



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 10, 2026 – 10:17 AM UTC

PDB ID : 3CZ5 / pdb_00003cz5
Title : Crystal structure of two-component response regulator, LuxR family, from Aurantimonas sp. SI85-9A1
Authors : Malashkevich, V.N.; Toro, R.; Wasserman, S.R.; Meyer, A.; Sauder, J.M.; Burley, S.K.; Almo, S.C.; New York SGX Research Center for Structural Genomics (NYSGXRC)
Deposited on : 2008-04-28
Resolution : 2.70 Å (reported)

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A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

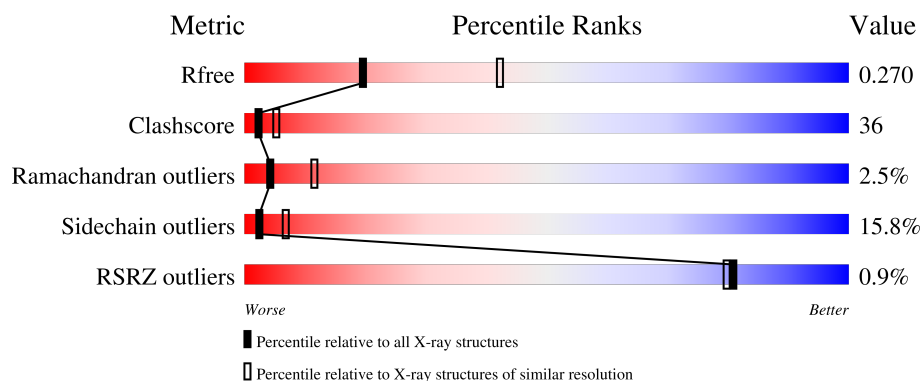
1 Overall quality at a glance

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))
R_{free}	180053	3538 (2.70-2.70)
Clashscore	190562	3843 (2.70-2.70)
Ramachandran outliers	187476	3778 (2.70-2.70)
Sidechain outliers	187428	3778 (2.70-2.70)
RSRZ outliers	180081	3538 (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 of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. 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	153	
1	B	153	
1	C	153	
1	D	153	

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 4431 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 Two-component response regulator, LuxR family.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	141	Total	C	N	O	S	0	0	0
			1081	676	196	205	4			
1	B	140	Total	C	N	O	S	0	0	0
			1077	674	195	204	4			
1	C	142	Total	C	N	O	S	0	0	0
			1092	682	200	206	4			
1	D	142	Total	C	N	O	S	0	0	0
			1092	682	200	206	4			

There are 44 discrepancies between the modelled and reference sequences:

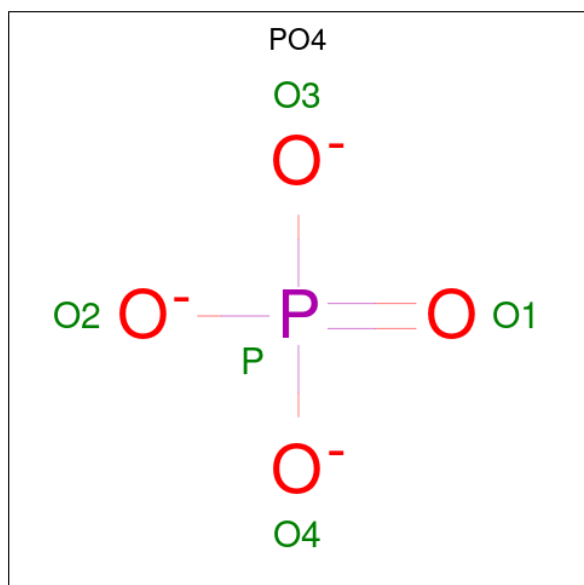
Chain	Residue	Modelled	Actual	Comment	Reference
A	1	MET	-	expression tag	UNP Q1YEP2
A	2	SER	-	expression tag	UNP Q1YEP2
A	3	LEU	-	expression tag	UNP Q1YEP2
A	146	GLU	-	expression tag	UNP Q1YEP2
A	147	GLY	-	expression tag	UNP Q1YEP2
A	148	HIS	-	expression tag	UNP Q1YEP2
A	149	HIS	-	expression tag	UNP Q1YEP2
A	150	HIS	-	expression tag	UNP Q1YEP2
A	151	HIS	-	expression tag	UNP Q1YEP2
A	152	HIS	-	expression tag	UNP Q1YEP2
A	153	HIS	-	expression tag	UNP Q1YEP2
B	1	MET	-	expression tag	UNP Q1YEP2
B	2	SER	-	expression tag	UNP Q1YEP2
B	3	LEU	-	expression tag	UNP Q1YEP2
B	146	GLU	-	expression tag	UNP Q1YEP2
B	147	GLY	-	expression tag	UNP Q1YEP2
B	148	HIS	-	expression tag	UNP Q1YEP2
B	149	HIS	-	expression tag	UNP Q1YEP2
B	150	HIS	-	expression tag	UNP Q1YEP2
B	151	HIS	-	expression tag	UNP Q1YEP2
B	152	HIS	-	expression tag	UNP Q1YEP2

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Chain	Residue	Modelled	Actual	Comment	Reference
B	153	HIS	-	expression tag	UNP Q1YEP2
C	1	MET	-	expression tag	UNP Q1YEP2
C	2	SER	-	expression tag	UNP Q1YEP2
C	3	LEU	-	expression tag	UNP Q1YEP2
C	146	GLU	-	expression tag	UNP Q1YEP2
C	147	GLY	-	expression tag	UNP Q1YEP2
C	148	HIS	-	expression tag	UNP Q1YEP2
C	149	HIS	-	expression tag	UNP Q1YEP2
C	150	HIS	-	expression tag	UNP Q1YEP2
C	151	HIS	-	expression tag	UNP Q1YEP2
C	152	HIS	-	expression tag	UNP Q1YEP2
C	153	HIS	-	expression tag	UNP Q1YEP2
D	1	MET	-	expression tag	UNP Q1YEP2
D	2	SER	-	expression tag	UNP Q1YEP2
D	3	LEU	-	expression tag	UNP Q1YEP2
D	146	GLU	-	expression tag	UNP Q1YEP2
D	147	GLY	-	expression tag	UNP Q1YEP2
D	148	HIS	-	expression tag	UNP Q1YEP2
D	149	HIS	-	expression tag	UNP Q1YEP2
D	150	HIS	-	expression tag	UNP Q1YEP2
D	151	HIS	-	expression tag	UNP Q1YEP2
D	152	HIS	-	expression tag	UNP Q1YEP2
D	153	HIS	-	expression tag	UNP Q1YEP2

- Molecule 2 is PHOSPHATE ION (CCD ID: PO4) (formula: O₄P).



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

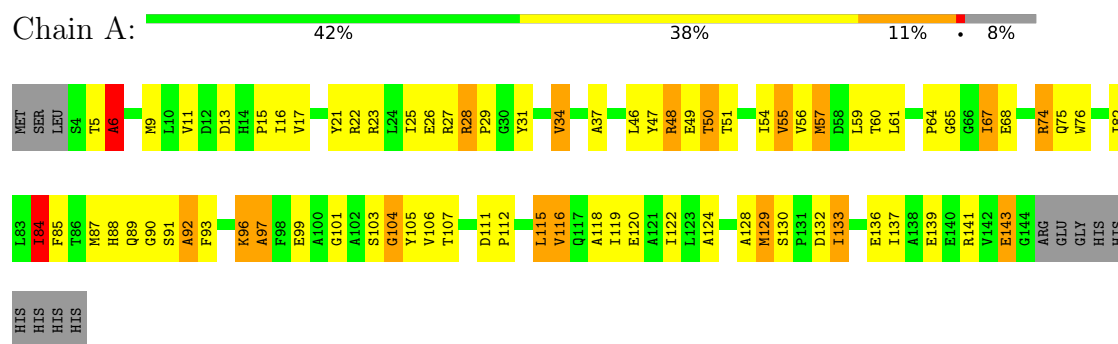
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	17	Total	O	0	0
			17	17		
3	B	25	Total	O	0	0
			25	25		
3	C	11	Total	O	0	0
			11	11		
3	D	16	Total	O	0	0
			16	16		

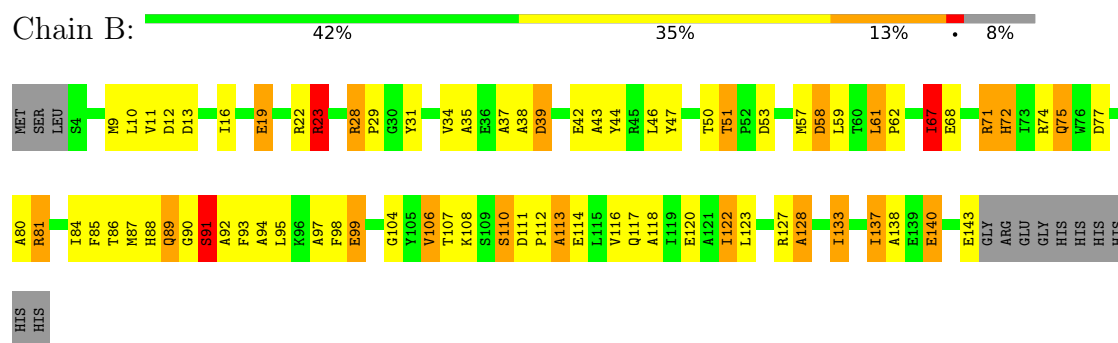
3 Residue-property plots [i](#)

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

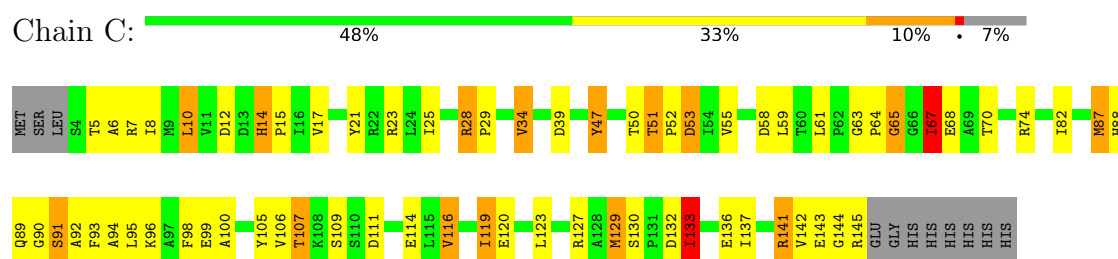
- Molecule 1: Two-component response regulator, LuxR family



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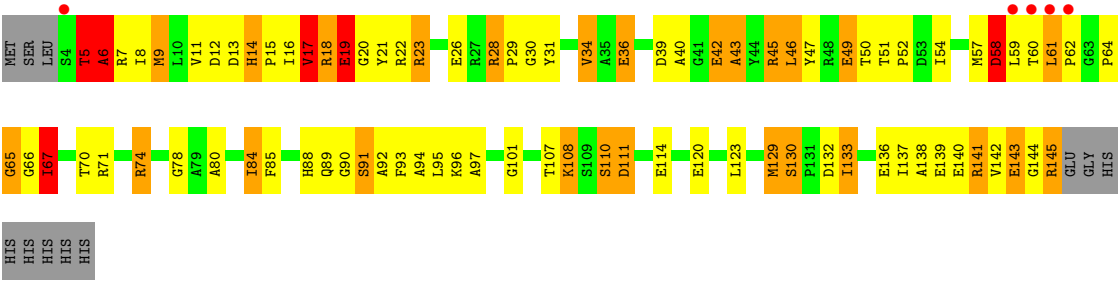


- Molecule 1: Two-component response regulator, LuxR family



- Molecule 1: Two-component response regulator, LuxR family





4 Data and refinement statistics

Property	Value	Source
Space group	P 42 21 2	Depositor
Cell constants a, b, c, α , β , γ	126.61Å 126.61Å 91.68Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	20.00 – 2.70 20.00 – 2.70	Depositor EDS
% Data completeness (in resolution range)	100.0 (20.00-2.70) 93.2 (20.00-2.70)	Depositor EDS
R_{merge}	0.17	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	7.65 (at 2.71Å)	Xtriage
Refinement program	REFMAC	Depositor
R, R_{free}	0.196 , 0.275 0.195 , 0.270	Depositor DCC
R_{free} test set	1018 reflections (5.19%)	wwPDB-VP
Wilson B-factor (Å ²)	48.9	Xtriage
Anisotropy	0.047	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 54.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.46$, $\langle L^2 \rangle = 0.29$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	4431	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 9.41% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 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: 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	1.57	8/1100 (0.7%)	1.67	18/1490 (1.2%)
1	B	1.57	9/1096 (0.8%)	1.67	17/1485 (1.1%)
1	C	1.45	3/1111 (0.3%)	1.64	23/1504 (1.5%)
1	D	1.58	12/1111 (1.1%)	1.59	18/1504 (1.2%)
All	All	1.54	32/4418 (0.7%)	1.64	76/5983 (1.3%)

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	B	0	1
1	D	0	1
All	All	0	2

All (32) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	84	ILE	CA-CB	-7.59	1.45	1.54
1	C	55	VAL	CA-CB	-7.55	1.44	1.54
1	B	122	ILE	CA-CB	-7.45	1.46	1.54
1	A	6	ALA	N-CA	6.97	1.55	1.46
1	A	116	VAL	CA-CB	-6.95	1.46	1.54
1	B	137	ILE	CA-CB	-6.59	1.46	1.54
1	D	19	GLU	CA-C	-6.51	1.44	1.52
1	D	130	SER	CA-C	6.41	1.60	1.52
1	D	43	ALA	CA-C	6.38	1.61	1.52
1	D	94	ALA	CA-CB	-6.36	1.43	1.53
1	B	118	ALA	CA-CB	-6.17	1.43	1.53
1	A	97	ALA	CA-C	-6.16	1.45	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	34	VAL	CA-CB	-5.93	1.47	1.54
1	C	51	THR	C-O	-5.88	1.21	1.23
1	B	35	ALA	CA-CB	-5.87	1.44	1.53
1	D	6	ALA	CA-C	-5.83	1.45	1.52
1	B	58	ASP	CA-C	-5.62	1.45	1.53
1	B	67	ILE	CA-CB	-5.60	1.47	1.54
1	D	71	ARG	CA-C	-5.55	1.45	1.52
1	A	68	GLU	CG-CD	5.54	1.66	1.52
1	A	130	SER	CA-C	5.52	1.60	1.53
1	D	45	ARG	CB-CG	-5.43	1.36	1.52
1	D	84	ILE	CA-CB	-5.40	1.47	1.54
1	C	28	ARG	C-O	-5.36	1.18	1.24
1	D	7	ARG	N-CA	-5.31	1.39	1.46
1	D	59	LEU	N-CA	5.27	1.52	1.46
1	B	16	ILE	CA-CB	-5.14	1.48	1.54
1	B	94	ALA	CA-CB	-5.12	1.45	1.53
1	B	38	ALA	CA-C	-5.06	1.46	1.52
1	D	58	ASP	CA-C	5.05	1.60	1.53
1	A	115	LEU	N-CA	-5.03	1.40	1.46
1	D	60	THR	CA-CB	5.00	1.59	1.52

All (76) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	97	ALA	N-CA-C	-11.03	99.27	111.07
1	C	130	SER	CA-C-N	-10.97	108.48	119.56
1	C	130	SER	C-N-CA	-10.97	108.48	119.56
1	A	124	ALA	N-CA-C	-9.45	101.52	113.23
1	A	99	GLU	N-CA-C	-8.66	101.77	111.82
1	D	59	LEU	N-CA-C	8.11	122.98	112.12
1	D	66	GLY	N-CA-C	-7.81	105.09	115.32
1	A	130	SER	CA-C-N	7.40	126.94	119.24
1	A	130	SER	C-N-CA	7.40	126.94	119.24
1	B	89	GLN	N-CA-C	7.37	121.08	109.81
1	C	14	HIS	CA-C-N	7.16	127.49	119.32
1	C	14	HIS	C-N-CA	7.16	127.49	119.32
1	C	133	ILE	N-CA-C	-7.11	103.92	110.82
1	C	55	VAL	CA-C-N	-7.10	112.89	122.98
1	C	55	VAL	C-N-CA	-7.10	112.89	122.98
1	D	42	GLU	N-CA-C	-7.05	103.02	111.69
1	C	53	ASP	N-CA-C	-6.94	104.29	112.89
1	C	67	ILE	CB-CA-C	-6.83	103.07	112.02

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	61	LEU	CA-C-N	-6.80	111.34	119.84
1	C	61	LEU	C-N-CA	-6.80	111.34	119.84
1	B	42	GLU	N-CA-C	-6.74	104.01	111.36
1	D	88	HIS	N-CA-C	6.56	119.99	110.28
1	D	70	THR	N-CA-C	-6.50	103.69	111.69
1	D	9	MET	N-CA-C	-6.50	98.61	109.07
1	C	34	VAL	N-CA-CB	-6.49	103.88	112.26
1	B	138	ALA	N-CA-C	-6.46	104.32	111.36
1	B	128	ALA	N-CA-C	6.34	119.83	109.06
1	D	22	ARG	N-CA-C	-6.28	104.52	111.36
1	A	56	VAL	CB-CA-C	-6.23	101.86	110.96
1	A	64	PRO	CA-C-N	-6.23	115.31	122.85
1	A	64	PRO	C-N-CA	-6.23	115.31	122.85
1	C	107	THR	CA-C-N	-6.12	109.06	121.18
1	C	107	THR	C-N-CA	-6.12	109.06	121.18
1	C	129	MET	N-CA-C	-6.10	99.86	109.50
1	A	16	ILE	N-CA-C	6.10	116.73	110.82
1	D	5	THR	N-CA-C	-6.09	98.88	108.14
1	A	48	ARG	CA-C-N	-6.08	113.00	122.67
1	A	48	ARG	C-N-CA	-6.08	113.00	122.67
1	B	16	ILE	N-CA-C	5.97	116.71	110.62
1	D	34	VAL	N-CA-CB	-5.97	104.11	112.35
1	C	123	LEU	N-CA-C	-5.94	105.52	112.89
1	B	94	ALA	N-CA-C	-5.92	104.91	111.36
1	B	58	ASP	N-CA-C	-5.86	102.80	110.53
1	B	67	ILE	N-CA-CB	-5.80	101.02	110.31
1	D	74	ARG	N-CA-C	-5.77	105.50	112.54
1	D	67	ILE	N-CA-C	-5.68	105.31	110.82
1	A	87	MET	N-CA-C	-5.67	106.53	113.50
1	A	84	ILE	CB-CA-C	-5.63	102.94	111.33
1	B	23	ARG	N-CA-C	-5.63	105.22	111.36
1	B	75	GLN	N-CA-C	-5.60	105.95	112.89
1	B	10	LEU	CB-CG-CD1	-5.55	94.05	110.70
1	D	84	ILE	CB-CA-C	-5.54	103.62	111.21
1	A	6	ALA	N-CA-C	5.47	122.45	110.80
1	B	51	THR	CA-C-N	5.47	125.93	120.52
1	B	51	THR	C-N-CA	5.47	125.93	120.52
1	B	10	LEU	CB-CA-C	-5.39	100.86	109.75
1	D	36	GLU	CB-CA-C	-5.36	103.62	111.23
1	C	23	ARG	N-CA-C	-5.35	105.53	111.36
1	C	47	TYR	N-CA-C	-5.31	105.57	111.36
1	D	141	ARG	N-CA-C	-5.29	105.93	112.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	23	ARG	CG-CD-NE	5.26	123.57	112.00
1	D	19	GLU	CA-C-N	5.25	126.74	120.13
1	D	19	GLU	C-N-CA	5.25	126.74	120.13
1	A	104	GLY	O-C-N	-5.19	119.32	123.27
1	A	34	VAL	N-CA-CB	-5.17	105.22	112.35
1	A	59	LEU	N-CA-C	-5.13	106.19	112.90
1	D	123	LEU	N-CA-C	-5.11	107.02	113.20
1	C	107	THR	O-C-N	-5.11	117.21	123.19
1	B	137	ILE	CB-CA-C	-5.10	105.44	111.97
1	C	100	ALA	N-CA-C	-5.10	107.12	113.19
1	B	72	HIS	N-CA-C	-5.10	105.37	111.03
1	B	58	ASP	CB-CA-C	-5.09	99.25	109.68
1	C	10	LEU	CA-C-N	-5.08	116.20	123.11
1	C	10	LEU	C-N-CA	-5.08	116.20	123.11
1	C	119	ILE	N-CA-C	-5.07	105.45	110.62
1	A	75	GLN	N-CA-C	-5.05	105.96	111.82

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	91	SER	Peptide
1	D	65	GLY	Peptide

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	1081	0	1074	70	1
1	B	1077	0	1071	76	1
1	C	1092	0	1087	52	0
1	D	1092	0	1087	113	0
2	A	10	0	0	1	0
2	B	5	0	0	0	0
2	C	5	0	0	0	0
3	A	17	0	0	0	0
3	B	25	0	0	5	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	C	11	0	0	0	0
3	D	16	0	0	4	0
All	All	4431	0	4319	311	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 36.

All (311) 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:B:88:HIS:HE1	1:B:93:PHE:CE1	1.34	1.44
1:C:88:HIS:CE1	1:C:93:PHE:HE1	1.42	1.36
1:A:88:HIS:NE2	1:A:93:PHE:HE1	1.22	1.33
1:B:88:HIS:CE1	1:B:93:PHE:CE1	2.18	1.29
1:C:88:HIS:CE1	1:C:93:PHE:CE1	2.21	1.28
1:A:88:HIS:NE2	1:A:93:PHE:CE1	2.01	1.27
1:D:18:ARG:HD2	1:D:18:ARG:O	1.43	1.17
1:D:18:ARG:HH21	1:D:18:ARG:CG	1.54	1.16
1:D:61:LEU:HB3	1:D:62:PRO:CD	1.77	1.14
1:A:48:ARG:HH12	1:A:76:TRP:NE1	1.45	1.12
1:A:48:ARG:NH1	1:A:76:TRP:NE1	1.97	1.11
1:D:18:ARG:HH21	1:D:18:ARG:HG3	1.13	1.11
1:B:9:MET:HE3	1:B:46:LEU:HB2	1.24	1.08
1:B:9:MET:CE	1:B:46:LEU:HB2	1.82	1.08
1:D:19:GLU:HG3	1:D:23:ARG:HD3	1.33	1.08
1:A:11:VAL:HG11	1:A:57:MET:HE3	1.31	1.07
1:D:28:ARG:NH2	1:D:120:GLU:OE2	1.87	1.07
1:D:61:LEU:HB3	1:D:62:PRO:HD2	1.28	1.06
1:A:57:MET:HE2	1:A:61:LEU:HD11	1.32	1.06
1:A:9:MET:HE1	1:A:46:LEU:HB2	1.36	1.04
1:B:88:HIS:CE1	1:B:93:PHE:HE1	1.63	1.04
1:D:17:VAL:CG1	1:D:18:ARG:H	1.73	1.00
1:D:18:ARG:C	1:D:20:GLY:H	1.62	0.99
1:D:17:VAL:HG13	1:D:18:ARG:H	1.26	0.98
1:D:107:THR:HG23	1:D:133:ILE:CD1	1.95	0.95
1:A:88:HIS:CD2	1:A:93:PHE:CE1	2.55	0.95
1:D:74:ARG:NH2	1:D:78:GLY:O	2.01	0.93
1:D:13:ASP:OD1	1:D:14:HIS:HD2	1.50	0.93
1:A:88:HIS:CD2	1:A:93:PHE:CD1	2.56	0.92
1:D:18:ARG:HG3	1:D:18:ARG:NH2	1.78	0.92
1:D:17:VAL:CG1	1:D:18:ARG:N	2.30	0.91

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:61:LEU:CB	1:D:62:PRO:HD2	2.01	0.90
1:D:144:GLY:C	1:D:145:ARG:HG2	1.94	0.90
1:B:88:HIS:CE1	1:B:93:PHE:CD1	2.60	0.90
1:B:71:ARG:CB	1:B:71:ARG:HH11	1.86	0.89
1:C:21:TYR:O	1:C:25:ILE:HG13	1.74	0.88
1:B:71:ARG:HD3	3:B:204:HOH:O	1.72	0.88
1:A:57:MET:CE	1:A:61:LEU:HD11	2.03	0.87
1:A:67:ILE:CD1	1:A:97:ALA:HA	2.04	0.87
1:D:18:ARG:CG	1:D:18:ARG:NH2	2.26	0.87
1:A:139:GLU:OE2	1:A:143:GLU:OE1	1.92	0.86
1:B:9:MET:HE3	1:B:46:LEU:CB	2.04	0.86
1:A:67:ILE:HD11	1:A:97:ALA:CA	2.04	0.86
1:B:71:ARG:CD	3:B:204:HOH:O	2.23	0.85
1:D:18:ARG:HH21	1:D:18:ARG:HG2	1.39	0.85
1:D:13:ASP:OD1	1:D:14:HIS:CD2	2.27	0.85
1:A:9:MET:CE	1:A:46:LEU:HB2	2.06	0.85
1:B:88:HIS:HE1	1:B:93:PHE:CD1	1.95	0.85
1:A:57:MET:HE2	1:A:61:LEU:CD1	2.08	0.84
1:D:144:GLY:O	1:D:145:ARG:CG	2.26	0.84
1:B:71:ARG:HH11	1:B:71:ARG:HB2	1.39	0.83
1:A:67:ILE:HD11	1:A:97:ALA:N	1.93	0.83
1:B:71:ARG:HB3	1:B:71:ARG:NH1	1.93	0.83
1:A:48:ARG:HH12	1:A:76:TRP:HE1	1.27	0.83
1:B:67:ILE:HG21	3:B:212:HOH:O	1.78	0.83
1:D:14:HIS:NE2	1:D:58:ASP:OD2	2.11	0.83
1:B:19:GLU:OE2	1:B:22:ARG:NH2	2.12	0.82
1:B:107:THR:HG23	1:B:133:ILE:HD11	1.62	0.81
1:B:107:THR:HG23	1:B:133:ILE:CD1	2.10	0.81
1:B:67:ILE:HG23	1:B:68:GLU:H	1.45	0.80
1:D:19:GLU:O	1:D:23:ARG:HG2	1.80	0.80
1:A:48:ARG:NH1	1:A:76:TRP:CD1	2.48	0.80
1:B:71:ARG:CB	1:B:71:ARG:NH1	2.44	0.80
1:B:11:VAL:HG11	1:B:57:MET:HE3	1.63	0.79
1:A:132:ASP:O	1:A:136:GLU:HG3	1.82	0.79
1:D:129:MET:HG2	1:D:133:ILE:HG22	1.65	0.79
1:D:17:VAL:HG12	1:D:18:ARG:N	1.98	0.78
1:D:5:THR:HA	1:D:30:GLY:O	1.85	0.77
1:B:67:ILE:HG23	1:B:68:GLU:OE2	1.84	0.77
1:A:67:ILE:HD11	1:A:97:ALA:HA	1.64	0.76
1:C:141:ARG:HH21	1:C:145:ARG:HH11	1.31	0.76
1:C:88:HIS:CE1	1:C:93:PHE:CD1	2.74	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:19:GLU:CG	1:D:23:ARG:HD3	2.16	0.75
1:B:91:SER:OG	1:B:137:ILE:HA	1.87	0.75
1:C:142:VAL:C	1:C:144:GLY:H	1.92	0.75
1:A:48:ARG:HH12	1:A:76:TRP:CD1	2.05	0.74
1:C:116:VAL:O	1:C:120:GLU:HG3	1.86	0.74
1:A:11:VAL:HB	1:A:57:MET:HG3	1.69	0.74
1:D:5:THR:O	1:D:6:ALA:HB2	1.88	0.73
1:C:90:GLY:O	1:C:92:ALA:N	2.22	0.73
1:A:88:HIS:HE2	1:A:93:PHE:HE1	0.76	0.72
1:D:16:ILE:O	1:D:16:ILE:HG22	1.88	0.72
1:A:48:ARG:NH1	1:A:76:TRP:CE2	2.57	0.71
1:D:61:LEU:HB3	1:D:62:PRO:HD3	1.70	0.71
1:B:39:ASP:C	1:B:39:ASP:OD1	2.33	0.70
1:B:86:THR:C	1:B:108:LYS:HG3	2.16	0.70
1:D:144:GLY:O	1:D:145:ARG:HG2	1.87	0.70
1:D:18:ARG:C	1:D:20:GLY:N	2.38	0.70
1:D:50:THR:O	1:D:51:THR:C	2.33	0.70
1:D:107:THR:HG23	1:D:133:ILE:HD11	1.74	0.70
1:D:142:VAL:C	1:D:144:GLY:N	2.49	0.69
1:B:88:HIS:HE1	1:B:93:PHE:HE1	0.79	0.69
1:C:87:MET:HE1	1:C:109:SER:HB3	1.75	0.69
1:C:132:ASP:O	1:C:136:GLU:HG3	1.93	0.69
1:D:92:ALA:O	1:D:93:PHE:C	2.34	0.69
1:D:144:GLY:C	1:D:145:ARG:CG	2.66	0.69
1:D:138:ALA:C	1:D:140:GLU:H	2.00	0.68
1:B:111:ASP:OD1	1:B:112:PRO:HD2	1.92	0.68
1:B:9:MET:HE1	1:B:46:LEU:HB2	1.74	0.68
1:A:74:ARG:HD2	1:A:101:GLY:HA3	1.75	0.67
1:A:107:THR:HG23	1:A:133:ILE:HD12	1.74	0.67
1:D:85:PHE:CE2	1:D:108:LYS:HD3	2.29	0.67
1:D:67:ILE:CD1	1:D:97:ALA:HA	2.24	0.67
1:B:107:THR:CG2	1:B:133:ILE:HD11	2.24	0.67
1:B:67:ILE:CG2	3:B:212:HOH:O	2.39	0.66
1:A:67:ILE:CD1	1:A:97:ALA:CA	2.67	0.66
1:D:14:HIS:CE1	1:D:58:ASP:OD2	2.49	0.66
1:D:67:ILE:HD11	1:D:97:ALA:HA	1.79	0.65
1:D:28:ARG:HG2	1:D:29:PRO:HD2	1.78	0.64
1:D:18:ARG:HD2	1:D:18:ARG:C	2.21	0.64
1:D:107:THR:CG2	1:D:133:ILE:CD1	2.75	0.64
1:D:19:GLU:HB2	1:D:23:ARG:HG2	1.79	0.64
1:C:88:HIS:NE2	1:C:93:PHE:HE1	1.89	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:107:THR:HG22	1:C:109:SER:H	1.63	0.63
1:B:127:ARG:HG3	1:B:128:ALA:N	2.13	0.62
1:A:11:VAL:CG1	1:A:57:MET:HE3	2.19	0.62
1:D:18:ARG:O	1:D:20:GLY:N	2.33	0.62
1:B:28:ARG:HG3	1:B:31:TYR:CD2	2.34	0.62
1:B:13:ASP:OD2	1:B:62:PRO:HD3	2.00	0.61
1:B:71:ARG:HD2	3:B:204:HOH:O	1.94	0.61
1:C:50:THR:O	1:C:51:THR:C	2.44	0.61
1:A:88:HIS:HD2	1:A:93:PHE:CD1	2.18	0.61
1:C:67:ILE:HG13	1:C:68:GLU:OE1	2.01	0.61
1:D:74:ARG:HG3	1:D:101:GLY:HA3	1.82	0.61
1:C:111:ASP:O	1:C:114:GLU:HB2	2.00	0.61
1:A:67:ILE:HD12	1:A:97:ALA:HA	1.83	0.61
1:D:138:ALA:C	1:D:140:GLU:N	2.56	0.60
1:C:88:HIS:HE1	1:C:93:PHE:CE1	2.11	0.60
1:B:11:VAL:HB	1:B:57:MET:HG3	1.84	0.60
1:B:44:TYR:CD1	1:B:72:HIS:CD2	2.89	0.60
1:B:116:VAL:O	1:B:120:GLU:HG3	2.02	0.60
1:C:88:HIS:ND1	1:C:93:PHE:CD1	2.70	0.60
1:D:142:VAL:C	1:D:144:GLY:H	2.07	0.59
1:D:65:GLY:HA3	1:D:67:ILE:HG22	1.83	0.59
1:D:132:ASP:O	1:D:136:GLU:HG3	2.02	0.59
1:B:91:SER:HB2	1:B:140:GLU:OE1	2.03	0.59
1:C:142:VAL:C	1:C:144:GLY:N	2.55	0.59
1:D:93:PHE:CD1	3:D:158:HOH:O	2.55	0.59
1:A:50:THR:O	1:A:51:THR:C	2.46	0.59
1:D:42:GLU:HG2	1:D:46:LEU:HD12	1.84	0.58
1:B:57:MET:HE2	1:B:61:LEU:HD11	1.85	0.58
1:D:18:ARG:O	1:D:18:ARG:CD	2.35	0.58
1:D:144:GLY:O	1:D:145:ARG:HG3	2.04	0.58
1:A:88:HIS:CD2	1:A:93:PHE:HD1	2.20	0.57
1:D:14:HIS:CD2	1:D:14:HIS:N	2.72	0.57
1:A:21:TYR:O	1:A:25:ILE:HG13	2.04	0.57
1:A:57:MET:CE	1:A:61:LEU:CD1	2.73	0.57
1:C:144:GLY:O	1:C:145:ARG:C	2.46	0.57
1:C:116:VAL:O	1:C:120:GLU:CG	2.52	0.57
1:B:28:ARG:CD	1:B:28:ARG:C	2.79	0.56
1:A:22:ARG:NH1	1:A:22:ARG:HG2	2.21	0.56
1:C:63:GLY:O	1:C:64:PRO:C	2.47	0.56
1:C:106:VAL:CG1	1:C:107:THR:N	2.69	0.56
1:D:110:SER:HB3	1:D:114:GLU:HG2	1.89	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:110:SER:CB	1:D:114:GLU:HG2	2.36	0.55
1:B:111:ASP:OD1	1:B:112:PRO:CD	2.54	0.55
1:B:22:ARG:NH1	1:B:23:ARG:HD2	2.22	0.54
1:A:55:VAL:HG13	1:A:82:ILE:HG13	1.90	0.54
1:A:22:ARG:HG2	1:A:22:ARG:HH11	1.73	0.54
1:B:53:ASP:O	1:B:81:ARG:HD3	2.08	0.54
1:D:140:GLU:C	1:D:142:VAL:H	2.14	0.54
1:B:9:MET:HE1	1:B:43:ALA:HA	1.89	0.54
1:D:142:VAL:O	1:D:144:GLY:N	2.40	0.54
1:D:110:SER:O	1:D:111:ASP:C	2.51	0.54
1:D:13:ASP:OD1	1:D:13:ASP:N	2.41	0.53
1:D:46:LEU:O	1:D:50:THR:OG1	2.26	0.53
1:C:12:ASP:OD1	1:C:58:ASP:OD2	2.26	0.53
1:D:90:GLY:HA2	3:D:160:HOH:O	2.08	0.53
1:D:138:ALA:O	1:D:140:GLU:N	2.41	0.53
1:B:50:THR:O	1:B:51:THR:C	2.52	0.53
1:A:107:THR:HG23	1:A:133:ILE:CD1	2.40	0.52
1:D:107:THR:HG23	1:D:133:ILE:HD13	1.85	0.52
1:B:107:THR:CG2	1:B:133:ILE:CD1	2.86	0.52
1:B:74:ARG:HA	1:B:77:ASP:O	2.10	0.52
1:D:85:PHE:CZ	1:D:108:LYS:HD3	2.45	0.52
1:D:18:ARG:NH2	1:D:18:ARG:HG2	2.11	0.52
1:C:98:PHE:CE1	1:C:127:ARG:HD2	2.45	0.52
1:C:106:VAL:HG12	1:C:107:THR:N	2.24	0.52
1:D:13:ASP:OD2	1:D:61:LEU:HA	2.10	0.52
1:D:129:MET:HG2	1:D:133:ILE:CG2	2.38	0.52
1:A:88:HIS:HD2	1:A:93:PHE:HD1	1.56	0.52
1:D:8:ILE:HG12	1:D:54:ILE:CG2	2.39	0.51
1:D:140:GLU:C	1:D:142:VAL:N	2.65	0.51
1:C:70:THR:O	1:C:74:ARG:HB2	2.10	0.51
1:D:9:MET:HB2	1:D:52:PRO:HG3	1.91	0.51
1:D:74:ARG:HD3	1:D:80:ALA:HB3	1.91	0.51
1:C:88:HIS:ND1	1:C:93:PHE:CE1	2.73	0.51
1:C:141:ARG:HH21	1:C:145:ARG:NH1	2.04	0.51
1:B:11:VAL:HG22	1:B:37:ALA:HB3	1.92	0.51
1:B:67:ILE:HG23	1:B:68:GLU:N	2.15	0.51
1:D:40:ALA:CB	1:D:64:PRO:HG2	2.41	0.51
1:A:104:GLY:HA2	1:A:128:ALA:O	2.10	0.51
1:B:113:ALA:O	1:B:117:GLN:HG3	2.11	0.50
1:B:97:ALA:O	1:B:98:PHE:C	2.50	0.50
1:C:47:TYR:CE2	1:C:52:PRO:HD2	2.47	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:107:THR:CG2	1:D:133:ILE:HD11	2.38	0.50
1:A:116:VAL:O	1:A:120:GLU:HG3	2.12	0.49
1:B:90:GLY:O	1:B:91:SER:C	2.53	0.49
1:D:93:PHE:CE1	3:D:158:HOH:O	2.55	0.49
1:A:5:THR:O	1:A:6:ALA:HB2	2.12	0.49
1:A:105:TYR:CD2	1:A:133:ILE:HD13	2.47	0.49
1:B:61:LEU:HB3	1:B:62:PRO:HD2	1.94	0.49
1:C:90:GLY:C	1:C:92:ALA:N	2.70	0.49
1:D:67:ILE:HD12	1:D:97:ALA:HA	1.95	0.49
1:D:28:ARG:HD3	1:D:31:TYR:CD2	2.48	0.49
1:A:61:LEU:HB2	1:A:65:GLY:HA2	1.94	0.48
1:D:39:ASP:OD1	1:D:42:GLU:CB	2.61	0.48
1:D:46:LEU:HA	1:D:49:GLU:HG3	1.95	0.48
1:A:60:THR:HB	2:A:201:PO4:O4	2.13	0.48
1:C:28:ARG:O	1:C:29:PRO:C	2.56	0.48
1:A:23:ARG:O	1:A:27:ARG:HG3	2.14	0.48
1:C:141:ARG:O	1:C:141:ARG:HG3	2.12	0.48
1:D:13:ASP:C	1:D:15:PRO:HD3	2.37	0.48
1:C:91:SER:HB3	1:C:137:ILE:HG13	1.95	0.48
1:B:58:ASP:HA	1:B:85:PHE:O	2.15	0.47
1:B:104:GLY:HA3	1:B:122:ILE:HD11	1.95	0.47
1:A:91:SER:HB3	1:A:137:ILE:HG13	1.95	0.47
1:B:95:LEU:O	1:B:99:GLU:HG3	2.14	0.47
1:B:28:ARG:HG3	1:B:31:TYR:CG	2.49	0.47
1:D:31:TYR:OH	1:D:120:GLU:HG3	2.14	0.47
1:D:40:ALA:HB3	1:D:64:PRO:HG2	1.96	0.47
1:D:16:ILE:O	1:D:16:ILE:CG2	2.59	0.47
1:B:87:MET:O	1:B:87:MET:HG3	2.14	0.47
1:B:107:THR:HG23	1:B:133:ILE:HD13	1.95	0.47
1:C:129:MET:HG2	1:C:133:ILE:CG2	2.45	0.47
1:A:28:ARG:HD2	1:A:29:PRO:O	2.14	0.47
1:A:91:SER:CB	1:A:137:ILE:HG13	2.44	0.47
1:C:90:GLY:C	1:C:92:ALA:H	2.23	0.46
1:D:110:SER:O	1:D:111:ASP:O	2.33	0.46
1:A:107:THR:CG2	1:A:133:ILE:CD1	2.93	0.46
1:B:71:ARG:HB3	1:B:71:ARG:CZ	2.45	0.46
1:C:8:ILE:HD12	1:C:8:ILE:N	2.30	0.46
1:D:133:ILE:HG23	1:D:137:ILE:HD12	1.98	0.46
1:C:88:HIS:ND1	1:C:93:PHE:HD1	2.14	0.46
1:A:84:ILE:HG22	1:A:85:PHE:N	2.29	0.46
1:C:67:ILE:CG1	1:C:68:GLU:OE1	2.63	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:67:ILE:HD11	1:D:97:ALA:CA	2.45	0.46
1:A:85:PHE:CD1	1:A:106:VAL:HG12	2.50	0.46
1:D:5:THR:CA	1:D:30:GLY:O	2.61	0.46
1:B:110:SER:HB2	1:B:114:GLU:HG3	1.98	0.46
1:A:107:THR:CG2	1:A:133:ILE:HD12	2.45	0.45
1:C:94:ALA:HA	1:C:105:TYR:CD1	2.52	0.45
1:A:28:ARG:HG3	1:A:31:TYR:CG	2.51	0.45
1:A:85:PHE:CE2	1:A:115:LEU:HD22	2.51	0.45
1:B:12:ASP:OD1	1:B:58:ASP:OD2	2.33	0.45
1:D:17:VAL:HG13	1:D:18:ARG:HG3	1.98	0.45
1:D:18:ARG:HD3	1:D:20:GLY:HA3	1.98	0.45
1:A:11:VAL:HG22	1:A:37:ALA:HB3	1.98	0.45
1:D:19:GLU:OE1	1:D:19:GLU:N	2.49	0.45
1:D:64:PRO:O	1:D:65:GLY:C	2.60	0.45
1:D:130:SER:O	1:D:133:ILE:N	2.49	0.45
1:C:133:ILE:HD12	1:C:133:ILE:HA	1.62	0.45
1:A:111:ASP:O	1:A:112:PRO:C	2.58	0.44
1:D:142:VAL:O	1:D:143:GLU:C	2.59	0.44
1:A:28:ARG:HG3	1:A:31:TYR:CD2	2.52	0.44
1:C:39:ASP:OD1	1:C:39:ASP:C	2.60	0.44
1:D:23:ARG:HD2	3:D:154:HOH:O	2.18	0.44
1:A:13:ASP:O	1:A:15:PRO:HD3	2.17	0.44
1:A:118:ALA:O	1:A:119:ILE:C	2.59	0.44
1:C:70:THR:HG23	1:C:82:ILE:HD12	2.00	0.44
1:C:95:LEU:O	1:C:96:LYS:C	2.59	0.44
1:A:22:ARG:HH11	1:A:22:ARG:CG	2.30	0.43
1:B:59:LEU:O	1:B:59:LEU:HG	2.13	0.43
1:B:90:GLY:C	1:B:92:ALA:H	2.26	0.43
1:C:141:ARG:NH2	1:C:145:ARG:HH11	2.08	0.43
1:A:47:TYR:O	1:A:51:THR:N	2.44	0.43
1:C:96:LYS:O	1:C:99:GLU:HB3	2.17	0.43
1:D:42:GLU:O	1:D:46:LEU:HB2	2.19	0.43
1:A:90:GLY:C	1:A:92:ALA:N	2.75	0.43
1:D:11:VAL:HB	1:D:57:MET:HA	2.00	0.43
1:B:91:SER:OG	1:B:137:ILE:CA	2.63	0.43
1:A:67:ILE:HD11	1:A:96:LYS:C	2.42	0.43
1:B:74:ARG:NH2	1:B:80:ALA:O	2.51	0.43
1:B:123:LEU:HA	1:B:123:LEU:HD23	1.73	0.43
1:C:10:LEU:HD12	1:C:10:LEU:HA	1.83	0.43
1:D:47:TYR:O	1:D:51:THR:N	2.51	0.43
1:D:64:PRO:C	1:D:65:GLY:O	2.61	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:90:GLY:C	1:B:92:ALA:N	2.75	0.42
1:D:9:MET:HE1	1:D:43:ALA:HA	2.01	0.42
1:D:67:ILE:CD1	1:D:97:ALA:CA	2.94	0.42
1:D:90:GLY:C	1:D:92:ALA:N	2.75	0.42
1:A:91:SER:HB2	1:A:137:ILE:HG12	2.02	0.42
1:B:28:ARG:O	1:B:31:TYR:HB2	2.19	0.42
1:C:7:ARG:N	1:C:53:ASP:OD2	2.42	0.42
1:B:11:VAL:HA	1:B:37:ALA:O	2.20	0.42
1:B:28:ARG:HA	1:B:29:PRO:HD3	1.90	0.42
1:C:59:LEU:O	1:C:59:LEU:HG	2.20	0.42
1:A:54:ILE:HG23	1:A:54:ILE:O	2.20	0.42
1:A:105:TYR:HD2	1:A:133:ILE:HD13	1.85	0.41
1:D:57:MET:HE2	1:D:57:MET:HB2	1.75	0.41
1:A:141:ARG:NH1	1:A:141:ARG:HG3	2.34	0.41
1:D:129:MET:O	1:D:130:SER:C	2.63	0.41
1:B:57:MET:HE2	1:B:61:LEU:CD1	2.49	0.41
1:C:59:LEU:HD11	1:C:67:ILE:CD1	2.51	0.41
1:B:28:ARG:CG	1:B:31:TYR:CD2	3.03	0.41
1:B:47:TYR:OH	1:B:77:ASP:OD2	2.36	0.41
1:C:64:PRO:C	1:C:65:GLY:O	2.63	0.41
1:D:47:TYR:CD1	1:D:47:TYR:C	2.99	0.41
1:D:45:ARG:O	1:D:49:GLU:HG3	2.21	0.41
1:D:91:SER:O	1:D:95:LEU:HG	2.20	0.41
1:B:85:PHE:HD1	1:B:106:VAL:HG12	1.86	0.41
1:B:143:GLU:H	1:B:143:GLU:HG2	1.43	0.41
1:C:116:VAL:H	1:C:116:VAL:HG23	1.49	0.41
1:D:39:ASP:OD1	1:D:42:GLU:HB2	2.21	0.41
1:D:67:ILE:HD11	1:D:96:LYS:C	2.46	0.41
1:D:129:MET:HE3	1:D:129:MET:HB2	1.89	0.41
1:A:129:MET:HE3	1:A:129:MET:HB2	1.85	0.40
1:B:85:PHE:CD1	1:B:106:VAL:HG12	2.57	0.40
1:D:18:ARG:HH11	1:D:21:TYR:HE2	1.69	0.40
1:A:141:ARG:HG3	1:A:141:ARG:HH11	1.87	0.40
1:C:14:HIS:HA	1:C:15:PRO:HD2	1.84	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:A:26:GLU:OE2	1:B:22:ARG:NH1[2_665]	2.10	0.10

5.3 Torsion angles

5.3.1 Protein backbone

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	139/153 (91%)	128 (92%)	9 (6%)	2 (1%)	9	23
1	B	138/153 (90%)	129 (94%)	8 (6%)	1 (1%)	18	41
1	C	140/153 (92%)	131 (94%)	5 (4%)	4 (3%)	3	9
1	D	140/153 (92%)	121 (86%)	12 (9%)	7 (5%)	1	3
All	All	557/612 (91%)	509 (91%)	34 (6%)	14 (2%)	4	11

All (14) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	91	SER
1	C	143	GLU
1	D	111	ASP
1	D	143	GLU
1	B	113	ALA
1	C	65	GLY
1	D	6	ALA
1	D	139	GLU
1	A	6	ALA
1	A	92	ALA
1	C	6	ALA
1	D	17	VAL
1	D	19	GLU
1	D	61	LEU

5.3.2 Protein sidechains

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	107/118 (91%)	90 (84%)	17 (16%)	2	7
1	B	107/118 (91%)	89 (83%)	18 (17%)	2	6
1	C	108/118 (92%)	98 (91%)	10 (9%)	8	21
1	D	108/118 (92%)	85 (79%)	23 (21%)	1	3
All	All	430/472 (91%)	362 (84%)	68 (16%)	2	7

All (68) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	17	VAL
1	A	28	ARG
1	A	34	VAL
1	A	49	GLU
1	A	50	THR
1	A	55	VAL
1	A	57	MET
1	A	67	ILE
1	A	74	ARG
1	A	84	ILE
1	A	89	GLN
1	A	96	LYS
1	A	103	SER
1	A	122	ILE
1	A	129	MET
1	A	133	ILE
1	A	143	GLU
1	B	19	GLU
1	B	23	ARG
1	B	28	ARG
1	B	34	VAL
1	B	39	ASP
1	B	61	LEU
1	B	67	ILE
1	B	71	ARG
1	B	75	GLN
1	B	81	ARG
1	B	84	ILE
1	B	89	GLN
1	B	91	SER
1	B	99	GLU
1	B	106	VAL
1	B	110	SER

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Mol	Chain	Res	Type
1	B	133	ILE
1	B	140	GLU
1	C	5	THR
1	C	17	VAL
1	C	34	VAL
1	C	67	ILE
1	C	87	MET
1	C	89	GLN
1	C	116	VAL
1	C	119	ILE
1	C	133	ILE
1	C	141	ARG
1	D	5	THR
1	D	12	ASP
1	D	14	HIS
1	D	17	VAL
1	D	18	ARG
1	D	19	GLU
1	D	26	GLU
1	D	28	ARG
1	D	34	VAL
1	D	36	GLU
1	D	46	LEU
1	D	49	GLU
1	D	58	ASP
1	D	67	ILE
1	D	84	ILE
1	D	89	GLN
1	D	91	SER
1	D	108	LYS
1	D	110	SER
1	D	129	MET
1	D	133	ILE
1	D	141	ARG
1	D	145	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (9) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	14	HIS
1	A	89	GLN
1	B	72	HIS

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Mol	Chain	Res	Type
1	B	88	HIS
1	C	88	HIS
1	C	89	GLN
1	D	14	HIS
1	D	89	GLN
1	D	135	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 oligosaccharides 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	PO4	A	202	-	4,4,4	1.25	0	6,6,6	2.61	3 (50%)
2	PO4	C	201	-	4,4,4	1.72	1 (25%)	6,6,6	1.20	0
2	PO4	B	201	-	4,4,4	1.09	0	6,6,6	1.02	1 (16%)
2	PO4	A	201	-	4,4,4	1.08	0	6,6,6	2.21	2 (33%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	201	PO4	P-O2	-2.80	1.46	1.54

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	202	PO4	O3-P-O1	-4.82	93.90	110.95
2	A	201	PO4	O4-P-O1	-4.54	94.90	110.95
2	A	202	PO4	O4-P-O2	2.74	116.44	107.91
2	A	202	PO4	O4-P-O3	2.73	116.40	107.91
2	A	201	PO4	O4-P-O2	2.41	115.41	107.91
2	B	201	PO4	O3-P-O2	2.09	114.41	107.91

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	201	PO4	1	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2		OWAB(Å ²)	Q<0.9
1	A	141/153 (92%)	-0.67	0	100 100	13, 25, 41, 51	0
1	B	140/153 (91%)	-0.62	0	100 100	12, 24, 39, 44	0
1	C	142/153 (92%)	-0.44	0	100 100	11, 28, 46, 57	0
1	D	142/153 (92%)	-0.14	5 (3%)	47 43	14, 29, 58, 77	0
All	All	565/612 (92%)	-0.47	5 (0%)	81 80	11, 27, 50, 77	0

All (5) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	61	LEU	5.7
1	D	60	THR	4.3
1	D	62	PRO	4.2
1	D	59	LEU	3.3
1	D	4	SER	2.4

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 oligosaccharides in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum,

median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
2	PO4	B	201	5/5	0.89	0.22	20,21,21,30	0
2	PO4	A	202	5/5	0.96	0.08	2,9,10,11	0
2	PO4	C	201	5/5	0.96	0.12	16,16,17,38	0
2	PO4	A	201	5/5	0.98	0.07	16,18,19,20	0

6.5 Other polymers [i](#)

There are no such residues in this entry.