



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 02:57 AM GMT

PDB ID : 2JH3  
Title : THE CRYSTAL STRUCTURE OF DR2241 FROM DEINOCOCCUS RADIODURANS AT 1.9 Å RESOLUTION REVEALS A MULTI-DOMAIN PROTEIN WITH STRUCTURAL SIMILARITY TO CHELATASES BUT ALSO WITH TWO ADDITIONAL NOVEL DOMAINS  
Authors : Leiros, H.-K.S.; Mcsweeney, S.M.  
Deposited on : 2007-02-20  
Resolution : 1.90 Å(reported)

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

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

MolProbity : 4.02b-467  
Mogul : 1.7 (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

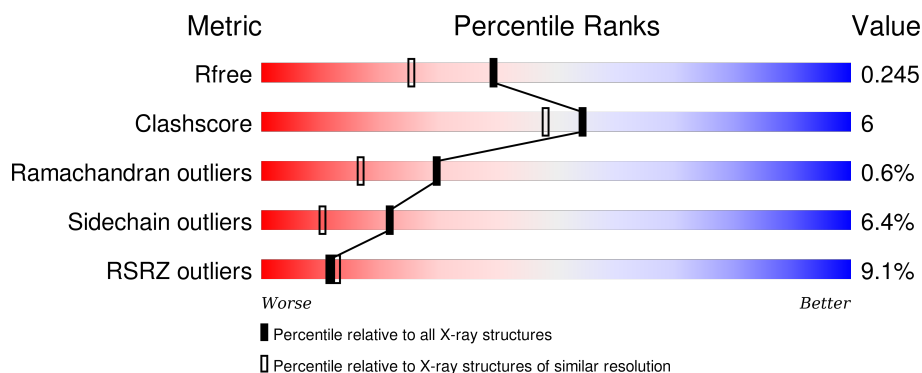
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 1.90 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	4755 (1.90-1.90)
Clashscore	102246	5398 (1.90-1.90)
Ramachandran outliers	100387	5338 (1.90-1.90)
Sidechain outliers	100360	5339 (1.90-1.90)
RSRZ outliers	91569	4766 (1.90-1.90)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions  $\leq 5\%$ . The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	474	<div> <div>6%</div> <div> <div></div> <div>79%</div> <div>14%</div> <div>• • •</div> </div> </div>
1	B	474	<div> <div>14%</div> <div> <div></div> <div>76%</div> <div>17%</div> <div>• • •</div> </div> </div>
1	C	474	<div> <div>4%</div> <div> <div></div> <div>78%</div> <div>15%</div> <div>• •</div> </div> </div>
1	D	474	<div> <div>12%</div> <div> <div></div> <div>80%</div> <div>13%</div> <div>• • •</div> </div> </div>

## 2 Entry composition [i](#)

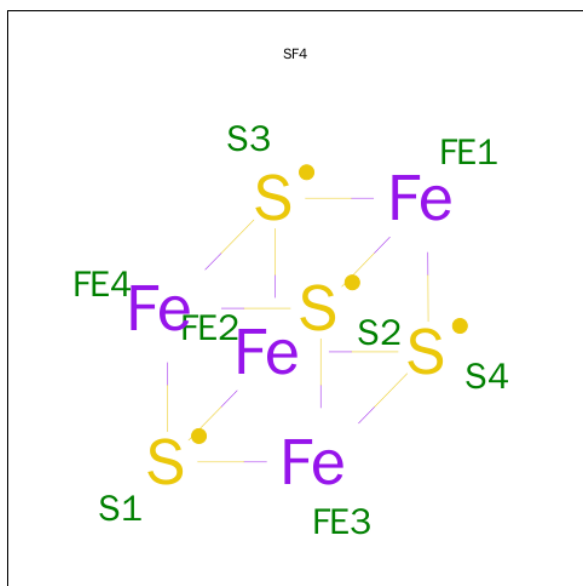
There are 3 unique types of molecules in this entry. The entry contains 14998 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 RIBOSOMAL PROTEIN S2-RELATED PROTEIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	459	Total	C	N	O	S	55	0	0
			3502	2188	667	641	6			
1	B	459	Total	C	N	O	S	101	0	0
			3502	2188	667	641	6			
1	C	459	Total	C	N	O	S	77	0	0
			3502	2188	667	641	6			
1	D	456	Total	C	N	O	S	104	0	0
			3476	2174	661	635	6			

- Molecule 2 is IRON/SULFUR CLUSTER (three-letter code: SF4) (formula: Fe<sub>4</sub>S<sub>4</sub>).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	Fe	S	0	0
			8	4	4		
2	B	1	Total	Fe	S	0	0
			8	4	4		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	C	1	Total 8	Fe 4	S 4	0	0
2	D	1	Total 8	Fe 4	S 4	0	0

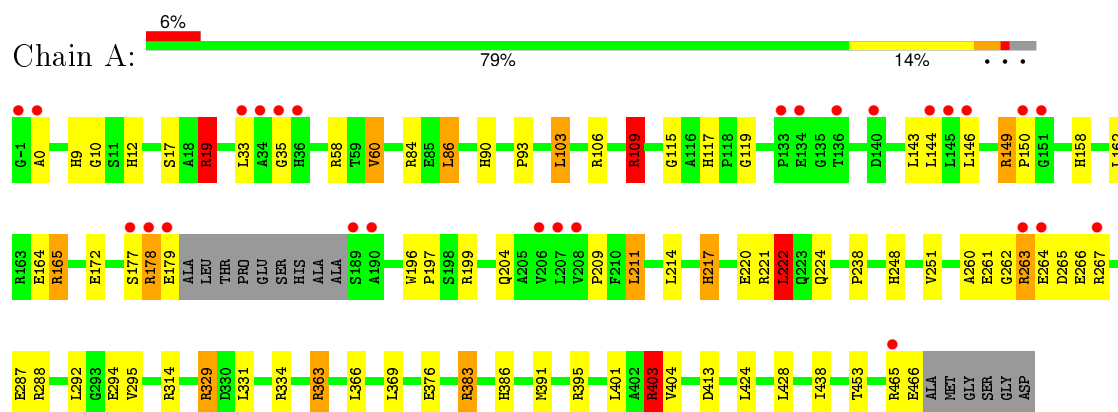
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	298	Total 298	O 298	0	0
3	B	184	Total 184	O 184	0	0
3	C	285	Total 285	O 285	0	0
3	D	217	Total 217	O 217	0	0

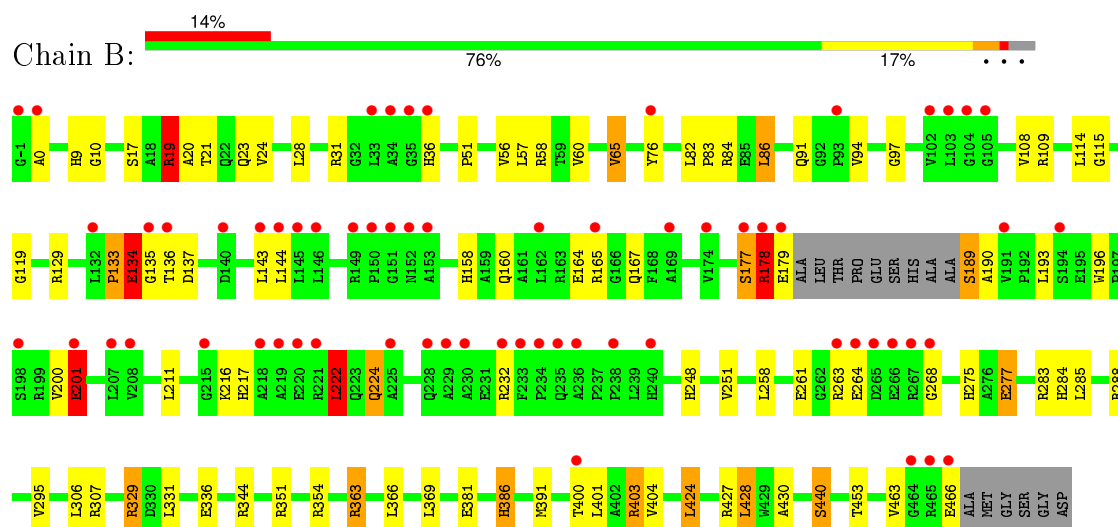
### 3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ( $RSRZ > 2$ ). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

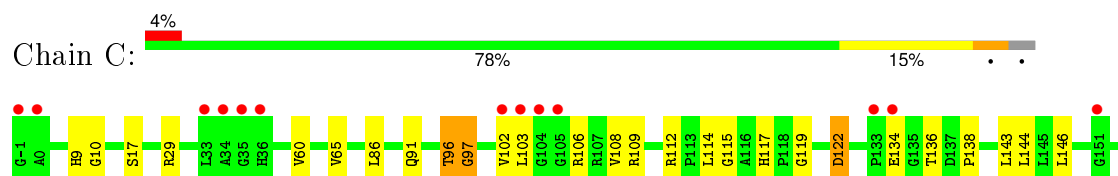
#### • Molecule 1: RIBOSOMAL PROTEIN S2-RELATED PROTEIN

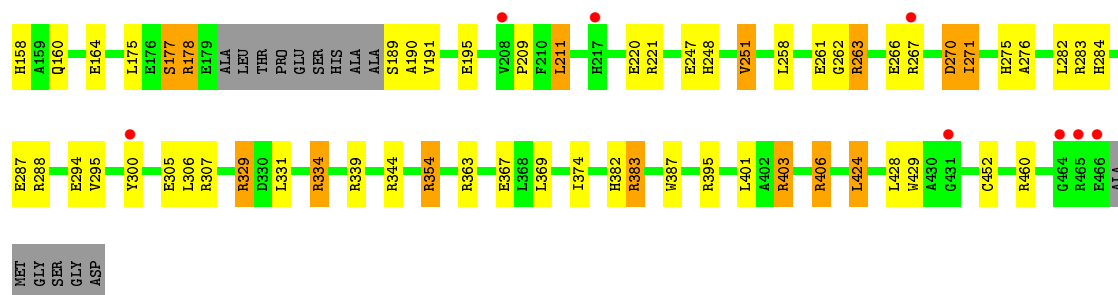


#### • Molecule 1: RIBOSOMAL PROTEIN S2-RELATED PROTEIN



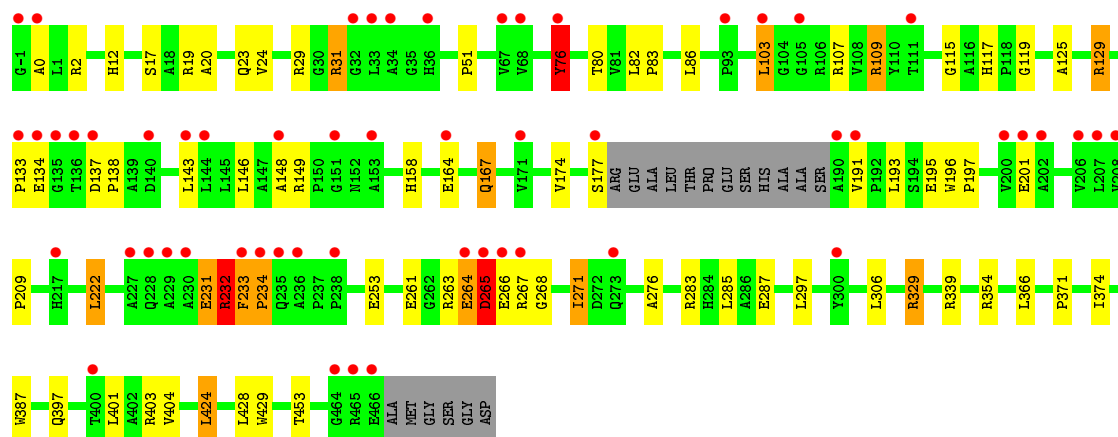
#### • Molecule 1: RIBOSOMAL PROTEIN S2-RELATED PROTEIN





• Molecule 1: RIBOSOMAL PROTEIN S2-RELATED PROTEIN

Chain D: 12% 80% 13%



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	124.78Å 128.69Å 135.08Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	20.00 – 1.90 19.93 – 1.90	Depositor EDS
% Data completeness (in resolution range)	98.7 (20.00-1.90) 98.7 (19.93-1.90)	Depositor EDS
$R_{merge}$	0.08	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.93 (at 1.90Å)	Xtriage
Refinement program	REFMAC 5.2.0005	Depositor
R, $R_{free}$	0.189 , 0.238 0.197 , 0.245	Depositor DCC
$R_{free}$ test set	3400 reflections (2.06%)	DCC
Wilson B-factor (Å <sup>2</sup> )	25.9	Xtriage
Anisotropy	0.048	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.35 , 55.8	EDS
Estimated twinning fraction	0.015 for k,h,-l	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.31$	Xtriage
Outliers	0 of 168541 reflections	Xtriage
$F_o, F_c$ correlation	0.96	EDS
Total number of atoms	14998	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	36.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.78% of the height of the origin peak. No significant pseudotranslation is detected.*

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

<sup>2</sup>Theoretical values of  $\langle |L| \rangle$ ,  $\langle L^2 \rangle$  for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 0.2 for perfectly twinned datasets.

## 5 Model quality ⓘ

### 5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: SF4

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	1.43	8/3580 (0.2%)	1.08	27/4882 (0.6%)
1	B	1.33	18/3580 (0.5%)	1.14	38/4882 (0.8%)
1	C	1.11	7/3580 (0.2%)	1.10	22/4882 (0.5%)
1	D	1.10	9/3554 (0.3%)	1.12	29/4848 (0.6%)
All	All	1.25	42/14294 (0.3%)	1.11	116/19494 (0.6%)

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	1	2
1	B	0	4
1	D	0	2
All	All	1	8

All (42) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	220	GLU	CD-OE1	51.89	1.82	1.25
1	B	277	GLU	CD-OE2	30.24	1.58	1.25
1	D	263	ARG	CD-NE	-26.41	1.01	1.46
1	B	277	GLU	CD-OE1	-26.07	0.96	1.25
1	B	386	HIS	CG-CD2	21.61	1.72	1.35
1	B	466	GLU	CB-CG	-18.14	1.17	1.52
1	A	19	ARG	CG-CD	17.62	1.96	1.51
1	A	178	ARG	CB-CG	17.54	2.00	1.52
1	B	277	GLU	CG-CD	16.02	1.75	1.51
1	D	76	TYR	CE1-CZ	15.77	1.59	1.38
1	C	221	ARG	CG-CD	-15.01	1.14	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	265	ASP	N-CA	-12.18	1.22	1.46
1	D	233	PHE	CG-CD1	12.12	1.56	1.38
1	D	234	PRO	CA-CB	-9.21	1.35	1.53
1	A	217	HIS	CB-CG	8.97	1.66	1.50
1	D	76	TYR	CZ-OH	-8.85	1.22	1.37
1	B	19	ARG	CD-NE	8.83	1.61	1.46
1	B	177	SER	C-N	8.75	1.54	1.34
1	C	403	ARG	CG-CD	8.70	1.73	1.51
1	B	386	HIS	CG-ND1	-8.63	1.19	1.38
1	D	232	ARG	CA-CB	-8.31	1.35	1.53
1	C	97	GLY	N-CA	8.09	1.58	1.46
1	B	217	HIS	CB-CG	7.95	1.64	1.50
1	B	91	GLN	CD-OE1	7.62	1.40	1.24
1	B	232	ARG	CB-CG	-7.59	1.32	1.52
1	A	60	VAL	CB-CG2	-7.44	1.37	1.52
1	D	167	GLN	CG-CD	-6.98	1.34	1.51
1	B	19	ARG	CB-CG	6.95	1.71	1.52
1	B	178	ARG	N-CA	6.94	1.60	1.46
1	C	452	CYS	CB-SG	-6.94	1.70	1.82
1	C	251	VAL	CB-CG2	-6.82	1.38	1.52
1	B	336	GLU	CB-CG	6.79	1.65	1.52
1	B	216	LYS	CB-CG	-6.64	1.34	1.52
1	D	2	ARG	CD-NE	-6.21	1.35	1.46
1	B	224	GLN	CB-CG	6.05	1.68	1.52
1	C	294	GLU	CG-CD	5.98	1.60	1.51
1	A	217	HIS	CG-ND1	5.83	1.51	1.38
1	D	265	ASP	CA-C	-5.60	1.38	1.52
1	B	91	GLN	CB-CG	-5.26	1.38	1.52
1	C	354	ARG	CD-NE	-5.23	1.37	1.46
1	A	294	GLU	CG-CD	5.11	1.59	1.51
1	B	189	SER	C-N	5.09	1.45	1.34

All (116) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	76	TYR	CB-CG-CD1	-18.94	109.64	121.00
1	B	189	SER	O-C-N	-15.57	97.78	122.70
1	D	233	PHE	CB-CG-CD1	13.55	130.29	120.80
1	B	354	ARG	NE-CZ-NH1	-13.05	113.78	120.30
1	C	354	ARG	NE-CZ-NH1	-12.78	113.91	120.30
1	C	354	ARG	NE-CZ-NH2	11.76	126.18	120.30
1	B	354	ARG	NE-CZ-NH2	11.23	125.92	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	84	ARG	NE-CZ-NH2	-10.60	115.00	120.30
1	C	329	ARG	NE-CZ-NH2	-10.44	115.08	120.30
1	D	354	ARG	NE-CZ-NH1	-10.32	115.14	120.30
1	C	96	THR	C-N-CA	-9.87	101.58	122.30
1	D	76	TYR	CG-CD1-CE1	-9.83	113.44	121.30
1	C	329	ARG	NE-CZ-NH1	9.79	125.19	120.30
1	B	177	SER	C-N-CA	9.52	145.49	121.70
1	B	19	ARG	CD-NE-CZ	-9.44	110.39	123.60
1	D	233	PHE	CZ-CE2-CD2	9.31	131.27	120.10
1	A	314	ARG	NE-CZ-NH1	9.27	124.94	120.30
1	B	386	HIS	CG-ND1-CE1	9.25	121.14	108.20
1	C	109	ARG	NE-CZ-NH2	-8.97	115.81	120.30
1	C	307	ARG	NE-CZ-NH1	8.63	124.62	120.30
1	B	91	GLN	CG-CD-OE1	-8.49	104.61	121.60
1	B	277	GLU	CG-CD-OE1	8.46	135.23	118.30
1	D	76	TYR	CD1-CG-CD2	8.29	127.02	117.90
1	A	288	ARG	NE-CZ-NH2	7.99	124.29	120.30
1	C	221	ARG	CG-CD-NE	-7.89	95.22	111.80
1	A	403	ARG	NE-CZ-NH2	-7.86	116.37	120.30
1	B	189	SER	CA-C-N	7.83	134.42	117.20
1	A	19	ARG	CG-CD-NE	7.79	128.17	111.80
1	B	386	HIS	CA-CB-CG	7.60	126.52	113.60
1	D	29	ARG	NE-CZ-NH1	7.59	124.09	120.30
1	C	221	ARG	CB-CG-CD	7.47	131.01	111.60
1	D	234	PRO	N-CA-CB	-7.46	94.35	103.30
1	D	148	ALA	O-C-N	7.40	134.54	122.70
1	D	354	ARG	NE-CZ-NH2	7.39	124.00	120.30
1	C	344	ARG	NE-CZ-NH2	7.38	123.99	120.30
1	D	233	PHE	CD1-CG-CD2	-7.31	108.80	118.30
1	A	314	ARG	NE-CZ-NH2	-7.29	116.66	120.30
1	B	201	GLU	CB-CA-C	-7.25	95.91	110.40
1	D	263	ARG	CD-NE-CZ	7.08	133.50	123.60
1	B	386	HIS	ND1-CG-CD2	-7.05	96.13	106.00
1	A	165	ARG	NE-CZ-NH2	-6.99	116.81	120.30
1	D	234	PRO	CA-CB-CG	6.93	117.96	104.80
1	A	84	ARG	NE-CZ-NH1	6.88	123.74	120.30
1	B	344	ARG	NE-CZ-NH2	6.88	123.74	120.30
1	A	220	GLU	CA-CB-CG	6.80	128.36	113.40
1	B	424	LEU	CA-CB-CG	6.76	130.85	115.30
1	C	263	ARG	NE-CZ-NH2	-6.75	116.92	120.30
1	B	189	SER	C-N-CA	6.68	138.40	121.70
1	A	329	ARG	NE-CZ-NH1	6.58	123.59	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	19	ARG	CG-CD-NE	6.58	125.61	111.80
1	B	178	ARG	CA-C-N	6.53	131.56	117.20
1	A	413	ASP	CB-CG-OD1	6.51	124.16	118.30
1	A	363	ARG	NE-CZ-NH1	6.51	123.55	120.30
1	D	329	ARG	NE-CZ-NH2	-6.48	117.06	120.30
1	D	149	ARG	C-N-CD	-6.46	106.38	120.60
1	A	109	ARG	NE-CZ-NH2	-6.46	117.07	120.30
1	C	96	THR	O-C-N	-6.43	112.27	123.20
1	A	334	ARG	NE-CZ-NH1	6.42	123.51	120.30
1	C	460	ARG	NE-CZ-NH2	-6.42	117.09	120.30
1	A	266	GLU	CB-CA-C	-6.38	97.65	110.40
1	A	265	ASP	N-CA-CB	6.34	122.02	110.60
1	B	329	ARG	NE-CZ-NH1	6.29	123.44	120.30
1	C	339	ARG	NE-CZ-NH1	6.28	123.44	120.30
1	B	84	ARG	NE-CZ-NH2	-6.21	117.19	120.30
1	B	134	GLU	CB-CA-C	6.09	122.58	110.40
1	D	354	ARG	CG-CD-NE	-6.08	99.03	111.80
1	B	277	GLU	OE1-CD-OE2	-6.05	116.03	123.30
1	A	403	ARG	NE-CZ-NH1	6.02	123.31	120.30
1	B	165	ARG	CB-CA-C	6.01	122.42	110.40
1	D	339	ARG	NE-CZ-NH1	6.01	123.31	120.30
1	D	109	ARG	NE-CZ-NH2	-5.96	117.32	120.30
1	D	263	ARG	CG-CD-NE	5.92	124.23	111.80
1	A	103	LEU	CA-CB-CG	5.89	128.84	115.30
1	A	222	LEU	CA-CB-CG	5.88	128.83	115.30
1	C	177	SER	C-N-CA	5.88	136.40	121.70
1	C	178	ARG	N-CA-C	5.86	126.81	111.00
1	B	283	ARG	NE-CZ-NH2	-5.78	117.41	120.30
1	A	383	ARG	NE-CZ-NH1	5.76	123.18	120.30
1	B	351	ARG	NE-CZ-NH1	-5.72	117.44	120.30
1	D	265	ASP	N-CA-CB	5.66	120.78	110.60
1	C	403	ARG	CB-CG-CD	-5.64	96.92	111.60
1	C	122	ASP	CB-CG-OD1	5.62	123.36	118.30
1	D	233	PHE	CG-CD1-CE1	5.60	126.96	120.80
1	A	466	GLU	CA-CB-CG	5.59	125.69	113.40
1	A	165	ARG	NE-CZ-NH1	5.56	123.08	120.30
1	B	232	ARG	CA-CB-CG	5.56	125.62	113.40
1	B	222	LEU	CA-CB-CG	5.46	127.85	115.30
1	A	465	ARG	CA-CB-CG	-5.42	101.47	113.40
1	B	277	GLU	CB-CG-CD	-5.42	99.58	114.20
1	A	149	ARG	CD-NE-CZ	-5.39	116.06	123.60
1	D	148	ALA	CA-C-N	-5.37	105.38	117.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	339	ARG	NE-CZ-NH2	-5.37	117.62	120.30
1	A	265	ASP	N-CA-C	5.36	125.47	111.00
1	B	86	LEU	CA-CB-CG	5.34	127.59	115.30
1	C	334	ARG	NE-CZ-NH1	5.33	122.96	120.30
1	B	307	ARG	NE-CZ-NH1	5.31	122.96	120.30
1	D	265	ASP	CB-CA-C	-5.29	99.83	110.40
1	C	424	LEU	CB-CG-CD1	5.28	119.98	111.00
1	C	395	ARG	CD-NE-CZ	-5.28	116.22	123.60
1	A	149	ARG	NE-CZ-NH1	-5.27	117.66	120.30
1	A	86	LEU	CB-CG-CD1	5.24	119.91	111.00
1	B	201	GLU	CB-CG-CD	-5.23	100.08	114.20
1	D	424	LEU	CA-CB-CG	5.16	127.18	115.30
1	B	363	ARG	NE-CZ-NH1	-5.16	117.72	120.30
1	B	428	LEU	CB-CG-CD1	5.16	119.77	111.00
1	B	277	GLU	CG-CD-OE2	-5.15	108.00	118.30
1	D	129	ARG	CD-NE-CZ	-5.15	116.39	123.60
1	B	165	ARG	CD-NE-CZ	5.14	130.79	123.60
1	B	354	ARG	CD-NE-CZ	5.14	130.79	123.60
1	D	329	ARG	NE-CZ-NH1	5.14	122.87	120.30
1	D	424	LEU	CB-CG-CD1	5.12	119.70	111.00
1	D	234	PRO	CB-CA-C	-5.11	99.23	112.00
1	B	217	HIS	CA-CB-CG	5.09	122.26	113.60
1	C	29	ARG	NE-CZ-NH1	5.08	122.84	120.30
1	B	263	ARG	CA-CB-CG	5.01	124.42	113.40
1	B	133	PRO	O-C-N	-5.01	114.68	122.70

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
1	A	265	ASP	CA

All (8) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	19	ARG	Sidechain
1	A	217	HIS	Sidechain
1	B	189	SER	Mainchain,Peptide
1	B	19	ARG	Sidechain
1	B	386	HIS	Sidechain
1	D	264	GLU	Mainchain
1	D	76	TYR	Sidechain

## 5.2 Too-close contacts ⓘ

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3502	0	3479	36	0
1	B	3502	0	3479	51	0
1	C	3502	0	3479	48	0
1	D	3476	0	3455	40	0
2	A	8	0	0	0	0
2	B	8	0	0	0	0
2	C	8	0	0	0	0
2	D	8	0	0	0	0
3	A	298	0	0	8	0
3	B	184	0	0	11	0
3	C	285	0	0	11	0
3	D	217	0	0	4	0
All	All	14998	0	13892	173	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 6.

All (173) 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:C:275:HIS:CE1	1:C:363:ARG:HH21	1.42	1.36
1:B:0:ALA:HB1	1:B:268:GLY:H	1.14	1.05
1:C:275:HIS:CE1	1:C:363:ARG:NH2	2.25	1.04
1:C:275:HIS:HE1	1:C:363:ARG:HH21	0.99	0.96
1:A:329:ARG:NH2	3:A:2183:HOH:O	1.97	0.95
1:D:329:ARG:NH2	3:D:2139:HOH:O	2.00	0.94
1:C:329:ARG:NH2	3:C:2199:HOH:O	2.06	0.89
1:B:178:ARG:O	1:B:179:GLU:HB3	1.72	0.88
1:B:0:ALA:HB1	1:B:268:GLY:N	1.90	0.86
1:D:283:ARG:O	1:D:287:GLU:HG3	1.79	0.83
1:C:195:GLU:OE2	3:C:2125:HOH:O	2.00	0.80
1:B:97:GLY:O	1:B:109:ARG:HD2	1.83	0.79
1:C:275:HIS:ND1	1:C:363:ARG:NH2	2.32	0.78
1:B:329:ARG:NH2	3:B:2101:HOH:O	2.17	0.76
1:B:51:PRO:HG3	3:B:2127:HOH:O	1.88	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:283:ARG:O	1:C:287:GLU:HG3	1.91	0.70
1:D:403:ARG:HG3	3:D:2183:HOH:O	1.92	0.69
1:C:220:GLU:OE1	3:C:2133:HOH:O	2.10	0.69
1:B:275:HIS:HE1	1:B:363:ARG:CZ	2.06	0.68
1:A:165:ARG:HG3	3:A:2106:HOH:O	1.92	0.67
1:C:270:ASP:OD1	3:C:2150:HOH:O	2.13	0.66
1:C:305:GLU:OE1	1:C:354:ARG:HD2	1.95	0.65
1:C:117:HIS:HE1	1:C:261:GLU:OE2	1.79	0.65
1:C:115:GLY:O	1:C:158:HIS:HE1	1.80	0.64
1:A:115:GLY:O	1:A:158:HIS:HE1	1.81	0.64
1:C:284:HIS:CE1	1:C:288:ARG:HH21	2.15	0.64
1:C:117:HIS:CD2	1:C:119:GLY:H	2.14	0.64
1:A:248:HIS:O	1:A:251:VAL:HG22	1.97	0.63
1:C:117:HIS:HD2	1:C:119:GLY:H	1.47	0.63
1:D:31:ARG:NH2	1:D:253:GLU:OE2	2.32	0.63
1:D:222:LEU:O	1:D:222:LEU:HD12	1.99	0.62
1:A:109:ARG:NH2	1:A:261:GLU:O	2.32	0.62
1:B:36:HIS:NE2	3:B:2013:HOH:O	2.20	0.62
1:B:178:ARG:O	1:B:179:GLU:CB	2.34	0.62
1:D:222:LEU:C	1:D:222:LEU:HD12	2.20	0.62
1:B:129:ARG:CD	1:B:167:GLN:OE1	2.48	0.62
1:A:383:ARG:HD3	3:A:2227:HOH:O	2.00	0.61
1:C:275:HIS:HE1	1:C:363:ARG:NH2	1.82	0.61
1:C:284:HIS:CE1	1:C:288:ARG:NH2	2.69	0.60
1:D:297:LEU:HD12	1:D:306:LEU:HG	1.83	0.60
1:A:0:ALA:HB1	1:A:267:ARG:O	2.01	0.60
1:A:117:HIS:CD2	1:A:119:GLY:H	2.20	0.60
1:B:0:ALA:CB	1:B:268:GLY:H	2.03	0.60
1:C:295:VAL:HG21	1:C:369:LEU:HD21	1.85	0.59
1:A:9:HIS:HD2	1:A:10:GLY:O	1.85	0.59
1:A:204:GLN:HE21	1:A:238:PRO:HG2	1.68	0.58
1:C:160:GLN:O	1:C:164:GLU:HG3	2.04	0.58
1:D:125:ALA:HB1	1:D:129:ARG:HH21	1.69	0.57
1:A:386:HIS:CE1	3:A:2235:HOH:O	2.58	0.57
1:A:292:LEU:HD22	1:A:438:ILE:HD12	1.87	0.56
1:D:133:PRO:O	1:D:134:GLU:C	2.40	0.56
1:B:277:GLU:OE1	1:B:277:GLU:CG	2.53	0.56
1:B:129:ARG:HD3	1:B:167:GLN:OE1	2.04	0.56
1:C:334:ARG:NE	3:C:2201:HOH:O	2.25	0.56
1:B:295:VAL:HG21	1:B:369:LEU:HD21	1.88	0.56
1:D:231:GLU:O	1:D:234:PRO:HD3	2.06	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:196:TRP:CG	1:D:197:PRO:HD3	2.40	0.55
1:B:57:LEU:O	1:B:60:VAL:HG22	2.07	0.55
1:B:20:ALA:O	1:B:24:VAL:HG23	2.07	0.55
1:C:382:HIS:C	1:C:383:ARG:HG2	2.25	0.54
1:C:209:PRO:HB3	1:C:211:LEU:HD22	1.89	0.54
1:B:129:ARG:HD2	1:B:167:GLN:OE1	2.08	0.54
1:B:65:VAL:HG13	1:B:108:VAL:HG22	1.90	0.54
1:B:248:HIS:O	1:B:251:VAL:HG22	2.08	0.54
1:C:65:VAL:CG1	1:C:108:VAL:HG22	2.37	0.54
1:C:248:HIS:O	1:C:251:VAL:HG22	2.07	0.54
1:D:387:TRP:CE3	1:D:429:TRP:HA	2.44	0.53
1:D:0:ALA:HA	1:D:268:GLY:HA3	1.90	0.53
1:D:109:ARG:HD2	3:D:2090:HOH:O	2.09	0.53
1:D:76:TYR:CZ	1:D:80:THR:HG21	2.44	0.53
1:C:9:HIS:HD2	1:C:10:GLY:O	1.91	0.53
1:B:400:THR:O	1:B:403:ARG:HB2	2.09	0.52
1:B:306:LEU:HD12	1:B:306:LEU:N	2.25	0.52
1:A:90:HIS:ND1	3:A:2064:HOH:O	2.34	0.51
1:A:260:ALA:O	1:A:263:ARG:HG2	2.10	0.51
1:B:109:ARG:NH1	3:B:2041:HOH:O	2.44	0.51
1:C:96:THR:HA	1:C:112:ARG:HD3	1.92	0.51
1:A:172:GLU:HG3	1:A:199:ARG:HB3	1.93	0.51
1:B:193:LEU:O	1:B:196:TRP:HB3	2.10	0.51
1:B:82:LEU:HB2	1:B:83:PRO:HD3	1.92	0.51
1:B:21:THR:OG1	3:B:2010:HOH:O	2.19	0.51
1:A:295:VAL:HG21	1:A:369:LEU:HD21	1.93	0.50
1:A:12:HIS:HE1	1:A:453:THR:OG1	1.94	0.50
1:B:275:HIS:CE1	1:B:363:ARG:CZ	2.93	0.50
1:B:94:VAL:O	3:B:2037:HOH:O	2.19	0.49
1:B:363:ARG:HD3	3:B:2062:HOH:O	2.13	0.49
1:C:263:ARG:HD2	1:C:266:GLU:OE2	2.12	0.49
1:B:264:GLU:HG3	3:B:2041:HOH:O	2.11	0.49
1:B:381:GLU:OE2	1:B:440:SER:OG	2.31	0.49
1:D:117:HIS:CD2	1:D:119:GLY:H	2.30	0.49
1:D:158:HIS:HD2	3:D:2065:HOH:O	1.95	0.49
1:C:146:LEU:HB3	1:C:209:PRO:HA	1.94	0.49
1:B:401:LEU:O	1:B:404:VAL:HG22	2.12	0.49
1:A:60:VAL:HG22	1:A:106:ARG:NE	2.27	0.48
1:B:114:LEU:HA	1:B:258:LEU:CD1	2.43	0.48
1:B:284:HIS:ND1	1:B:288:ARG:NH2	2.61	0.48
1:A:395:ARG:NH1	1:D:23:GLN:OE1	2.47	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:115:GLY:O	1:B:158:HIS:HE1	1.96	0.48
1:D:12:HIS:HE1	1:D:453:THR:OG1	1.96	0.48
1:A:162:LEU:HA	1:A:165:ARG:HD2	1.96	0.48
1:C:102:VAL:HG13	3:C:2076:HOH:O	2.13	0.47
1:D:146:LEU:HB3	1:D:209:PRO:HA	1.95	0.47
1:A:386:HIS:HE1	3:A:2235:HOH:O	1.96	0.47
1:A:177:SER:OG	1:A:221:ARG:NH2	2.47	0.47
1:A:146:LEU:HB3	1:A:209:PRO:HA	1.96	0.47
1:C:115:GLY:O	1:C:158:HIS:CE1	2.66	0.47
1:D:193:LEU:HD21	1:D:222:LEU:HD13	1.97	0.47
1:B:285:LEU:C	1:B:285:LEU:HD23	2.35	0.47
1:A:149:ARG:HB3	1:A:150:PRO:HD2	1.97	0.47
1:B:403:ARG:HG3	1:B:463:VAL:HG11	1.97	0.46
1:B:114:LEU:HA	1:B:258:LEU:HD11	1.95	0.46
1:A:209:PRO:HB3	1:A:211:LEU:HD22	1.97	0.46
1:C:65:VAL:HG13	1:C:108:VAL:HA	1.96	0.46
1:D:138:PRO:HB2	1:D:167:GLN:O	2.15	0.46
1:D:232:ARG:C	1:D:233:PHE:CD2	2.88	0.46
1:D:397:GLN:HB3	1:D:401:LEU:HB3	1.97	0.46
1:D:103:LEU:N	1:D:103:LEU:HD23	2.30	0.46
1:A:149:ARG:CB	1:A:150:PRO:HD2	2.46	0.46
1:B:222:LEU:O	1:B:222:LEU:HD12	2.16	0.46
1:C:300:TYR:HB2	3:C:2168:HOH:O	2.15	0.46
1:D:109:ARG:NH2	1:D:261:GLU:O	2.49	0.46
1:A:403:ARG:HG2	3:A:2296:HOH:O	2.16	0.46
1:C:271:ILE:HD13	1:C:276:ALA:HB2	1.98	0.45
1:D:115:GLY:O	1:D:158:HIS:HE1	1.99	0.45
1:C:106:ARG:HG2	3:C:2077:HOH:O	2.15	0.45
1:D:401:LEU:O	1:D:404:VAL:HG22	2.17	0.45
1:C:97:GLY:HA2	1:C:262:GLY:HA3	1.98	0.45
1:A:117:HIS:HD2	1:A:119:GLY:H	1.62	0.45
1:B:201:GLU:OE1	1:B:201:GLU:N	2.50	0.45
1:B:28:LEU:HD23	1:B:31:ARG:HD2	1.98	0.45
1:C:382:HIS:C	1:C:383:ARG:CG	2.85	0.45
1:D:137:ASP:HA	1:D:138:PRO:HD3	1.83	0.44
1:D:231:GLU:O	1:D:233:PHE:N	2.51	0.44
1:A:376:GLU:OE2	3:A:2224:HOH:O	2.21	0.44
1:B:160:GLN:O	1:B:164:GLU:HG3	2.18	0.44
1:D:271:ILE:HD13	1:D:276:ALA:HB2	1.99	0.43
1:C:387:TRP:CE3	1:C:429:TRP:HA	2.53	0.43
1:A:196:TRP:CG	1:A:197:PRO:HD3	2.53	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:19:ARG:HG2	1:D:23:GLN:NE2	2.33	0.43
1:B:137:ASP:OD1	1:B:137:ASP:C	2.57	0.43
1:C:306:LEU:HD12	1:C:306:LEU:N	2.34	0.43
1:B:427:ARG:HG3	1:B:430:ALA:HB3	2.01	0.42
1:B:136:THR:HG22	1:B:137:ASP:N	2.35	0.42
1:D:82:LEU:HB2	1:D:83:PRO:HD3	2.01	0.42
1:C:103:LEU:O	1:C:106:ARG:HB2	2.20	0.42
1:A:33:LEU:C	1:A:35:GLY:H	2.23	0.42
1:D:125:ALA:HB1	1:D:129:ARG:NH2	2.33	0.42
1:A:60:VAL:CG2	1:A:106:ARG:NE	2.82	0.42
1:A:211:LEU:HD23	1:A:214:LEU:HD13	2.00	0.42
1:C:102:VAL:CG1	3:C:2076:HOH:O	2.67	0.42
1:D:285:LEU:C	1:D:285:LEU:HD23	2.40	0.42
1:C:300:TYR:CB	3:C:2168:HOH:O	2.66	0.42
1:D:20:ALA:O	1:D:24:VAL:HG23	2.20	0.42
1:C:136:THR:O	1:C:138:PRO:HD3	2.19	0.42
1:A:262:GLY:O	1:A:264:GLU:N	2.53	0.42
1:C:282:LEU:HD13	1:C:282:LEU:C	2.40	0.41
1:D:51:PRO:HB3	1:D:371:PRO:HB3	2.02	0.41
1:B:196:TRP:CZ3	1:B:200:VAL:HG21	2.55	0.41
1:B:23:GLN:OE1	3:B:2011:HOH:O	2.22	0.41
1:C:60:VAL:HG23	1:C:106:ARG:NE	2.36	0.41
1:A:401:LEU:O	1:A:404:VAL:HG22	2.21	0.41
1:D:231:GLU:C	1:D:233:PHE:N	2.74	0.41
1:B:133:PRO:O	1:B:134:GLU:C	2.57	0.41
1:C:190:ALA:HA	3:C:2122:HOH:O	2.20	0.41
1:B:19:ARG:NH2	3:B:2009:HOH:O	2.53	0.41
1:B:9:HIS:HD2	1:B:10:GLY:O	2.04	0.41
1:D:271:ILE:CD1	1:D:276:ALA:HB2	2.50	0.41
1:B:76:TYR:CD2	1:C:134:GLU:HB3	2.56	0.41
1:A:222:LEU:HD12	1:A:222:LEU:C	2.42	0.41
1:C:406:ARG:H	1:C:406:ARG:HG2	1.71	0.41
1:D:174:VAL:HG12	1:D:191:VAL:HG23	2.02	0.40
1:C:114:LEU:HA	1:C:258:LEU:HD11	2.03	0.40
1:B:453:THR:HG22	3:B:2020:HOH:O	2.21	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	455/474 (96%)	438 (96%)	17 (4%)	0	100	100
1	B	455/474 (96%)	431 (95%)	19 (4%)	5 (1%)	17	6
1	C	455/474 (96%)	436 (96%)	17 (4%)	2 (0%)	39	27
1	D	452/474 (95%)	425 (94%)	24 (5%)	3 (1%)	26	14
All	All	1817/1896 (96%)	1730 (95%)	77 (4%)	10 (1%)	30	17

All (10) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	178	ARG
1	B	190	ALA
1	C	178	ARG
1	B	119	GLY
1	B	135	GLY
1	B	261	GLU
1	C	177	SER
1	D	266	GLU
1	D	232	ARG
1	D	265	ASP

### 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	351/360 (98%)	327 (93%)	24 (7%)	20	9

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	B	351/360 (98%)	330 (94%)	21 (6%)	24	12
1	C	351/360 (98%)	328 (93%)	23 (7%)	21	10
1	D	348/360 (97%)	327 (94%)	21 (6%)	24	12
All	All	1401/1440 (97%)	1312 (94%)	89 (6%)	22	10

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

Mol	Chain	Res	Type
1	A	17	SER
1	A	19	ARG
1	A	58	ARG
1	A	86	LEU
1	A	93	PRO
1	A	103	LEU
1	A	109	ARG
1	A	143	LEU
1	A	144	LEU
1	A	164	GLU
1	A	178	ARG
1	A	179	GLU
1	A	211	LEU
1	A	222	LEU
1	A	224	GLN
1	A	263	ARG
1	A	287	GLU
1	A	331	LEU
1	A	363	ARG
1	A	366	LEU
1	A	391	MET
1	A	403	ARG
1	A	424	LEU
1	A	428	LEU
1	B	17	SER
1	B	19	ARG
1	B	56	VAL
1	B	58	ARG
1	B	65	VAL
1	B	86	LEU
1	B	134	GLU
1	B	143	LEU
1	B	144	LEU

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Mol	Chain	Res	Type
1	B	177	SER
1	B	201	GLU
1	B	211	LEU
1	B	222	LEU
1	B	224	GLN
1	B	331	LEU
1	B	366	LEU
1	B	391	MET
1	B	403	ARG
1	B	424	LEU
1	B	428	LEU
1	B	440	SER
1	C	17	SER
1	C	86	LEU
1	C	91	GLN
1	C	122	ASP
1	C	143	LEU
1	C	144	LEU
1	C	175	LEU
1	C	189	SER
1	C	191	VAL
1	C	211	LEU
1	C	247	GLU
1	C	267	ARG
1	C	270	ASP
1	C	271	ILE
1	C	331	LEU
1	C	367	GLU
1	C	374	ILE
1	C	383	ARG
1	C	401	LEU
1	C	403	ARG
1	C	406	ARG
1	C	424	LEU
1	C	428	LEU
1	D	17	SER
1	D	31	ARG
1	D	86	LEU
1	D	103	LEU
1	D	107	ARG
1	D	143	LEU
1	D	164	GLU

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Mol	Chain	Res	Type
1	D	177	SER
1	D	195	GLU
1	D	201	GLU
1	D	222	LEU
1	D	231	GLU
1	D	232	ARG
1	D	264	GLU
1	D	265	ASP
1	D	267	ARG
1	D	271	ILE
1	D	366	LEU
1	D	374	ILE
1	D	424	LEU
1	D	428	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (25) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	9	HIS
1	A	12	HIS
1	A	36	HIS
1	A	117	HIS
1	A	127	GLN
1	A	158	HIS
1	A	204	GLN
1	A	397	GLN
1	B	9	HIS
1	B	12	HIS
1	B	117	HIS
1	B	158	HIS
1	B	160	GLN
1	B	275	HIS
1	B	397	GLN
1	C	9	HIS
1	C	12	HIS
1	C	117	HIS
1	C	158	HIS
1	C	397	GLN
1	D	9	HIS
1	D	12	HIS
1	D	117	HIS
1	D	204	GLN

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Mol	Chain	Res	Type
1	D	397	GLN

### 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](#)

4 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	SF4	A	650	1	0,12,12	0.00	-	0,24,24	0.00	-
2	SF4	B	650	1	0,12,12	0.00	-	0,24,24	0.00	-
2	SF4	C	650	1	0,12,12	0.00	-	0,24,24	0.00	-
2	SF4	D	650	1	0,12,12	0.00	-	0,24,24	0.00	-

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	SF4	A	650	1	-	0/0/48/48	0/6/5/5

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	SF4	B	650	1	-	0/0/48/48	0/6/5/5
2	SF4	C	650	1	-	0/0/48/48	0/6/5/5
2	SF4	D	650	1	-	0/0/48/48	0/6/5/5

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.

No monomer is involved in short contacts.

## 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 ⓘ

### 6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95<sup>th</sup> percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
1	A	459/474 (96%)	0.18	27 (5%) 26 29	15, 30, 52, 62	25 (5%)
1	B	458/474 (96%)	0.64	64 (13%) 4 4	19, 39, 74, 105	33 (7%)
1	C	456/474 (96%)	0.18	21 (4%) 36 39	15, 29, 48, 67	26 (5%)
1	D	456/474 (96%)	0.51	55 (12%) 6 6	19, 37, 65, 75	36 (7%)
All	All	1829/1896 (96%)	0.38	167 (9%) 11 13	15, 33, 63, 105	120 (6%)

All (167) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	105	GLY	9.8
1	A	33	LEU	8.9
1	B	179	GLU	8.0
1	B	264	GLU	7.9
1	A	-1	GLY	6.7
1	D	177	SER	6.0
1	A	34	ALA	5.9
1	C	33	LEU	5.7
1	D	-1	GLY	5.7
1	B	266	GLU	5.6
1	B	104	GLY	5.6
1	C	104	GLY	5.4
1	B	466	GLU	5.4
1	B	144	LEU	5.4
1	D	230	ALA	5.4
1	B	151	GLY	5.4
1	D	200	VAL	5.3
1	D	34	ALA	5.2
1	B	234	PRO	5.1
1	B	-1	GLY	5.0
1	B	36	HIS	5.0

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Mol	Chain	Res	Type	RSRZ
1	A	189	SER	4.7
1	B	34	ALA	4.7
1	B	236	ALA	4.7
1	D	33	LEU	4.7
1	D	135	GLY	4.6
1	B	153	ALA	4.6
1	C	-1	GLY	4.6
1	B	33	LEU	4.5
1	D	266	GLU	4.5
1	C	34	ALA	4.5
1	D	267	ARG	4.4
1	A	36	HIS	4.4
1	A	134	GLU	4.4
1	B	143	LEU	4.4
1	D	202	ALA	4.3
1	A	35	GLY	4.3
1	D	217	HIS	4.2
1	B	267	ARG	4.2
1	D	201	GLU	4.2
1	C	36	HIS	4.1
1	D	36	HIS	4.1
1	B	268	GLY	4.1
1	C	465	ARG	4.0
1	B	229	ALA	4.0
1	D	105	GLY	4.0
1	A	190	ALA	4.0
1	A	264	GLU	4.0
1	A	136	THR	3.9
1	D	300	TYR	3.9
1	B	221	ARG	3.8
1	D	234	PRO	3.8
1	D	137	ASP	3.7
1	D	466	GLU	3.7
1	D	190	ALA	3.7
1	B	465	ARG	3.6
1	B	145	LEU	3.6
1	B	150	PRO	3.6
1	A	179	GLU	3.5
1	B	228	GLN	3.5
1	D	76	TYR	3.5
1	D	465	ARG	3.5
1	A	144	LEU	3.4

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Mol	Chain	Res	Type	RSRZ
1	D	151	GLY	3.4
1	B	208	VAL	3.4
1	B	149	ARG	3.4
1	D	140	ASP	3.4
1	B	207	LEU	3.3
1	C	102	VAL	3.3
1	C	466	GLU	3.3
1	D	265	ASP	3.3
1	B	132	LEU	3.3
1	D	264	GLU	3.2
1	A	208	VAL	3.2
1	D	144	LEU	3.2
1	A	140	ASP	3.1
1	C	464	GLY	3.1
1	A	145	LEU	3.1
1	D	207	LEU	3.1
1	A	133	PRO	3.1
1	B	263	ARG	3.1
1	C	0	ALA	3.1
1	B	220	GLU	3.1
1	B	218	ALA	3.1
1	D	238	PRO	3.1
1	D	206	VAL	3.1
1	C	103	LEU	3.1
1	B	146	LEU	3.0
1	D	134	GLU	3.0
1	A	263	ARG	3.0
1	B	215	GLY	3.0
1	C	217	HIS	3.0
1	B	230	ALA	3.0
1	A	151	GLY	3.0
1	D	229	ALA	3.0
1	A	178	ARG	2.9
1	D	400	THR	2.9
1	B	140	ASP	2.9
1	A	150	PRO	2.9
1	B	169	ALA	2.9
1	D	464	GLY	2.9
1	D	273	GLN	2.8
1	B	194	SER	2.8
1	A	465	ARG	2.8
1	B	235	GLN	2.8

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Mol	Chain	Res	Type	RSRZ
1	D	153	ALA	2.8
1	A	267	ARG	2.8
1	B	198	SER	2.8
1	C	134	GLU	2.8
1	D	164	GLU	2.8
1	B	233	PHE	2.8
1	D	103	LEU	2.7
1	A	206	VAL	2.7
1	D	68	VAL	2.7
1	D	235	GLN	2.7
1	B	0	ALA	2.7
1	B	103	LEU	2.7
1	C	35	GLY	2.7
1	D	133	PRO	2.6
1	B	464	GLY	2.6
1	C	208	VAL	2.6
1	B	105	GLY	2.6
1	B	135	GLY	2.5
1	B	240	HIS	2.5
1	D	171	VAL	2.5
1	B	238	PRO	2.5
1	A	177	SER	2.5
1	D	228	GLN	2.5
1	B	201	GLU	2.5
1	D	227	ALA	2.5
1	D	93	PRO	2.5
1	B	177	SER	2.4
1	B	136	THR	2.4
1	B	178	ARG	2.4
1	D	67	VAL	2.4
1	A	0	ALA	2.4
1	B	400	THR	2.4
1	A	207	LEU	2.4
1	B	165	ARG	2.4
1	D	233	PHE	2.3
1	C	431	GLY	2.3
1	D	191	VAL	2.3
1	B	232	ARG	2.3
1	B	265	ASP	2.3
1	C	300	TYR	2.3
1	C	133	PRO	2.2
1	B	219	ALA	2.2

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Mol	Chain	Res	Type	RSRZ
1	B	225	ALA	2.2
1	D	148	ALA	2.2
1	B	93	PRO	2.2
1	D	143	LEU	2.2
1	B	162	LEU	2.2
1	D	32	GLY	2.1
1	B	76	TYR	2.1
1	B	35	GLY	2.1
1	C	151	GLY	2.1
1	B	102	VAL	2.1
1	B	191	VAL	2.1
1	D	111	THR	2.1
1	D	0	ALA	2.1
1	D	236	ALA	2.1
1	B	174	VAL	2.1
1	A	146	LEU	2.0
1	D	208	VAL	2.0
1	B	152	ASN	2.0
1	C	267	ARG	2.0
1	D	136	THR	2.0

## 6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

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

## 6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
2	SF4	A	650	8/8	1.00	0.10	-0.12	16,17,19,19	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
2	SF4	C	650	8/8	1.00	0.10	-0.23	17,18,21,21	0
2	SF4	B	650	8/8	1.00	0.09	-0.35	19,20,21,21	0
2	SF4	D	650	8/8	1.00	0.08	-0.41	20,21,23,23	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.