Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 12:34 AM GMT

PDB ID	:	2ARK
Title	:	Structure of a flavodoxin from Aquifex aeolicus
Authors	:	Cuff, M.E.; Quartey, P.; Zhou, M.; Cymborowski, M.; Minor, W.; Joachimiak, A.; Midwest Center for Structural Genomics (MCSG)
Deposited on	:	2005-08-19
Resolution	:	2.40 Å(reported)

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

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

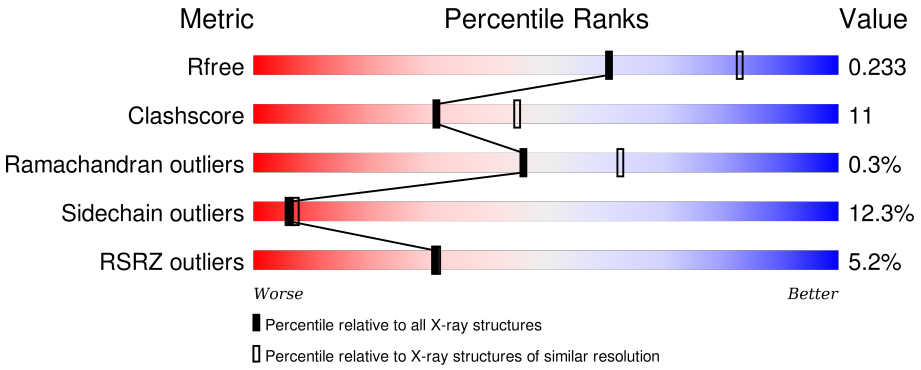
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	trunk26865

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 2.40 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	2919 (2.40-2.40)
Clashscore	102246	3407 (2.40-2.40)
Ramachandran outliers	100387	3351 (2.40-2.40)
Sidechain outliers	100360	3352 (2.40-2.40)
RSRZ outliers	91569	2928 (2.40-2.40)

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	188	4% 74% 20% 5% ••
1	B	188	5% 77% 18% • ••
1	C	188	4% 78% 16% • ••
1	D	188	7% 73% 19% 6% ••
1	E	188	4% 68% 23% 5% • •

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Mol	Chain	Length	Quality of chain
1	F	188	

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	PO4	A	501	-	-	X	-
2	PO4	F	506	-	-	-	X
3	GOL	A	509	-	-	-	X

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 9119 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 Flavodoxin.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	187	Total	C	N	O	S	Se	0	0	0
			1445	917	251	267	3	7			
1	B	186	Total	C	N	O	S	Se	0	0	0
			1439	914	250	265	3	7			
1	C	186	Total	C	N	O	S	Se	0	0	0
			1439	914	249	266	3	7			
1	D	187	Total	C	N	O	S	Se	0	0	0
			1445	917	251	267	3	7			
1	E	185	Total	C	N	O	S	Se	0	0	0
			1434	911	248	265	3	7			
1	F	185	Total	C	N	O	S	Se	0	0	0
			1431	910	248	263	3	7			

There are 60 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-2	SER	-	CLONING ARTIFACT	UNP O67866
A	-1	ASN	-	CLONING ARTIFACT	UNP O67866
A	0	ALA	-	CLONING ARTIFACT	UNP O67866
A	1	MSE	MET	MODIFIED RESIDUE	UNP O67866
A	18	MSE	MET	MODIFIED RESIDUE	UNP O67866
A	61	MSE	MET	MODIFIED RESIDUE	UNP O67866
A	68	MSE	MET	MODIFIED RESIDUE	UNP O67866
A	106	MSE	MET	MODIFIED RESIDUE	UNP O67866
A	111	MSE	MET	MODIFIED RESIDUE	UNP O67866
A	113	MSE	MET	MODIFIED RESIDUE	UNP O67866
B	-2	SER	-	CLONING ARTIFACT	UNP O67866
B	-1	ASN	-	CLONING ARTIFACT	UNP O67866
B	0	ALA	-	CLONING ARTIFACT	UNP O67866
B	1	MSE	MET	MODIFIED RESIDUE	UNP O67866
B	18	MSE	MET	MODIFIED RESIDUE	UNP O67866
B	61	MSE	MET	MODIFIED RESIDUE	UNP O67866
B	68	MSE	MET	MODIFIED RESIDUE	UNP O67866

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Chain	Residue	Modelled	Actual	Comment	Reference
B	106	MSE	MET	MODIFIED RESIDUE	UNP O67866
B	111	MSE	MET	MODIFIED RESIDUE	UNP O67866
B	113	MSE	MET	MODIFIED RESIDUE	UNP O67866
C	-2	SER	-	CLONING ARTIFACT	UNP O67866
C	-1	ASN	-	CLONING ARTIFACT	UNP O67866
C	0	ALA	-	CLONING ARTIFACT	UNP O67866
C	1	MSE	MET	MODIFIED RESIDUE	UNP O67866
C	18	MSE	MET	MODIFIED RESIDUE	UNP O67866
C	61	MSE	MET	MODIFIED RESIDUE	UNP O67866
C	68	MSE	MET	MODIFIED RESIDUE	UNP O67866
C	106	MSE	MET	MODIFIED RESIDUE	UNP O67866
C	111	MSE	MET	MODIFIED RESIDUE	UNP O67866
C	113	MSE	MET	MODIFIED RESIDUE	UNP O67866
D	-2	SER	-	CLONING ARTIFACT	UNP O67866
D	-1	ASN	-	CLONING ARTIFACT	UNP O67866
D	0	ALA	-	CLONING ARTIFACT	UNP O67866
D	1	MSE	MET	MODIFIED RESIDUE	UNP O67866
D	18	MSE	MET	MODIFIED RESIDUE	UNP O67866
D	61	MSE	MET	MODIFIED RESIDUE	UNP O67866
D	68	MSE	MET	MODIFIED RESIDUE	UNP O67866
D	106	MSE	MET	MODIFIED RESIDUE	UNP O67866
D	111	MSE	MET	MODIFIED RESIDUE	UNP O67866
D	113	MSE	MET	MODIFIED RESIDUE	UNP O67866
E	-2	SER	-	CLONING ARTIFACT	UNP O67866
E	-1	ASN	-	CLONING ARTIFACT	UNP O67866
E	0	ALA	-	CLONING ARTIFACT	UNP O67866
E	1	MSE	MET	MODIFIED RESIDUE	UNP O67866
E	18	MSE	MET	MODIFIED RESIDUE	UNP O67866
E	61	MSE	MET	MODIFIED RESIDUE	UNP O67866
E	68	MSE	MET	MODIFIED RESIDUE	UNP O67866
E	106	MSE	MET	MODIFIED RESIDUE	UNP O67866
E	111	MSE	MET	MODIFIED RESIDUE	UNP O67866
E	113	MSE	MET	MODIFIED RESIDUE	UNP O67866
F	-2	SER	-	CLONING ARTIFACT	UNP O67866
F	-1	ASN	-	CLONING ARTIFACT	UNP O67866
F	0	ALA	-	CLONING ARTIFACT	UNP O67866
F	1	MSE	MET	MODIFIED RESIDUE	UNP O67866
F	18	MSE	MET	MODIFIED RESIDUE	UNP O67866
F	61	MSE	MET	MODIFIED RESIDUE	UNP O67866
F	68	MSE	MET	MODIFIED RESIDUE	UNP O67866
F	106	MSE	MET	MODIFIED RESIDUE	UNP O67866
F	111	MSE	MET	MODIFIED RESIDUE	UNP O67866

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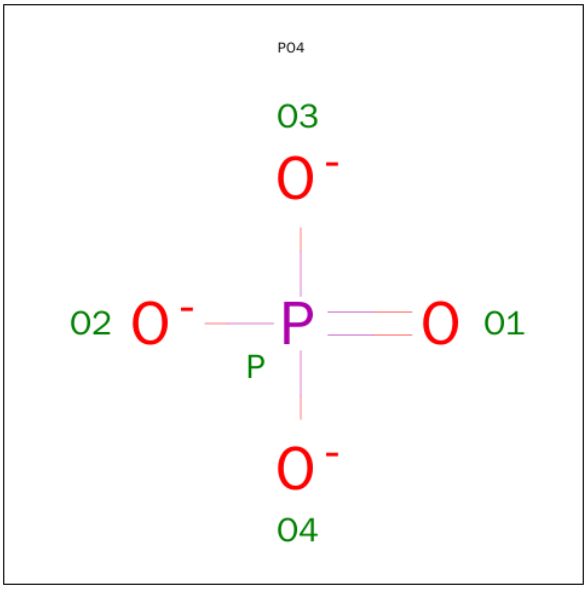
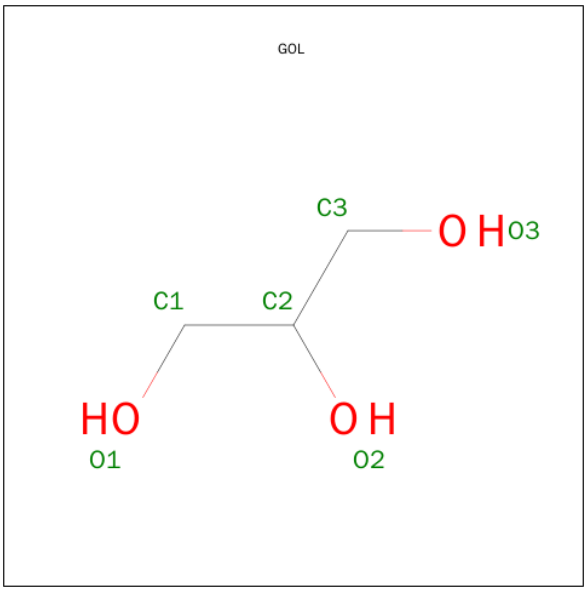
Chain	Residue	Modelled	Actual	Comment	Reference
F	113	MSE	MET	MODIFIED RESIDUE	UNP O67866

- Molecule 2 is PHOSPHATE ION (three-letter code: PO4) (formula: O_4P).



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

- Molecule 3 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).



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

- Molecule 4 is water.

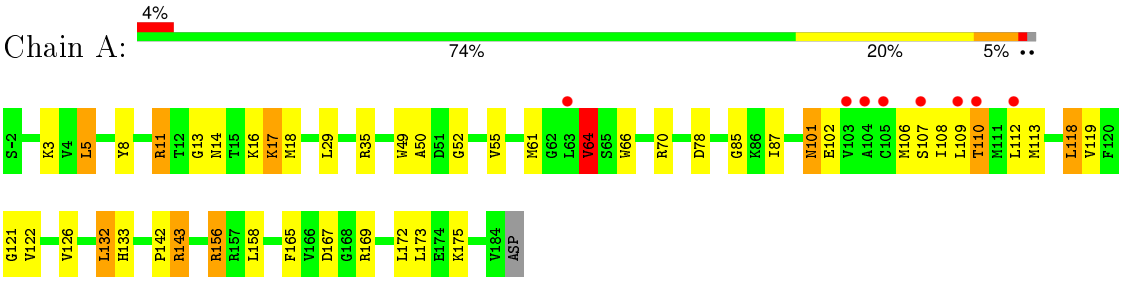
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	69	Total O 69 69	0	0
4	B	95	Total O 95 95	0	0
4	C	55	Total O 55 55	0	0
4	D	75	Total O 75 75	0	0
4	E	42	Total O 42 42	0	0
4	F	84	Total O 84 84	0	0

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.

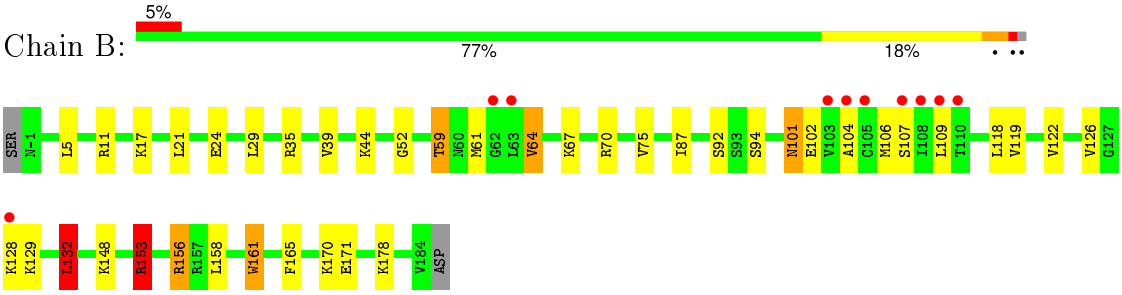
- Molecule 1: Flavodoxin

Chain A:



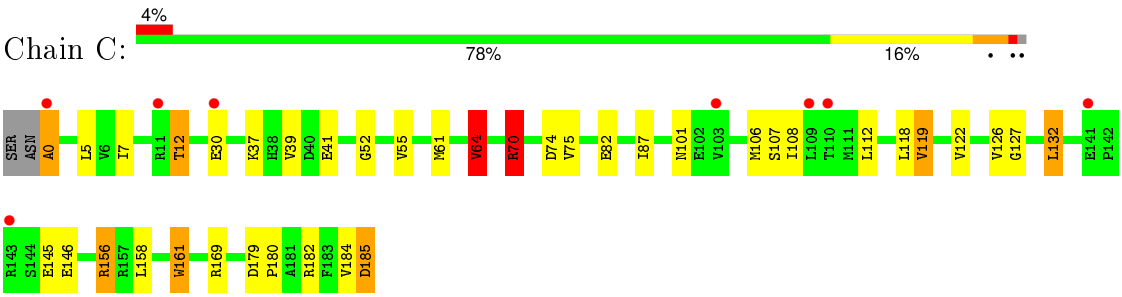
- Molecule 1: Flavodoxin

Chain B:



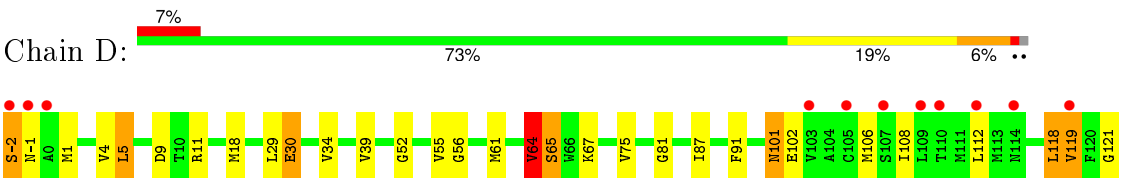
- Molecule 1: Flavodoxin

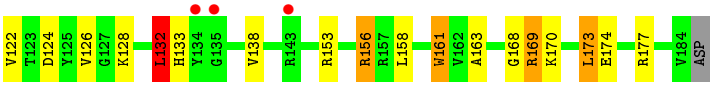
Chain C:



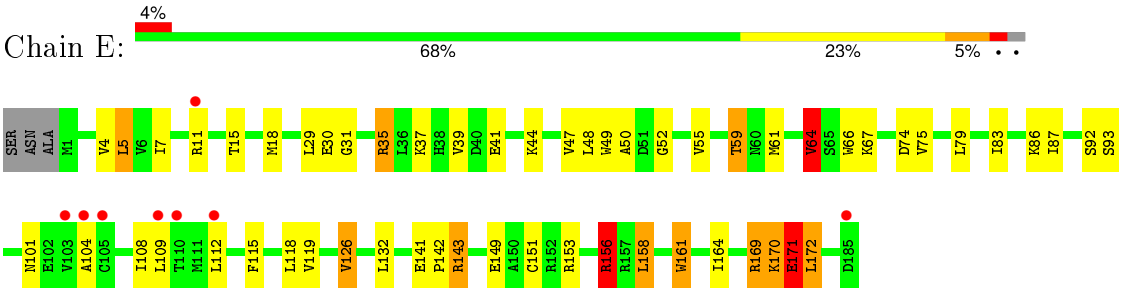
- Molecule 1: Flavodoxin

Chain D:

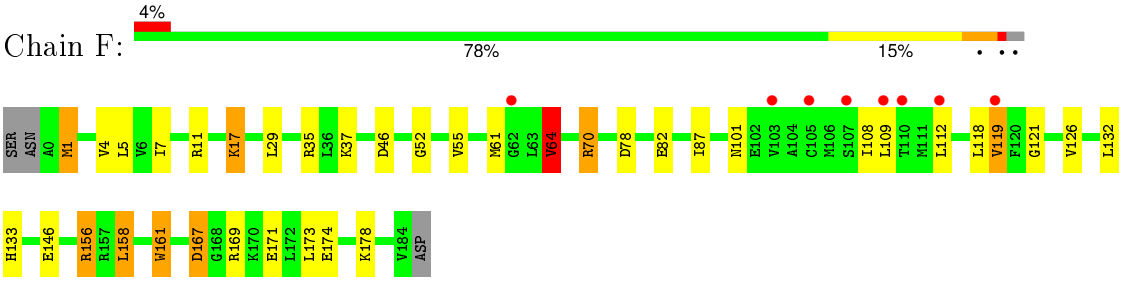




• Molecule 1: Flavodoxin



• Molecule 1: Flavodoxin



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 32 2 1	Depositor
Cell constants a, b, c, α, β, γ	112.85Å 112.85Å 150.65Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	36.00 – 2.40 36.94 – 2.40	Depositor EDS
% Data completeness (in resolution range)	99.6 (36.00-2.40) 99.6 (36.94-2.40)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	3.02 (at 2.39Å)	Xtriage
Refinement program	REFMAC 5.2.0005	Depositor
R, R_{free}	0.171 , 0.235 0.169 , 0.233	Depositor DCC
R_{free} test set	2202 reflections (5.30%)	DCC
Wilson B-factor (Å^2)	38.5	Xtriage
Anisotropy	0.506	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.33 , 49.0	EDS
Estimated twinning fraction	0.037 for -h,-k,l	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.51$, $< L^2 > = 0.34$	Xtriage
Outliers	1 of 43827 reflections (0.002%)	Xtriage
F_o,F_c correlation	0.96	EDS
Total number of atoms	9119	wwPDB-VP
Average B, all atoms (Å^2)	29.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.39% 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, 0.375 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: GOL, PO4

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	0.80	0/1464	0.89	6/1956 (0.3%)
1	B	0.75	0/1458	0.95	6/1948 (0.3%)
1	C	0.93	3/1458 (0.2%)	1.06	8/1948 (0.4%)
1	D	1.11	4/1464 (0.3%)	0.92	8/1956 (0.4%)
1	E	1.46	9/1454 (0.6%)	0.97	7/1944 (0.4%)
1	F	0.70	0/1450	0.83	4/1937 (0.2%)
All	All	0.99	16/8748 (0.2%)	0.94	39/11689 (0.3%)

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	E	0	1

All (16) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	-2	SER	CB-OG	27.80	1.78	1.42
1	E	171	GLU	CD-OE2	25.95	1.54	1.25
1	E	169	ARG	CZ-NH2	24.22	1.64	1.33
1	E	171	GLU	CD-OE1	23.67	1.51	1.25
1	C	169	ARG	CZ-NH2	13.32	1.50	1.33
1	D	-2	SER	CA-CB	11.38	1.70	1.52
1	C	169	ARG	NE-CZ	11.15	1.47	1.33
1	E	169	ARG	CG-CD	10.93	1.79	1.51
1	C	0	ALA	N-CA	10.84	1.68	1.46
1	E	30	GLU	CD-OE2	10.74	1.37	1.25
1	E	30	GLU	C-O	10.51	1.43	1.23
1	D	-2	SER	N-CA	9.73	1.65	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	E	30	GLU	CD-OE1	8.81	1.35	1.25
1	E	30	GLU	C-N	5.98	1.43	1.33
1	D	65	SER	CB-OG	-5.13	1.35	1.42
1	E	31	GLY	C-O	5.01	1.31	1.23

All (39) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	169	ARG	NE-CZ-NH1	-22.91	108.84	120.30
1	E	169	ARG	NE-CZ-NH2	15.00	127.80	120.30
1	C	169	ARG	NE-CZ-NH2	14.29	127.44	120.30
1	E	169	ARG	NE-CZ-NH1	-9.42	115.59	120.30
1	B	156	ARG	NE-CZ-NH1	8.98	124.79	120.30
1	C	70	ARG	NE-CZ-NH1	-8.62	115.99	120.30
1	C	0	ALA	N-CA-CB	8.54	122.05	110.10
1	B	132	LEU	CA-CB-CG	8.52	134.88	115.30
1	C	70	ARG	NE-CZ-NH2	8.26	124.43	120.30
1	A	70	ARG	NE-CZ-NH1	-8.07	116.27	120.30
1	B	156	ARG	NE-CZ-NH2	-7.83	116.38	120.30
1	D	132	LEU	CA-CB-CG	7.34	132.18	115.30
1	E	171	GLU	OE1-CD-OE2	7.25	132.00	123.30
1	B	153	ARG	NE-CZ-NH2	-7.09	116.76	120.30
1	A	64	VAL	CB-CA-C	-7.06	97.99	111.40
1	D	-2	SER	CA-CB-OG	-6.99	92.34	111.20
1	A	70	ARG	NE-CZ-NH2	6.60	123.60	120.30
1	E	156	ARG	NE-CZ-NH1	6.55	123.57	120.30
1	D	156	ARG	NE-CZ-NH1	6.40	123.50	120.30
1	D	64	VAL	CB-CA-C	-6.36	99.32	111.40
1	E	64	VAL	CB-CA-C	-6.34	99.35	111.40
1	C	64	VAL	CB-CA-C	-6.17	99.67	111.40
1	B	64	VAL	CB-CA-C	-6.15	99.72	111.40
1	D	156	ARG	NE-CZ-NH2	-6.09	117.25	120.30
1	F	64	VAL	CB-CA-C	-6.04	99.92	111.40
1	D	118	LEU	CA-CB-CG	5.97	129.02	115.30
1	A	156	ARG	NE-CZ-NH1	5.87	123.23	120.30
1	A	118	LEU	CA-CB-CG	5.83	128.70	115.30
1	E	156	ARG	NE-CZ-NH2	-5.71	117.44	120.30
1	D	5	LEU	CA-CB-CG	5.57	128.10	115.30
1	A	156	ARG	NE-CZ-NH2	-5.56	117.52	120.30
1	D	65	SER	N-CA-CB	-5.53	102.21	110.50
1	B	132	LEU	CB-CG-CD1	5.43	120.23	111.00
1	E	74	ASP	N-CA-C	5.36	125.46	111.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	F	156	ARG	NE-CZ-NH1	5.24	122.92	120.30
1	F	70	ARG	NE-CZ-NH1	-5.16	117.72	120.30
1	C	169	ARG	CD-NE-CZ	-5.10	116.46	123.60
1	C	156	ARG	NE-CZ-NH1	5.08	122.84	120.30
1	F	156	ARG	NE-CZ-NH2	-5.03	117.79	120.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	E	171	GLU	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	1445	0	1450	48	0
1	B	1439	0	1445	34	0
1	C	1439	0	1443	28	0
1	D	1445	0	1450	31	0
1	E	1434	0	1438	43	0
1	F	1431	0	1439	20	1
2	A	5	0	0	3	0
2	B	5	0	0	1	0
2	C	5	0	0	1	0
2	D	5	0	0	0	0
2	E	5	0	0	1	0
2	F	5	0	0	1	0
3	A	12	0	16	0	0
3	B	6	0	8	1	0
3	C	12	0	16	3	0
3	D	6	0	8	1	0
4	A	69	0	0	3	0
4	B	95	0	0	7	0
4	C	55	0	0	1	0
4	D	75	0	0	3	0
4	E	42	0	0	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	F	84	0	0	4	1
All	All	9119	0	8713	188	1

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 11.

All (188) 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:169:ARG:CG	1:E:169:ARG:CD	1.79	1.55
1:C:0:ALA:N	1:C:0:ALA:CA	1.68	1.50
1:F:1:MSE:CE	1:F:1:MSE:SE	2.14	1.46
1:C:61:MSE:SE	1:C:61:MSE:CE	2.17	1.42
1:A:61:MSE:CE	1:A:61:MSE:SE	2.17	1.42
1:E:61:MSE:SE	1:E:61:MSE:CE	2.18	1.41
1:D:61:MSE:CE	1:D:61:MSE:SE	2.18	1.41
1:D:-2:SER:CB	1:D:-2:SER:OG	1.78	1.29
1:E:15:THR:HA	1:E:18:MSE:HE3	1.32	1.12
1:B:122:VAL:HB	1:B:132:LEU:HD22	1.36	1.06
1:A:143:ARG:HH21	1:A:143:ARG:HG2	1.22	1.03
1:C:12:THR:HG22	2:C:503:PO4:O3	1.62	0.99
1:E:59:THR:HG22	1:E:92:SER:OG	1.64	0.97
1:E:169:ARG:CB	1:E:169:ARG:CD	2.57	0.82
1:A:11:ARG:N	2:A:501:PO4:O2	2.13	0.81
1:E:169:ARG:HB2	1:E:171:GLU:OE1	1.82	0.80
1:F:11:ARG:N	2:F:506:PO4:O1	2.14	0.79
1:B:11:ARG:N	2:B:502:PO4:O1	2.13	0.79
1:E:18:MSE:CE	1:E:93:SER:HB2	2.13	0.78
1:F:1:MSE:HG2	1:F:167:ASP:OD1	1.84	0.78
1:D:122:VAL:HB	1:D:132:LEU:HD22	1.66	0.77
1:C:184:VAL:O	1:C:185:ASP:HB2	1.84	0.75
1:A:78:ASP:HB2	4:A:553:HOH:O	1.87	0.75
1:E:18:MSE:HE2	1:E:93:SER:HB2	1.71	0.73
1:E:15:THR:HA	1:E:18:MSE:CE	2.16	0.71
1:A:106:MSE:O	1:A:110:THR:HG22	1.91	0.70
1:A:110:THR:HG21	3:C:508:GOL:O2	1.91	0.70
1:A:143:ARG:HG2	1:A:143:ARG:NH2	2.01	0.69
1:C:107:SER:HB3	3:C:508:GOL:H12	1.75	0.68
4:A:564:HOH:O	1:B:170:LYS:HE3	1.94	0.68
1:B:67:LYS:CE	4:B:569:HOH:O	2.42	0.67
1:A:14:ASN:N	2:A:501:PO4:O3	2.28	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:B:510:GOL:H2	3:C:511:GOL:H32	1.78	0.66
1:A:106:MSE:O	1:A:110:THR:CG2	2.43	0.66
1:E:169:ARG:HG3	1:E:172:LEU:HD21	1.78	0.65
1:A:52:GLY:HA2	1:A:87:ILE:O	1.98	0.64
1:B:59:THR:HG22	1:B:92:SER:OG	1.96	0.64
1:A:143:ARG:HH21	1:A:143:ARG:CG	2.04	0.64
1:E:18:MSE:HE1	1:E:93:SER:CB	2.28	0.64
1:A:11:ARG:HH11	1:A:11:ARG:CG	2.10	0.64
1:E:169:ARG:CG	1:E:169:ARG:NE	2.60	0.63
1:E:64:VAL:HG13	1:E:108:ILE:HG12	1.81	0.63
1:B:59:THR:HB	1:B:104:ALA:HB2	1.79	0.62
1:A:106:MSE:HE1	1:B:106:MSE:CE	2.29	0.62
1:B:59:THR:CG2	1:B:94:SER:HB3	2.30	0.62
1:B:59:THR:HB	1:B:104:ALA:CB	2.31	0.61
1:E:143:ARG:HH11	1:E:143:ARG:HB3	1.66	0.60
1:A:11:ARG:HH11	1:A:11:ARG:HG2	1.66	0.60
1:A:167:ASP:HB2	4:A:526:HOH:O	2.00	0.60
1:A:11:ARG:HG3	2:A:501:PO4:O2	2.02	0.59
1:B:67:LYS:HE2	4:B:569:HOH:O	2.00	0.59
1:A:11:ARG:HH11	1:A:11:ARG:HB3	1.67	0.59
1:D:-2:SER:CA	1:D:-2:SER:OG	2.51	0.59
1:E:18:MSE:CE	1:E:93:SER:CB	2.81	0.58
1:C:74:ASP:OD2	4:C:548:HOH:O	2.17	0.58
1:B:107:SER:HA	3:D:507:GOL:H11	1.86	0.57
1:D:67:LYS:HE3	4:D:554:HOH:O	2.04	0.57
1:E:47:VAL:O	1:E:86:LYS:HE3	2.04	0.57
1:A:107:SER:HA	1:A:110:THR:HG23	1.85	0.56
1:F:121:GLY:HA3	1:F:133:HIS:O	2.04	0.56
1:A:106:MSE:CE	1:B:106:MSE:CE	2.83	0.56
1:B:44:LYS:HE3	4:B:544:HOH:O	2.05	0.56
1:C:55:VAL:HG21	1:C:112:LEU:HD21	1.86	0.56
1:C:161:TRP:CE3	1:C:161:TRP:HA	2.41	0.56
1:E:18:MSE:HE1	1:E:93:SER:HB2	1.88	0.56
1:A:66:TRP:CD2	1:C:70:ARG:HG2	2.41	0.56
1:B:122:VAL:HB	1:B:132:LEU:CD2	2.25	0.55
1:F:4:VAL:HG13	1:F:158:LEU:HD13	1.86	0.55
1:B:61:MSE:HE2	4:B:557:HOH:O	2.06	0.55
1:B:70:ARG:HD2	4:B:558:HOH:O	2.07	0.55
1:C:82:GLU:O	1:D:177:ARG:HG2	2.07	0.55
1:D:121:GLY:HA3	1:D:133:HIS:O	2.06	0.55
1:F:109:LEU:HD22	1:F:119:VAL:HG13	1.89	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:11:ARG:N	2:E:505:PO4:O4	2.35	0.55
1:B:128:LYS:HD2	1:B:129:LYS:HG3	1.88	0.55
1:A:3:LYS:HE2	1:A:49:TRP:O	2.07	0.54
1:E:161:TRP:HA	1:E:161:TRP:CE3	2.43	0.54
1:C:106:MSE:HE2	1:D:106:MSE:HE2	1.90	0.54
1:A:172:LEU:HD23	1:A:175:LYS:HD2	1.90	0.54
1:B:59:THR:HG21	1:B:94:SER:HB3	1.88	0.54
1:B:153:ARG:NH2	4:B:534:HOH:O	2.38	0.53
1:C:52:GLY:HA2	1:C:87:ILE:O	2.08	0.53
1:B:59:THR:HG21	1:B:101:ASN:HA	1.91	0.52
1:E:29:LEU:HA	1:E:156:ARG:HH21	1.74	0.52
1:E:161:TRP:HA	1:E:161:TRP:HE3	1.74	0.52
1:A:106:MSE:CE	1:B:106:MSE:HE2	2.41	0.51
1:C:161:TRP:HA	1:C:161:TRP:HE3	1.74	0.51
1:D:55:VAL:HG21	1:D:112:LEU:HD21	1.93	0.51
1:C:30:GLU:CD	1:C:30:GLU:H	2.15	0.50
1:C:106:MSE:HE1	1:D:106:MSE:HE1	1.93	0.50
1:C:0:ALA:C	1:C:0:ALA:N	2.59	0.50
1:C:64:VAL:HG13	1:C:108:ILE:HG12	1.92	0.50
1:A:11:ARG:HH11	1:A:11:ARG:CB	2.24	0.49
1:E:59:THR:HG21	1:E:101:ASN:HA	1.94	0.49
1:D:173:LEU:HD22	1:D:177:ARG:HD3	1.95	0.49
1:A:143:ARG:CG	1:A:143:ARG:NH2	2.69	0.49
1:D:101:ASN:HD22	1:D:102:GLU:N	2.11	0.48
1:C:119:VAL:HG12	1:D:119:VAL:HG12	1.95	0.48
1:B:59:THR:HG23	1:B:94:SER:HB3	1.94	0.48
1:D:30:GLU:HB2	4:D:532:HOH:O	2.13	0.48
1:D:9:ASP:OD2	1:D:65:SER:OG	2.21	0.48
1:A:122:VAL:HB	1:A:132:LEU:HG	1.96	0.48
1:C:7:ILE:HA	1:C:37:LYS:O	2.13	0.48
1:E:4:VAL:HG13	1:E:158:LEU:HD13	1.94	0.48
1:E:141:GLU:HG2	1:E:142:PRO:HD2	1.96	0.48
1:E:59:THR:HB	1:E:104:ALA:HB2	1.96	0.47
1:D:18:MSE:HE3	1:D:138:VAL:HG23	1.96	0.47
1:E:48:LEU:HD21	1:E:79:LEU:HD22	1.96	0.47
1:A:66:TRP:CG	1:C:70:ARG:HG2	2.50	0.47
1:C:182:ARG:NH2	1:D:81:GLY:O	2.47	0.47
1:E:126:VAL:HG22	1:E:149:GLU:HG3	1.96	0.47
1:A:66:TRP:CZ2	1:C:70:ARG:HD3	2.50	0.46
1:A:8:TYR:CZ	1:A:16:LYS:HG3	2.51	0.46
1:E:55:VAL:HG21	1:E:112:LEU:HD21	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:106:MSE:HE1	1:B:106:MSE:HE1	1.97	0.46
1:E:170:LYS:CB	1:E:170:LYS:NZ	2.79	0.46
1:B:67:LYS:NZ	4:B:569:HOH:O	2.12	0.46
1:F:64:VAL:HG13	1:F:108:ILE:HG12	1.99	0.46
1:F:61:MSE:HA	1:F:61:MSE:HE2	1.97	0.45
1:E:29:LEU:CA	1:E:156:ARG:HH21	2.29	0.45
1:F:61:MSE:HE3	4:F:567:HOH:O	2.17	0.45
1:E:109:LEU:HD22	1:E:119:VAL:HG13	1.98	0.45
1:E:5:LEU:HB2	1:E:50:ALA:HB2	1.98	0.45
1:E:7:ILE:HA	1:E:37:LYS:O	2.17	0.45
1:F:55:VAL:HG21	1:F:112:LEU:HD21	1.99	0.45
1:A:55:VAL:HG21	1:A:112:LEU:HD21	1.99	0.45
1:E:18:MSE:HG2	1:E:151:CYS:SG	2.56	0.45
1:D:4:VAL:HB	1:D:34:VAL:HG22	1.99	0.45
1:A:165:PHE:HB3	1:B:165:PHE:HB3	1.99	0.44
1:B:59:THR:HG23	1:B:94:SER:CB	2.47	0.44
1:E:44:LYS:HG3	4:E:508:HOH:O	2.17	0.44
1:B:101:ASN:HD22	1:B:102:GLU:H	1.64	0.44
1:E:35:ARG:HD3	1:E:49:TRP:CZ3	2.52	0.44
1:A:5:LEU:HB2	1:A:50:ALA:HB2	1.99	0.44
1:F:4:VAL:CG1	1:F:158:LEU:HD13	2.48	0.44
1:D:64:VAL:HG13	1:D:108:ILE:HG12	1.99	0.44
1:A:8:TYR:CE1	1:A:16:LYS:HG3	2.52	0.43
1:C:127:GLY:HA3	1:C:146:GLU:HG2	1.99	0.43
1:D:173:LEU:HD22	1:D:177:ARG:CD	2.48	0.43
1:F:52:GLY:HA2	1:F:87:ILE:O	2.18	0.43
1:E:83:ILE:HD11	1:E:115:PHE:CD2	2.54	0.43
1:E:59:THR:HB	1:E:104:ALA:CB	2.49	0.43
1:D:52:GLY:HA2	1:D:87:ILE:O	2.18	0.43
1:A:64:VAL:HG13	1:A:108:ILE:HG12	2.00	0.43
1:C:184:VAL:O	1:C:185:ASP:CB	2.63	0.43
1:C:122:VAL:HB	1:C:132:LEU:HG	2.01	0.43
1:E:52:GLY:HA2	1:E:87:ILE:O	2.19	0.43
1:E:18:MSE:HE1	1:E:93:SER:N	2.34	0.42
1:D:56:GLY:HA2	1:D:91:PHE:O	2.19	0.42
1:F:161:TRP:HA	1:F:161:TRP:CE3	2.54	0.42
1:A:18:MSE:HG2	1:A:142:PRO:HG3	2.01	0.42
1:B:52:GLY:HA2	1:B:87:ILE:O	2.19	0.42
1:F:146:GLU:OE2	4:F:558:HOH:O	2.21	0.42
1:D:124:ASP:OD2	1:D:153:ARG:HD2	2.20	0.42
1:A:113:MSE:SE	1:B:109:LEU:HD13	2.70	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:66:TRP:CE2	1:C:70:ARG:HG2	2.54	0.42
1:A:35:ARG:HD3	1:A:49:TRP:CZ3	2.55	0.42
1:B:101:ASN:HD22	1:B:102:GLU:N	2.17	0.42
1:A:3:LYS:HG2	1:A:49:TRP:CE2	2.55	0.42
1:E:164:ILE:HG23	1:E:170:LYS:HG3	2.00	0.42
1:D:11:ARG:HE	1:D:11:ARG:HB3	1.70	0.42
1:A:13:GLY:O	1:A:17:LYS:HD2	2.19	0.42
1:A:106:MSE:O	1:A:110:THR:HG23	2.19	0.41
1:A:101:ASN:HD22	1:A:102:GLU:N	2.18	0.41
1:D:174:GLU:HA	1:D:174:GLU:OE2	2.20	0.41
1:E:126:VAL:CG2	1:E:149:GLU:HG3	2.50	0.41
1:D:161:TRP:HA	1:D:161:TRP:CE3	2.56	0.41
1:C:106:MSE:CE	1:D:106:MSE:CE	2.98	0.41
1:F:161:TRP:HE3	1:F:161:TRP:HA	1.85	0.41
1:A:109:LEU:HD22	1:A:119:VAL:HB	2.02	0.41
1:B:21:LEU:HD13	1:B:148:LYS:HA	2.03	0.41
1:B:161:TRP:HA	1:B:161:TRP:CE3	2.55	0.41
1:A:121:GLY:HA3	1:A:133:HIS:O	2.21	0.41
1:C:179:ASP:HA	1:C:180:PRO:HD3	1.92	0.41
1:F:1:MSE:CG	1:F:167:ASP:OD1	2.62	0.41
1:A:11:ARG:NH1	1:A:11:ARG:HB3	2.34	0.41
1:D:163:ALA:HB1	1:D:169:ARG:HG3	2.02	0.41
1:B:122:VAL:CB	1:B:132:LEU:HD22	2.25	0.41
1:D:67:LYS:CE	4:D:554:HOH:O	2.66	0.41
1:F:64:VAL:HG13	1:F:108:ILE:CG1	2.51	0.41
1:D:161:TRP:HE3	1:D:161:TRP:HA	1.86	0.41
1:F:37:LYS:HD2	1:F:46:ASP:OD2	2.21	0.41
1:F:169:ARG:NH1	4:F:549:HOH:O	2.53	0.41
1:F:174:GLU:HG2	4:F:534:HOH:O	2.21	0.40
1:D:168:GLY:O	1:D:170:LYS:N	2.54	0.40
1:E:66:TRP:CH2	1:E:67:LYS:HE2	2.56	0.40
1:A:85:GLY:HA2	1:A:118:LEU:HD23	2.03	0.40
1:A:113:MSE:HE1	1:B:106:MSE:HE1	2.03	0.40

All (1) 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:F:17:LYS:NZ	4:F:553:HOH:O[6_765]	2.11	0.09

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	185/188 (98%)	181 (98%)	2 (1%)	2 (1%)	17 25
1	B	184/188 (98%)	179 (97%)	5 (3%)	0	100 100
1	C	184/188 (98%)	181 (98%)	3 (2%)	0	100 100
1	D	185/188 (98%)	178 (96%)	7 (4%)	0	100 100
1	E	183/188 (97%)	180 (98%)	3 (2%)	0	100 100
1	F	183/188 (97%)	175 (96%)	7 (4%)	1 (0%)	34 48
All	All	1104/1128 (98%)	1074 (97%)	27 (2%)	3 (0%)	46 63

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	169	ARG
1	F	64	VAL
1	A	64	VAL

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	149/143 (104%)	136 (91%)	13 (9%)	13 19
1	B	148/143 (104%)	128 (86%)	20 (14%)	5 5
1	C	148/143 (104%)	131 (88%)	17 (12%)	7 9
1	D	149/143 (104%)	130 (87%)	19 (13%)	5 6

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	E	148/143 (104%)	130 (88%)	18 (12%)	6 7
1	F	147/143 (103%)	125 (85%)	22 (15%)	3 4
All	All	889/858 (104%)	780 (88%)	109 (12%)	6 7

All (109) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	5	LEU
1	A	11	ARG
1	A	17	LYS
1	A	29	LEU
1	A	64	VAL
1	A	101	ASN
1	A	110	THR
1	A	126	VAL
1	A	132	LEU
1	A	143	ARG
1	A	156	ARG
1	A	158	LEU
1	A	173	LEU
1	B	5	LEU
1	B	17	LYS
1	B	24	GLU
1	B	29	LEU
1	B	35	ARG
1	B	39	VAL
1	B	59	THR
1	B	64	VAL
1	B	75	VAL
1	B	101	ASN
1	B	118	LEU
1	B	119	VAL
1	B	126	VAL
1	B	132	LEU
1	B	153	ARG
1	B	156	ARG
1	B	158	LEU
1	B	161	TRP
1	B	171	GLU
1	B	178	LYS
1	C	5	LEU

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Mol	Chain	Res	Type
1	C	12	THR
1	C	39	VAL
1	C	41	GLU
1	C	64	VAL
1	C	70	ARG
1	C	75	VAL
1	C	101	ASN
1	C	118	LEU
1	C	119	VAL
1	C	126	VAL
1	C	132	LEU
1	C	145	GLU
1	C	156	ARG
1	C	158	LEU
1	C	161	TRP
1	C	185	ASP
1	D	-1	ASN
1	D	1	MSE
1	D	5	LEU
1	D	29	LEU
1	D	30	GLU
1	D	39	VAL
1	D	64	VAL
1	D	75	VAL
1	D	101	ASN
1	D	118	LEU
1	D	119	VAL
1	D	126	VAL
1	D	128	LYS
1	D	132	LEU
1	D	156	ARG
1	D	158	LEU
1	D	161	TRP
1	D	169	ARG
1	D	173	LEU
1	E	5	LEU
1	E	35	ARG
1	E	39	VAL
1	E	41	GLU
1	E	59	THR
1	E	64	VAL
1	E	75	VAL

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Mol	Chain	Res	Type
1	E	118	LEU
1	E	126	VAL
1	E	132	LEU
1	E	143	ARG
1	E	153	ARG
1	E	156	ARG
1	E	158	LEU
1	E	161	TRP
1	E	170	LYS
1	E	171	GLU
1	E	172	LEU
1	F	1	MSE
1	F	5	LEU
1	F	7	ILE
1	F	17	LYS
1	F	29	LEU
1	F	35	ARG
1	F	64	VAL
1	F	70	ARG
1	F	78	ASP
1	F	82	GLU
1	F	101	ASN
1	F	118	LEU
1	F	119	VAL
1	F	126	VAL
1	F	132	LEU
1	F	156	ARG
1	F	158	LEU
1	F	161	TRP
1	F	167	ASP
1	F	171	GLU
1	F	173	LEU
1	F	178	LYS

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	38	HIS
1	A	60	ASN
1	A	101	ASN
1	B	60	ASN
1	B	101	ASN

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Mol	Chain	Res	Type
1	D	60	ASN
1	D	101	ASN
1	E	60	ASN
1	F	60	ASN
1	F	101	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

12 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	PO4	A	501	-	4,4,4	1.24	0	6,6,6	0.26	0
3	GOL	A	509	-	5,5,5	0.44	0	5,5,5	0.75	0
3	GOL	A	512	-	5,5,5	0.39	0	5,5,5	0.37	0
2	PO4	B	502	-	4,4,4	0.82	0	6,6,6	0.33	0
3	GOL	B	510	-	5,5,5	0.36	0	5,5,5	0.62	0
2	PO4	C	503	-	4,4,4	0.40	0	6,6,6	0.28	0
3	GOL	C	508	-	5,5,5	0.32	0	5,5,5	0.55	0
3	GOL	C	511	-	5,5,5	0.29	0	5,5,5	0.59	0
2	PO4	D	504	-	4,4,4	0.43	0	6,6,6	0.31	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
3	GOL	D	507	-	5,5,5	0.23	0	5,5,5	0.74	0
2	PO4	E	505	-	4,4,4	0.32	0	6,6,6	0.29	0
2	PO4	F	506	-	4,4,4	0.86	0	6,6,6	0.34	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
2	PO4	A	501	-	-	0/0/0/0	0/0/0/0
3	GOL	A	509	-	-	0/4/4/4	0/0/0/0
3	GOL	A	512	-	-	0/4/4/4	0/0/0/0
2	PO4	B	502	-	-	0/0/0/0	0/0/0/0
3	GOL	B	510	-	-	0/4/4/4	0/0/0/0
2	PO4	C	503	-	-	0/0/0/0	0/0/0/0
3	GOL	C	508	-	-	0/4/4/4	0/0/0/0
3	GOL	C	511	-	-	0/4/4/4	0/0/0/0
2	PO4	D	504	-	-	0/0/0/0	0/0/0/0
3	GOL	D	507	-	-	0/4/4/4	0/0/0/0
2	PO4	E	505	-	-	0/0/0/0	0/0/0/0
2	PO4	F	506	-	-	0/0/0/0	0/0/0/0

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

9 monomers are involved in 11 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	501	PO4	3	0
2	B	502	PO4	1	0
3	B	510	GOL	1	0
2	C	503	PO4	1	0
3	C	508	GOL	2	0
3	C	511	GOL	1	0
3	D	507	GOL	1	0
2	E	505	PO4	1	0
2	F	506	PO4	1	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	180/188 (95%)	-0.23	8 (4%)	38	39	19, 28, 37, 44	0
1	B	179/188 (95%)	-0.16	10 (5%)	28	28	18, 27, 35, 46	0
1	C	179/188 (95%)	0.08	8 (4%)	37	38	20, 28, 36, 48	0
1	D	180/188 (95%)	0.01	14 (7%)	16	15	13, 28, 40, 51	0
1	E	178/188 (94%)	-0.01	8 (4%)	37	38	17, 28, 36, 49	0
1	F	178/188 (94%)	-0.25	8 (4%)	37	38	21, 28, 36, 52	0
All	All	1074/1128 (95%)	-0.09	56 (5%)	31	31	13, 28, 36, 52	0

All (56) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	103	VAL	4.5
1	A	103	VAL	4.4
1	E	185	ASP	4.3
1	C	103	VAL	4.1
1	D	0	ALA	4.0
1	B	103	VAL	4.0
1	E	103	VAL	4.0
1	A	110	THR	3.6
1	B	104	ALA	3.5
1	E	110	THR	3.3
1	D	112	LEU	3.3
1	D	105	CYS	3.3
1	B	128	LYS	3.2
1	B	110	THR	3.2
1	C	110	THR	3.1
1	D	109	LEU	3.0
1	E	109	LEU	3.0
1	D	119	VAL	2.9
1	D	-2	SER	2.9

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Mol	Chain	Res	Type	RSRZ
1	D	143	ARG	2.9
1	C	0	ALA	2.9
1	D	110	THR	2.9
1	F	103	VAL	2.8
1	F	110	THR	2.8
1	D	107	SER	2.7
1	A	105	CYS	2.7
1	E	105	CYS	2.7
1	B	107	SER	2.6
1	B	109	LEU	2.6
1	D	-1	ASN	2.6
1	E	11	ARG	2.5
1	C	109	LEU	2.5
1	A	112	LEU	2.5
1	B	63	LEU	2.5
1	D	134	TYR	2.5
1	A	109	LEU	2.4
1	B	105	CYS	2.4
1	A	104	ALA	2.4
1	D	114	ASN	2.3
1	C	30	GLU	2.3
1	E	112	LEU	2.3
1	F	109	LEU	2.3
1	F	62	GLY	2.3
1	A	107	SER	2.2
1	C	141	GLU	2.2
1	A	63	LEU	2.2
1	F	105	CYS	2.2
1	C	143	ARG	2.2
1	F	107	SER	2.2
1	F	112	LEU	2.1
1	D	135	GLY	2.1
1	E	104	ALA	2.1
1	F	119	VAL	2.1
1	B	62	GLY	2.1
1	B	108	ILE	2.1
1	C	11	ARG	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
3	GOL	A	509	6/6	0.87	0.38	21.63	43,46,49,49	0
2	PO4	F	506	5/5	0.95	0.24	3.25	33,35,37,38	5
2	PO4	A	501	5/5	0.95	0.22	1.65	18,23,24,25	5
2	PO4	B	502	5/5	0.95	0.18	1.12	34,36,39,40	5
3	GOL	D	507	6/6	0.87	0.34	0.30	35,39,41,42	0
2	PO4	C	503	5/5	0.88	0.17	0.28	48,50,52,53	0
2	PO4	E	505	5/5	0.93	0.15	0.13	32,35,36,37	0
2	PO4	D	504	5/5	0.95	0.13	-0.16	48,50,51,52	0
3	GOL	C	508	6/6	0.89	0.27	-0.55	35,38,38,38	0
3	GOL	A	512	6/6	0.73	0.99	-	61,64,64,65	0
3	GOL	B	510	6/6	0.68	0.25	-	73,75,76,76	0
3	GOL	C	511	6/6	0.69	0.34	-	59,61,61,62	0

6.5 Other polymers (i)

There are no such residues in this entry.