	1:F:48:LEU:HA	1.81	0.41
1:B:48:LEU:HD12	1:B:48:LEU:HA	1.81	0.41
1:C:48:LEU:HA	1:C:48:LEU:HD12	1.81	0.41
1:A:240:ASP:HA	1:A:241:PRO:HD2	1.73	0.41
1:F:80:ASP:HA	1:F:81:PRO:HD2	1.63	0.41
1:A:298:GLN:HB3	3:A:633:HOH:O	2.19	0.41
1:A:17:ARG:HD2	2:D:500:NDP:H2A	2.02	0.41
1:C:262:GLY:O	1:D:252:ARG:NH2	2.49	0.41
2:A:500:NDP:H2A	1:D:17:ARG:HD2	2.03	0.41
1:C:80:ASP:HB3	1:C:83:LYS:HG3	2.03	0.41
1:E:262:GLY:O	1:F:252:ARG:NH2	2.49	0.40
1:D:190:MET:HB3	1:D:245:ARG:HH21	1.86	0.40
1:C:190:MET:HB3	1:C:245:ARG:HH21	1.86	0.40
1:B:254:ILE:HG12	1:B:268:ALA:HB2	2.02	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:254:ILE:HG12	1:E:268:ALA:HB2	2.02	0.40
1:D:254:ILE:HG12	1:D:268:ALA:HB2	2.03	0.40
1:D:80:ASP:HB3	1:D:83:LYS:HG3	2.03	0.40
1:B:190:MET:HB3	1:B:245:ARG:HH21	1.86	0.40
1:B:80:ASP:HB3	1:B:83:LYS:HG3	2.03	0.40
1:B:314:MET:HA	1:B:315:PRO:HD3	1.75	0.40
1:B:278:ARG:HD2	3:B:504:HOH:O	2.19	0.40
1:F:254:ILE:HG12	1:F:268:ALA:HB2	2.03	0.40
1:F:190:MET:HB3	1:F:245:ARG:HH21	1.86	0.40
1:F:80:ASP:HB3	1:F:83:LYS:HG3	2.03	0.40
2:B:500:NDP:N6A	1:C:13:THR:O	2.51	0.40
1:C:254:ILE:HG12	1:C:268:ALA:HB2	2.03	0.40
1:E:80:ASP:HB3	1:E:83:LYS:HG3	2.03	0.40
1:A:80:ASP:HB3	1:A:83:LYS:HG3	2.03	0.40
1:A:190:MET:HB3	1:A:245:ARG:HH21	1.86	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	379/381 (100%)	365 (96%)	13 (3%)	1 (0%)	46	75
1	B	379/381 (100%)	365 (96%)	13 (3%)	1 (0%)	46	75
1	C	379/381 (100%)	365 (96%)	13 (3%)	1 (0%)	46	75
1	D	379/381 (100%)	365 (96%)	13 (3%)	1 (0%)	46	75
1	E	379/381 (100%)	365 (96%)	13 (3%)	1 (0%)	46	75
1	F	379/381 (100%)	365 (96%)	13 (3%)	1 (0%)	46	75
All	All	2274/2286 (100%)	2190 (96%)	78 (3%)	6 (0%)	46	75

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	275	THR
1	B	275	THR
1	C	275	THR
1	D	275	THR
1	E	275	THR
1	F	275	THR

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	290/308 (94%)	258 (89%)	32 (11%)	8	18
1	B	290/308 (94%)	258 (89%)	32 (11%)	8	18
1	C	290/308 (94%)	258 (89%)	32 (11%)	8	18
1	D	290/308 (94%)	258 (89%)	32 (11%)	8	18
1	E	290/308 (94%)	258 (89%)	32 (11%)	8	18
1	F	290/308 (94%)	258 (89%)	32 (11%)	8	18
All	All	1740/1848 (94%)	1548 (89%)	192 (11%)	8	18

All (192) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	2	THR
1	A	13	THR
1	A	17	ARG
1	A	24	ARG
1	A	28	GLU
1	A	29	ASP
1	A	44	LEU
1	A	48	LEU
1	A	86	ASP
1	A	91	ASP
1	A	103	TYR
1	A	105	ILE
1	A	110	LEU

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Mol	Chain	Res	Type
1	A	129	LYS
1	A	151	LYS
1	A	152	LEU
1	A	165	ARG
1	A	172	ARG
1	A	187	SER
1	A	188	ASP
1	A	240	ASP
1	A	256	GLN
1	A	260	ARG
1	A	271	TYR
1	A	274	THR
1	A	311	GLN
1	A	313	MET
1	A	318	ILE
1	A	342	VAL
1	A	343	ARG
1	A	350	MET
1	A	377	ARG
1	B	2	THR
1	B	13	THR
1	B	17	ARG
1	B	24	ARG
1	B	28	GLU
1	B	29	ASP
1	B	44	LEU
1	B	48	LEU
1	B	86	ASP
1	B	91	ASP
1	B	103	TYR
1	B	105	ILE
1	B	110	LEU
1	B	129	LYS
1	B	151	LYS
1	B	152	LEU
1	B	165	ARG
1	B	172	ARG
1	B	187	SER
1	B	188	ASP
1	B	240	ASP
1	B	256	GLN
1	B	260	ARG

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Mol	Chain	Res	Type
1	B	271	TYR
1	B	274	THR
1	B	311	GLN
1	B	313	MET
1	B	318	ILE
1	B	342	VAL
1	B	343	ARG
1	B	350	MET
1	B	377	ARG
1	C	2	THR
1	C	13	THR
1	C	17	ARG
1	C	24	ARG
1	C	28	GLU
1	C	29	ASP
1	C	44	LEU
1	C	48	LEU
1	C	86	ASP
1	C	91	ASP
1	C	103	TYR
1	C	105	ILE
1	C	110	LEU
1	C	129	LYS
1	C	151	LYS
1	C	152	LEU
1	C	165	ARG
1	C	172	ARG
1	C	187	SER
1	C	188	ASP
1	C	240	ASP
1	C	256	GLN
1	C	260	ARG
1	C	271	TYR
1	C	274	THR
1	C	311	GLN
1	C	313	MET
1	C	318	ILE
1	C	342	VAL
1	C	343	ARG
1	C	350	MET
1	C	377	ARG
1	D	2	THR

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Mol	Chain	Res	Type
1	D	13	THR
1	D	17	ARG
1	D	24	ARG
1	D	28	GLU
1	D	29	ASP
1	D	44	LEU
1	D	48	LEU
1	D	86	ASP
1	D	91	ASP
1	D	103	TYR
1	D	105	ILE
1	D	110	LEU
1	D	129	LYS
1	D	151	LYS
1	D	152	LEU
1	D	165	ARG
1	D	172	ARG
1	D	187	SER
1	D	188	ASP
1	D	240	ASP
1	D	256	GLN
1	D	260	ARG
1	D	271	TYR
1	D	274	THR
1	D	311	GLN
1	D	313	MET
1	D	318	ILE
1	D	342	VAL
1	D	343	ARG
1	D	350	MET
1	D	377	ARG
1	E	2	THR
1	E	13	THR
1	E	17	ARG
1	E	24	ARG
1	E	28	GLU
1	E	29	ASP
1	E	44	LEU
1	E	48	LEU
1	E	86	ASP
1	E	91	ASP
1	E	103	TYR

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Mol	Chain	Res	Type
1	E	105	ILE
1	E	110	LEU
1	E	129	LYS
1	E	151	LYS
1	E	152	LEU
1	E	165	ARG
1	E	172	ARG
1	E	187	SER
1	E	188	ASP
1	E	240	ASP
1	E	256	GLN
1	E	260	ARG
1	E	271	TYR
1	E	274	THR
1	E	311	GLN
1	E	313	MET
1	E	318	ILE
1	E	342	VAL
1	E	343	ARG
1	E	350	MET
1	E	377	ARG
1	F	2	THR
1	F	13	THR
1	F	17	ARG
1	F	24	ARG
1	F	28	GLU
1	F	29	ASP
1	F	44	LEU
1	F	48	LEU
1	F	86	ASP
1	F	91	ASP
1	F	103	TYR
1	F	105	ILE
1	F	110	LEU
1	F	129	LYS
1	F	151	LYS
1	F	152	LEU
1	F	165	ARG
1	F	172	ARG
1	F	187	SER
1	F	188	ASP
1	F	240	ASP

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Mol	Chain	Res	Type
1	F	256	GLN
1	F	260	ARG
1	F	271	TYR
1	F	274	THR
1	F	311	GLN
1	F	313	MET
1	F	318	ILE
1	F	342	VAL
1	F	343	ARG
1	F	350	MET
1	F	377	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (16) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	124	HIS
1	A	256	GLN
1	A	338	ASN
1	B	124	HIS
1	B	338	ASN
1	C	124	HIS
1	C	256	GLN
1	C	338	ASN
1	D	46	GLN
1	D	124	HIS
1	D	338	ASN
1	E	124	HIS
1	E	256	GLN
1	E	338	ASN
1	F	124	HIS
1	F	338	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 carbohydrates in this entry.

5.6 Ligand geometry (i)

6 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	NDP	A	500	-	42,52,52	1.22	4 (9%)	55,80,80	1.68	8 (14%)
2	NDP	B	500	-	42,52,52	1.23	4 (9%)	55,80,80	1.68	8 (14%)
2	NDP	C	500	-	42,52,52	1.23	4 (9%)	55,80,80	1.68	8 (14%)
2	NDP	D	500	-	42,52,52	1.22	4 (9%)	55,80,80	1.68	8 (14%)
2	NDP	E	500	-	42,52,52	1.22	4 (9%)	55,80,80	1.68	8 (14%)
2	NDP	F	500	-	42,52,52	1.23	4 (9%)	55,80,80	1.68	8 (14%)

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	NDP	A	500	-	-	0/30/77/77	0/5/5/5
2	NDP	B	500	-	-	0/30/77/77	0/5/5/5
2	NDP	C	500	-	-	0/30/77/77	0/5/5/5
2	NDP	D	500	-	-	0/30/77/77	0/5/5/5
2	NDP	E	500	-	-	0/30/77/77	0/5/5/5
2	NDP	F	500	-	-	0/30/77/77	0/5/5/5

All (24) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	500	NDP	C4N-C5N	-3.68	1.41	1.49
2	F	500	NDP	C4N-C5N	-3.67	1.41	1.49

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	E	500	NDP	C4N-C5N	-3.67	1.41	1.49
2	A	500	NDP	C4N-C5N	-3.66	1.41	1.49
2	C	500	NDP	C4N-C5N	-3.65	1.41	1.49
2	D	500	NDP	C4N-C5N	-3.65	1.41	1.49
2	C	500	NDP	P2B-O2B	-2.97	1.51	1.60
2	E	500	NDP	P2B-O2B	-2.96	1.51	1.60
2	B	500	NDP	P2B-O2B	-2.96	1.51	1.60
2	D	500	NDP	P2B-O2B	-2.95	1.51	1.60
2	F	500	NDP	P2B-O2B	-2.95	1.51	1.60
2	A	500	NDP	P2B-O2B	-2.94	1.51	1.60
2	C	500	NDP	PN-O5D	-2.31	1.48	1.59
2	D	500	NDP	PN-O5D	-2.31	1.48	1.59
2	F	500	NDP	PN-O5D	-2.30	1.48	1.59
2	B	500	NDP	PN-O5D	-2.29	1.48	1.59
2	A	500	NDP	PN-O5D	-2.29	1.48	1.59
2	E	500	NDP	PN-O5D	-2.28	1.48	1.59
2	C	500	NDP	C6N-C5N	3.13	1.39	1.33
2	E	500	NDP	C6N-C5N	3.13	1.39	1.33
2	A	500	NDP	C6N-C5N	3.14	1.39	1.33
2	B	500	NDP	C6N-C5N	3.15	1.39	1.33
2	D	500	NDP	C6N-C5N	3.16	1.39	1.33
2	F	500	NDP	C6N-C5N	3.19	1.39	1.33

All (48) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	500	NDP	C1D-N1N-C2N	-6.01	110.44	120.91
2	E	500	NDP	C1D-N1N-C2N	-6.01	110.44	120.91
2	C	500	NDP	C1D-N1N-C2N	-5.99	110.47	120.91
2	F	500	NDP	C1D-N1N-C2N	-5.98	110.49	120.91
2	D	500	NDP	C1D-N1N-C2N	-5.97	110.50	120.91
2	A	500	NDP	C1D-N1N-C2N	-5.97	110.51	120.91
2	D	500	NDP	C4N-C5N-C6N	-2.84	117.89	122.58
2	F	500	NDP	C4N-C5N-C6N	-2.84	117.90	122.58
2	B	500	NDP	C4N-C5N-C6N	-2.83	117.91	122.58
2	E	500	NDP	C4N-C5N-C6N	-2.83	117.92	122.58
2	A	500	NDP	C4N-C5N-C6N	-2.82	117.92	122.58
2	C	500	NDP	C4N-C5N-C6N	-2.80	117.96	122.58
2	E	500	NDP	PN-O3-PA	-2.79	124.88	132.73
2	A	500	NDP	PN-O3-PA	-2.79	124.89	132.73
2	B	500	NDP	PN-O3-PA	-2.79	124.90	132.73
2	D	500	NDP	PN-O3-PA	-2.78	124.91	132.73

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	F	500	NDP	PN-O3-PA	-2.78	124.92	132.73
2	C	500	NDP	PN-O3-PA	-2.78	124.94	132.73
2	D	500	NDP	O4D-C1D-N1N	-2.60	102.58	108.07
2	E	500	NDP	O4D-C1D-N1N	-2.60	102.58	108.07
2	F	500	NDP	O4D-C1D-N1N	-2.60	102.58	108.07
2	A	500	NDP	O4D-C1D-N1N	-2.59	102.61	108.07
2	B	500	NDP	O4D-C1D-N1N	-2.59	102.61	108.07
2	C	500	NDP	O4D-C1D-N1N	-2.58	102.63	108.07
2	E	500	NDP	O2A-PA-O3	-2.07	95.72	105.09
2	A	500	NDP	O2A-PA-O3	-2.06	95.73	105.09
2	D	500	NDP	O2A-PA-O3	-2.06	95.76	105.09
2	B	500	NDP	O2A-PA-O3	-2.06	95.76	105.09
2	C	500	NDP	O2A-PA-O3	-2.05	95.77	105.09
2	F	500	NDP	O2A-PA-O3	-2.05	95.80	105.09
2	C	500	NDP	C5N-C4N-C3N	2.41	119.17	112.52
2	D	500	NDP	C5N-C4N-C3N	2.42	119.20	112.52
2	F	500	NDP	C5N-C4N-C3N	2.43	119.21	112.52
2	A	500	NDP	C5N-C4N-C3N	2.43	119.22	112.52
2	B	500	NDP	C5N-C4N-C3N	2.44	119.23	112.52
2	E	500	NDP	C5N-C4N-C3N	2.44	119.25	112.52
2	A	500	NDP	C1D-N1N-C6N	3.76	129.23	120.81
2	E	500	NDP	C1D-N1N-C6N	3.77	129.25	120.81
2	C	500	NDP	C1D-N1N-C6N	3.77	129.25	120.81
2	F	500	NDP	C1D-N1N-C6N	3.77	129.25	120.81
2	D	500	NDP	C1D-N1N-C6N	3.77	129.25	120.81
2	B	500	NDP	C1D-N1N-C6N	3.79	129.30	120.81
2	D	500	NDP	C1B-N9A-C4A	6.77	137.15	126.94
2	F	500	NDP	C1B-N9A-C4A	6.79	137.17	126.94
2	B	500	NDP	C1B-N9A-C4A	6.79	137.18	126.94
2	A	500	NDP	C1B-N9A-C4A	6.80	137.20	126.94
2	E	500	NDP	C1B-N9A-C4A	6.81	137.21	126.94
2	C	500	NDP	C1B-N9A-C4A	6.82	137.22	126.94

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

4 monomers are involved in 7 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	500	NDP	2	0
2	B	500	NDP	2	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	C	500	NDP	1	0
2	D	500	NDP	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^{th} 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	381/381 (100%)	-0.15	0 100 100	29, 40, 62, 72	0
1	B	381/381 (100%)	0.01	8 (2%) 67 68	29, 40, 62, 72	0
1	C	381/381 (100%)	0.23	29 (7%) 17 15	29, 40, 62, 72	0
1	D	381/381 (100%)	-0.19	1 (0%) 94 95	29, 40, 62, 72	0
1	E	381/381 (100%)	-0.09	3 (0%) 87 88	29, 40, 62, 72	0
1	F	381/381 (100%)	-0.15	2 (0%) 91 93	29, 40, 62, 72	0
All	All	2286/2286 (100%)	-0.06	43 (1%) 70 70	29, 40, 62, 72	0

All (43) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	1	ALA	6.0
1	C	88	SER	5.4
1	C	93	ILE	3.9
1	B	5	ALA	3.7
1	C	121	ALA	3.7
1	C	115	ALA	3.7
1	C	118	ALA	3.6
1	C	373	TRP	3.4
1	C	90	PHE	3.3
1	C	1	ALA	3.2
1	C	68	GLU	3.2
1	F	1	ALA	3.0
1	C	96	ASP	2.9
1	C	119	PHE	2.9
1	B	79	VAL	2.8
1	B	379	GLY	2.7
1	C	193	ASN	2.6
1	C	79	VAL	2.6
1	C	141	MET	2.5

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Mol	Chain	Res	Type	RSRZ
1	C	89	ASN	2.5
1	E	90	PHE	2.4
1	C	35	ALA	2.3
1	C	145	ALA	2.3
1	B	13	THR	2.3
1	B	378	GLN	2.3
1	C	97	PRO	2.2
1	E	93	ILE	2.2
1	C	113	GLU	2.2
1	D	86	ASP	2.2
1	B	2	THR	2.2
1	C	81	PRO	2.2
1	C	114	PHE	2.2
1	E	86	ASP	2.2
1	C	99	ILE	2.1
1	C	353	VAL	2.1
1	C	340	LYS	2.1
1	C	85	TYR	2.1
1	C	112	ALA	2.1
1	C	62	LEU	2.1
1	B	90	PHE	2.0
1	C	341	PRO	2.0
1	C	148	ALA	2.0
1	F	79	VAL	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^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
2	NDP	C	500	48/48	0.93	0.18	-0.20	38,40,41,41	0
2	NDP	D	500	48/48	0.97	0.15	-0.55	38,40,41,41	0
2	NDP	B	500	48/48	0.96	0.14	-0.61	38,40,41,41	0
2	NDP	E	500	48/48	0.97	0.15	-0.90	38,40,41,41	0
2	NDP	F	500	48/48	0.96	0.13	-0.93	38,40,41,41	0
2	NDP	A	500	48/48	0.96	0.14	-1.21	38,40,41,41	0

6.5 Other polymers (i)

There are no such residues in this entry.