



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 15, 2017 – 03:34 am GMT

PDB ID : 1X86  
Title : Crystal Structure of the DH/PH domains of Leukemia-associated RhoGEF in complex with RhoA  
Authors : Kristelly, R.; Gao, G.; Tesmer, J.J.  
Deposited on : 2004-08-17  
Resolution : 3.22 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	:	1.7.2 (RC1), CSD as538be (2017)
Xtriage (Phenix)	:	1.9-1692
EDS	:	trunk28620
Percentile statistics	:	20161228.v01 (using entries in the PDB archive December 28th 2016)
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)	:	recalc28949

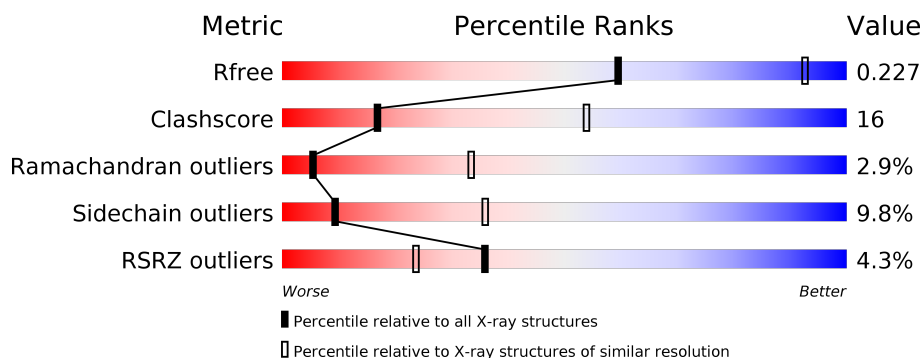
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 3.22 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))
$R_{free}$	100719	1036 (3.24-3.20)
Clashscore	112137	1161 (3.24-3.20)
Ramachandran outliers	110173	1140 (3.24-3.20)
Sidechain outliers	110143	1139 (3.24-3.20)
RSRZ outliers	101464	1040 (3.24-3.20)

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	385	<div> <div>52%</div> <div>35%</div> <div>7%</div> <div>6%</div> </div>
1	C	385	<div> <div>3%</div> <div>59%</div> <div>31%</div> <div>6%</div> </div>
1	E	385	<div> <div>7%</div> <div>48%</div> <div>33%</div> <div>6%</div> <div>13%</div> </div>
1	G	385	<div> <div>8%</div> <div>44%</div> <div>32%</div> <div>5%</div> <div>18%</div> </div>
2	B	196	<div> <div>50%</div> <div>37%</div> <div>8%</div> </div>
2	D	196	<div> <div>59%</div> <div>28%</div> <div>5%</div> <div>8%</div> </div>

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Mol	Chain	Length	Quality of chain
2	F	196	
2	H	196	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	PO4	B	401	-	-	-	X
3	PO4	F	403	-	-	-	X
3	PO4	H	404	-	-	-	X

## 2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 16981 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 Rho guanine nucleotide exchange factor 12.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	362	Total	C	N	O	S	0	0	0
			2964	1873	528	551	12			
1	C	362	Total	C	N	O	S	0	0	0
			2964	1873	528	551	12			
1	E	336	Total	C	N	O	S	0	0	0
			2767	1754	494	509	10			
1	G	314	Total	C	N	O	S	0	0	0
			2584	1643	460	471	10			

There are 52 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	764	GLY	THR	CLONING ARTIFACT	UNP Q9NZN5
A	765	SER	ASP	CLONING ARTIFACT	UNP Q9NZN5
A	973	PHE	TYR	ENGINEERED	UNP Q9NZN5
A	1139	VAL	-	CLONING ARTIFACT	UNP Q9NZN5
A	1140	ASP	-	CLONING ARTIFACT	UNP Q9NZN5
A	1141	GLY	-	CLONING ARTIFACT	UNP Q9NZN5
A	1142	GLY	-	CLONING ARTIFACT	UNP Q9NZN5
A	1143	HIS	-	EXPRESSION TAG	UNP Q9NZN5
A	1144	HIS	-	EXPRESSION TAG	UNP Q9NZN5
A	1145	HIS	-	EXPRESSION TAG	UNP Q9NZN5
A	1146	HIS	-	EXPRESSION TAG	UNP Q9NZN5
A	1147	HIS	-	EXPRESSION TAG	UNP Q9NZN5
A	1148	HIS	-	EXPRESSION TAG	UNP Q9NZN5
C	764	GLY	THR	CLONING ARTIFACT	UNP Q9NZN5
C	765	SER	ASP	CLONING ARTIFACT	UNP Q9NZN5
C	973	PHE	TYR	ENGINEERED	UNP Q9NZN5
C	1139	VAL	-	CLONING ARTIFACT	UNP Q9NZN5
C	1140	ASP	-	CLONING ARTIFACT	UNP Q9NZN5
C	1141	GLY	-	CLONING ARTIFACT	UNP Q9NZN5
C	1142	GLY	-	CLONING ARTIFACT	UNP Q9NZN5
C	1143	HIS	-	EXPRESSION TAG	UNP Q9NZN5

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Chain	Residue	Modelled	Actual	Comment	Reference
C	1144	HIS	-	EXPRESSION TAG	UNP Q9NZN5
C	1145	HIS	-	EXPRESSION TAG	UNP Q9NZN5
C	1146	HIS	-	EXPRESSION TAG	UNP Q9NZN5
C	1147	HIS	-	EXPRESSION TAG	UNP Q9NZN5
C	1148	HIS	-	EXPRESSION TAG	UNP Q9NZN5
E	764	GLY	THR	CLONING ARTIFACT	UNP Q9NZN5
E	765	SER	ASP	CLONING ARTIFACT	UNP Q9NZN5
E	973	PHE	TYR	ENGINEERED	UNP Q9NZN5
E	1139	VAL	-	CLONING ARTIFACT	UNP Q9NZN5
E	1140	ASP	-	CLONING ARTIFACT	UNP Q9NZN5
E	1141	GLY	-	CLONING ARTIFACT	UNP Q9NZN5
E	1142	GLY	-	CLONING ARTIFACT	UNP Q9NZN5
E	1143	HIS	-	EXPRESSION TAG	UNP Q9NZN5
E	1144	HIS	-	EXPRESSION TAG	UNP Q9NZN5
E	1145	HIS	-	EXPRESSION TAG	UNP Q9NZN5
E	1146	HIS	-	EXPRESSION TAG	UNP Q9NZN5
E	1147	HIS	-	EXPRESSION TAG	UNP Q9NZN5
E	1148	HIS	-	EXPRESSION TAG	UNP Q9NZN5
G	764	GLY	THR	CLONING ARTIFACT	UNP Q9NZN5
G	765	SER	ASP	CLONING ARTIFACT	UNP Q9NZN5
G	973	PHE	TYR	ENGINEERED	UNP Q9NZN5
G	1139	VAL	-	CLONING ARTIFACT	UNP Q9NZN5
G	1140	ASP	-	CLONING ARTIFACT	UNP Q9NZN5
G	1141	GLY	-	CLONING ARTIFACT	UNP Q9NZN5
G	1142	GLY	-	CLONING ARTIFACT	UNP Q9NZN5
G	1143	HIS	-	EXPRESSION TAG	UNP Q9NZN5
G	1144	HIS	-	EXPRESSION TAG	UNP Q9NZN5
G	1145	HIS	-	EXPRESSION TAG	UNP Q9NZN5
G	1146	HIS	-	EXPRESSION TAG	UNP Q9NZN5
G	1147	HIS	-	EXPRESSION TAG	UNP Q9NZN5
G	1148	HIS	-	EXPRESSION TAG	UNP Q9NZN5

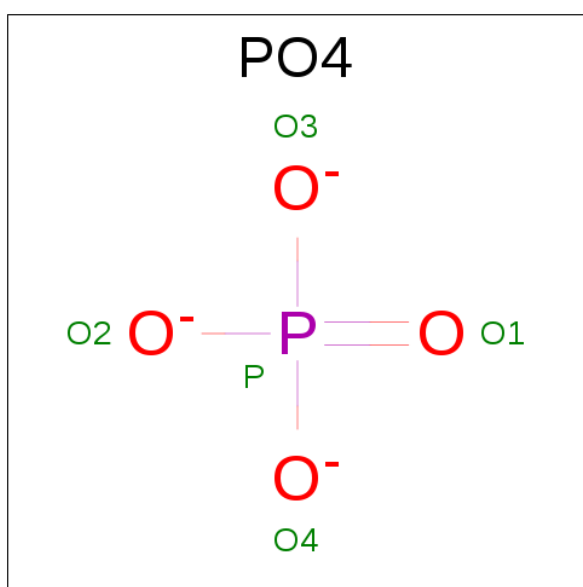
- Molecule 2 is a protein called Transforming protein RhoA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	180	Total	C	N	O	S	0	0	0
			1423	900	241	272	10			
2	D	180	Total	C	N	O	S	0	0	0
			1423	900	241	272	10			
2	F	179	Total	C	N	O	S	0	0	0
			1418	897	240	271	10			
2	H	179	Total	C	N	O	S	0	0	0
			1418	897	240	271	10			

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	-2	GLY	-	CLONING ARTIFACT	UNP P61586
B	-1	GLU	-	CLONING ARTIFACT	UNP P61586
B	0	PHE	-	CLONING ARTIFACT	UNP P61586
D	-2	GLY	-	CLONING ARTIFACT	UNP P61586
D	-1	GLU	-	CLONING ARTIFACT	UNP P61586
D	0	PHE	-	CLONING ARTIFACT	UNP P61586
F	-2	GLY	-	CLONING ARTIFACT	UNP P61586
F	-1	GLU	-	CLONING ARTIFACT	UNP P61586
F	0	PHE	-	CLONING ARTIFACT	UNP P61586
H	-2	GLY	-	CLONING ARTIFACT	UNP P61586
H	-1	GLU	-	CLONING ARTIFACT	UNP P61586
H	0	PHE	-	CLONING ARTIFACT	UNP P61586

- Molecule 3 is PHOSPHATE ION (three-letter code: PO4) (formula: O<sub>4</sub>P).

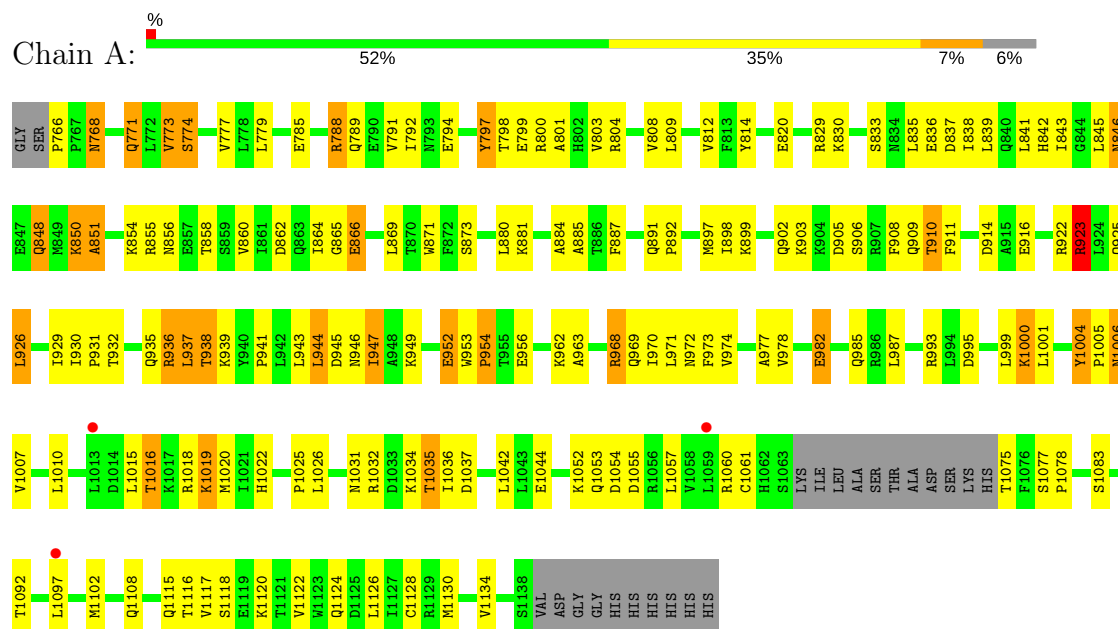


Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	B	1	Total O P 5 4 1	0	0
3	D	1	Total O P 5 4 1	0	0
3	F	1	Total O P 5 4 1	0	0
3	H	1	Total O P 5 4 1	0	0

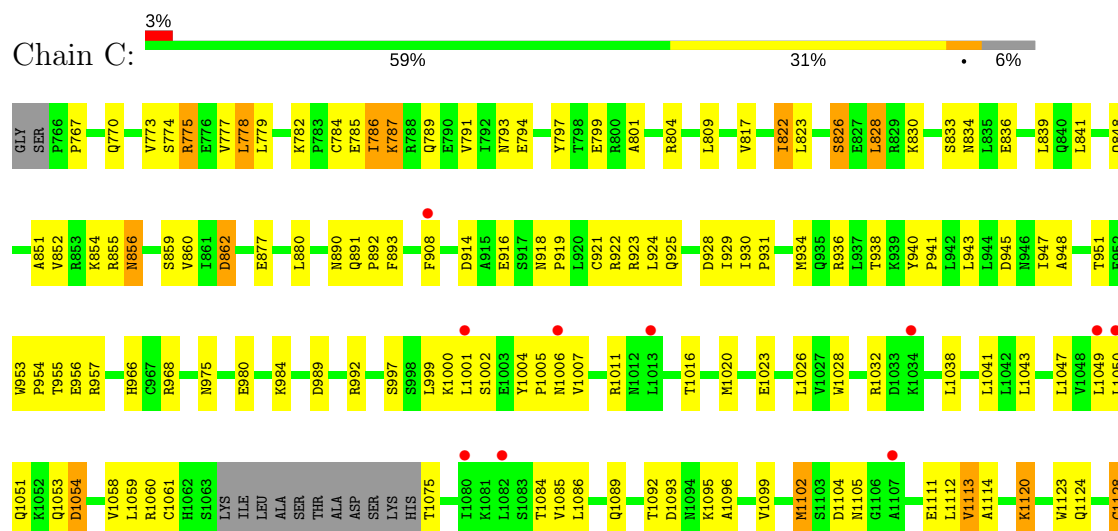
### 3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of 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: Rho guanine nucleotide exchange factor 12

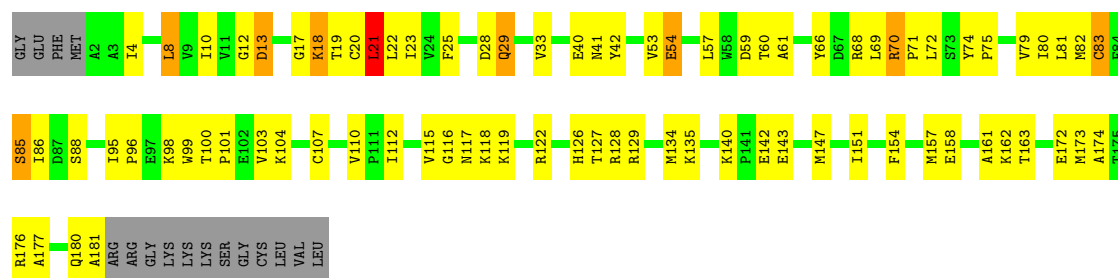


- Molecule 1: Rho guanine nucleotide exchange factor 12



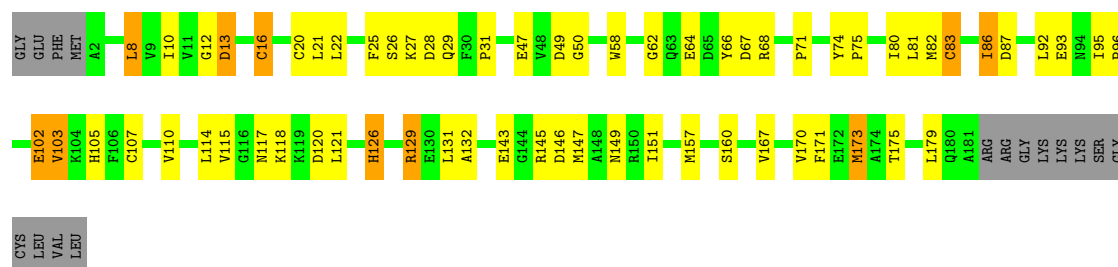






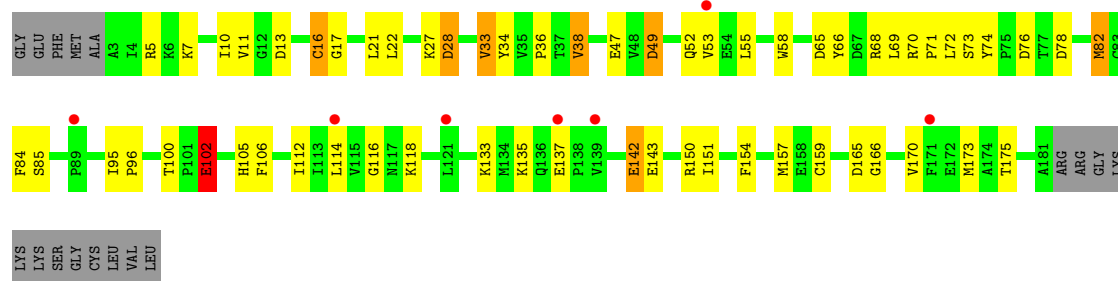
### • Molecule 2: Transforming protein RhoA

Chain D: 59% 28% 5% 8%



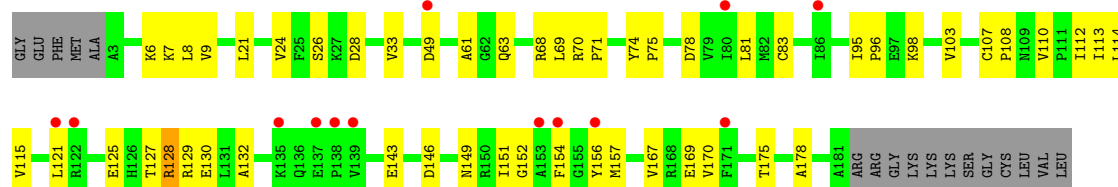
### • Molecule 2: Transforming protein RhoA

Chain F: 4% 61% 27% 9%



### • Molecule 2: Transforming protein RhoA

Chain H: 7% 65% 26% 9%



## 4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	296.42Å 95.24Å 157.34Å 90.00° 94.19° 90.00°	Depositor
Resolution (Å)	15.00 – 3.22 47.00 – 3.19	Depositor EDS
% Data completeness (in resolution range)	90.4 (15.00-3.22) 88.9 (47.00-3.19)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.85 (at 3.19Å)	Xtriage
Refinement program	REFMAC 5.2.0005	Depositor
R, $R_{free}$	0.227 , 0.279 0.229 , 0.227	Depositor DCC
$R_{free}$ test set	3238 reflections (5.32%)	DCC
Wilson B-factor (Å <sup>2</sup> )	86.6	Xtriage
Anisotropy	0.423	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.27 , 77.1	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.44$ , $\langle L^2 \rangle = 0.27$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.93	EDS
Total number of atoms	16981	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	44.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.12% 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, 0.333 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	0.97	3/3010 (0.1%)	0.97	6/4060 (0.1%)
1	C	0.63	1/3010 (0.0%)	0.73	0/4060
1	E	0.73	3/2806 (0.1%)	0.75	0/3779
1	G	0.88	9/2622 (0.3%)	0.77	3/3532 (0.1%)
2	B	1.09	1/1451 (0.1%)	1.05	2/1963 (0.1%)
2	D	0.73	2/1451 (0.1%)	0.78	0/1963
2	F	0.67	2/1446 (0.1%)	0.71	1/1956 (0.1%)
2	H	0.47	0/1446	0.61	0/1956
All	All	0.80	21/17242 (0.1%)	0.81	12/23269 (0.1%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	2
1	E	0	1
1	G	0	2
All	All	0	5

All (21) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	G	982	GLU	CD-OE2	19.11	1.46	1.25
1	G	980	GLU	CD-OE2	13.09	1.40	1.25
1	G	980	GLU	CD-OE1	8.76	1.35	1.25
1	G	1108	GLN	CD-NE2	8.74	1.54	1.32
2	B	83	CYS	CB-SG	-8.64	1.67	1.82
2	D	83	CYS	CB-SG	-7.91	1.68	1.82
1	E	1058	VAL	C-O	7.52	1.37	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	G	982	GLU	CD-OE1	6.90	1.33	1.25
2	F	82	MET	CG-SD	6.25	1.97	1.81
1	G	889	SER	CB-OG	6.23	1.50	1.42
1	A	850	LYS	CD-CE	6.14	1.66	1.51
2	F	102	GLU	C-O	-6.12	1.11	1.23
1	A	771	GLN	CG-CD	5.98	1.64	1.51
1	G	890	ASN	C-O	5.54	1.33	1.23
1	C	921	CYS	CB-SG	-5.54	1.72	1.81
1	A	952	GLU	CG-CD	5.52	1.60	1.51
1	E	956	GLU	CG-CD	5.51	1.60	1.51
1	G	850	LYS	CD-CE	5.49	1.65	1.51
2	D	20	CYS	CB-SG	-5.31	1.73	1.81
1	G	807	LYS	CD-CE	5.31	1.64	1.51
1	E	850	LYS	CD-CE	5.23	1.64	1.51

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	968	ARG	NE-CZ-NH2	-6.89	116.86	120.30
1	G	982	GLU	OE1-CD-OE2	6.60	131.22	123.30
2	F	142	GLU	OE1-CD-OE2	-6.45	115.56	123.30
1	A	809	LEU	CB-CG-CD2	-5.90	100.97	111.00
2	B	21	LEU	CA-CB-CG	5.47	127.88	115.30
1	G	800	ARG	NE-CZ-NH2	-5.22	117.69	120.30
1	A	936	ARG	NE-CZ-NH1	5.13	122.87	120.30
1	G	800	ARG	NE-CZ-NH1	5.12	122.86	120.30
1	A	968	ARG	NE-CZ-NH1	5.08	122.84	120.30
2	B	70	ARG	NE-CZ-NH2	-5.08	117.76	120.30
1	A	788	ARG	NE-CZ-NH2	-5.08	117.76	120.30
1	A	923	ARG	NE-CZ-NH2	-5.05	117.77	120.30

There are no chirality outliers.

All (5) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	1006	ASN	Peptide
1	A	766	PRO	Peptide
1	E	766	PRO	Peptide
1	G	1038	LEU	Peptide
1	G	1108	GLN	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	2964	0	3047	87	0
1	C	2964	0	3047	78	0
1	E	2767	0	2861	104	0
1	G	2584	0	2671	101	0
2	B	1423	0	1415	69	0
2	D	1423	0	1415	47	0
2	F	1418	0	1410	35	0
2	H	1418	0	1410	38	0
3	B	5	0	0	1	0
3	D	5	0	0	0	0
3	F	5	0	0	0	0
3	H	5	0	0	0	0
All	All	16981	0	17276	536	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 16.

All (536) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:929:ILE:O	1:A:932:THR:HG23	1.54	1.06
1:G:975:ASN:OD1	2:H:68:ARG:HB2	1.56	1.05
2:F:10:ILE:HG21	2:F:22:LEU:HD11	1.52	0.88
1:A:848:GLN:O	1:A:851:ALA:HB3	1.75	0.85
2:D:8:LEU:HD21	2:D:81:LEU:HD12	1.62	0.81
2:B:85:SER:OG	2:B:118:LYS:HD3	1.80	0.81
2:B:80:ILE:HD12	2:B:103:VAL:HG13	1.63	0.80
1:G:1042:LEU:HD21	1:G:1130:MET:HG3	1.61	0.80
1:E:817:VAL:HB	1:E:911:PHE:CZ	2.17	0.80
1:G:891:GLN:OE1	1:G:931:PRO:HB3	1.82	0.80
1:A:891:GLN:HE22	2:B:72:LEU:HB3	1.49	0.77
1:A:1097:LEU:HD21	1:A:1124:GLN:HB2	1.67	0.77
1:A:935:GLN:O	1:A:938:THR:HG22	1.86	0.76
1:E:923:ARG:O	2:F:5:ARG:NH2	2.19	0.76
1:E:902:GLN:NE2	1:E:912:VAL:HG11	2.01	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:8:LEU:O	2:D:8:LEU:HD23	1.89	0.73
2:H:121:LEU:HD22	2:H:127:THR:HG21	1.70	0.73
1:A:814:TYR:C	1:A:814:TYR:CD2	2.62	0.72
1:A:970:ILE:O	1:A:974:VAL:HG23	1.90	0.72
2:B:157:MET:CE	2:B:173:MET:SD	2.79	0.71
1:C:794:GLU:HA	1:C:797:TYR:CE2	2.25	0.70
1:A:789:GLN:NE2	1:A:860:VAL:HG13	2.06	0.70
1:C:784:CYS:SG	1:C:785:GLU:N	2.63	0.70
1:G:987:LEU:HD11	1:G:1020:MET:HB2	1.73	0.70
2:D:21:LEU:HD11	2:D:167:VAL:HG13	1.74	0.70
2:B:82:MET:HG2	2:B:95:ILE:HD12	1.75	0.69
2:B:12:GLY:O	2:B:13:ASP:O	2.11	0.69
1:G:831:ILE:HG12	1:G:897:MET:HG2	1.74	0.68
1:G:837:ASP:OD1	1:G:837:ASP:N	2.26	0.68
1:A:974:VAL:O	1:A:978:VAL:HG23	1.93	0.68
2:B:82:MET:CE	2:B:103:VAL:HG21	2.24	0.68
1:G:1040:THR:HG23	1:G:1048:VAL:O	1.95	0.67
1:G:924:LEU:HD22	1:G:928:ASP:CB	2.24	0.67
2:D:120:ASP:OD1	2:D:160:SER:OG	2.13	0.66
1:E:868:LEU:HD21	1:E:944:LEU:HD11	1.78	0.66
1:C:1096:ALA:HB2	1:C:1113:VAL:HB	1.77	0.66
1:C:1099:VAL:HG21	1:C:1112:LEU:HD12	1.79	0.64
1:E:1087:VAL:HA	1:E:1098:PHE:O	1.96	0.64
2:B:71:PRO:HA	2:B:74:TYR:HD2	1.62	0.64
2:D:157:MET:HB2	2:D:173:MET:CE	2.26	0.64
1:G:833:SER:HB3	1:G:890:ASN:HD22	1.63	0.64
1:C:1000:LYS:C	1:C:1002:SER:H	2.01	0.64
1:G:831:ILE:HG12	1:G:897:MET:CG	2.28	0.64
1:G:806:LEU:HB3	1:G:839:LEU:HD12	1.79	0.63
1:G:1021:ILE:O	1:G:1021:ILE:HG22	1.98	0.63
1:A:987:LEU:HD22	1:A:1015:LEU:HB3	1.79	0.63
2:H:107:CYS:HB3	2:H:110:VAL:HG21	1.81	0.63
1:E:1047:LEU:HD23	1:E:1080:ILE:HD12	1.79	0.63
1:A:941:PRO:O	1:A:945:ASP:OD2	2.17	0.63
1:G:984:LYS:HZ1	1:G:1016:THR:HB	1.63	0.63
1:E:1095:LYS:HE2	1:E:1117:VAL:HG22	1.81	0.62
2:F:71:PRO:HA	2:F:74:TYR:CD2	2.34	0.62
2:B:66:TYR:HB3	2:B:69:LEU:HD12	1.82	0.62
1:E:768:ASN:HD21	1:E:771:GLN:HB2	1.65	0.62
1:A:1025:PRO:HG2	1:A:1115:GLN:HE22	1.65	0.61
1:A:993:ARG:HH12	1:A:1057:LEU:HD21	1.65	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:1004:TYR:O	1:C:1006:ASN:N	2.34	0.61
1:C:999:LEU:HD11	1:C:1007:VAL:HG13	1.82	0.61
2:D:87:ASP:O	2:D:131:LEU:HD11	2.00	0.61
1:C:1000:LYS:O	1:C:1002:SER:N	2.33	0.60
1:E:924:LEU:HD22	1:E:928:ASP:HB3	1.84	0.60
1:C:794:GLU:HA	1:C:797:TYR:CD2	2.36	0.60
1:E:1049:LEU:HD11	1:E:1080:ILE:HD11	1.83	0.60
2:B:80:ILE:HD12	2:B:103:VAL:CG1	2.31	0.60
2:D:8:LEU:O	2:D:8:LEU:CD2	2.50	0.60
1:E:1027:VAL:HB	1:E:1113:VAL:HB	1.84	0.60
1:G:924:LEU:HD22	1:G:928:ASP:HB3	1.84	0.59
1:C:1095:LYS:HB3	1:C:1114:ALA:O	2.03	0.59
1:C:833:SER:OG	1:C:834:ASN:N	2.35	0.59
1:G:1021:ILE:O	1:G:1022:HIS:HB2	2.02	0.59
1:C:767:PRO:HG3	1:G:779:LEU:HD23	1.85	0.59
1:C:1020:MET:HE3	1:C:1023:GLU:HB3	1.83	0.59
1:A:1035:THR:O	1:A:1035:THR:OG1	2.14	0.59
1:C:1096:ALA:HA	1:C:1113:VAL:HA	1.84	0.58
2:F:116:GLY:N	2:F:157:MET:O	2.34	0.58
1:A:987:LEU:HD11	1:A:1020:MET:HB2	1.85	0.58
2:B:79:VAL:HG21	2:B:174:ALA:HB1	1.85	0.58
2:B:118:LYS:HG3	2:B:161:ALA:HB2	1.85	0.58
1:G:795:LEU:HA	1:G:943:LEU:HD13	1.86	0.58
2:F:68:ARG:O	2:F:71:PRO:HD2	2.03	0.58
1:C:955:THR:HB	1:E:811:GLN:OE1	2.04	0.58
1:A:854:LYS:O	1:A:855:ARG:C	2.40	0.58
2:D:66:TYR:O	2:D:68:ARG:N	2.38	0.57
1:E:770:GLN:NE2	1:E:790:GLU:OE2	2.36	0.57
2:H:21:LEU:HD11	2:H:167:VAL:HG13	1.84	0.57
2:H:81:LEU:HD23	2:H:113:ILE:HB	1.87	0.57
2:B:66:TYR:CB	2:B:69:LEU:HD12	2.34	0.57
2:B:86:ILE:O	2:B:86:ILE:HG22	2.03	0.57
1:E:882:HIS:O	1:E:886:THR:HG23	2.04	0.57
1:G:987:LEU:HD11	1:G:1020:MET:CB	2.33	0.57
1:E:944:LEU:HB3	1:E:964:ALA:HB2	1.87	0.57
1:C:1043:LEU:HD23	1:C:1043:LEU:N	2.20	0.57
1:A:869:LEU:HD23	1:A:963:ALA:HB2	1.87	0.57
2:D:126:HIS:C	2:D:126:HIS:ND1	2.57	0.57
2:D:62:GLY:N	2:D:64:GLU:OE1	2.36	0.56
1:G:975:ASN:OD1	2:H:68:ARG:CB	2.44	0.56
1:A:1016:THR:HG23	1:A:1016:THR:O	2.04	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1097:LEU:HD11	1:A:1124:GLN:N	2.21	0.56
2:B:118:LYS:HA	2:B:161:ALA:HB2	1.86	0.56
2:B:28:ASP:O	2:B:29:GLN:HB2	2.05	0.56
1:C:830:LYS:NZ	1:C:893:PHE:HB3	2.21	0.56
1:C:934:MET:O	1:C:938:THR:HG23	2.05	0.56
1:G:891:GLN:C	1:G:891:GLN:HE21	2.08	0.56
1:E:848:GLN:O	1:E:851:ALA:HB3	2.05	0.56
2:F:16:CYS:SG	2:F:84:PHE:HA	2.46	0.56
1:C:877:GLU:OE1	1:C:966:HIS:ND1	2.39	0.56
2:B:107:CYS:HB3	2:B:110:VAL:HG21	1.88	0.56
1:C:930:ILE:N	1:C:931:PRO:HD2	2.21	0.56
1:E:951:THR:HG22	1:E:957:ARG:HB2	1.86	0.56
1:E:881:LYS:HD3	1:E:973:PHE:CG	2.41	0.56
1:G:891:GLN:HE21	1:G:892:PRO:N	2.04	0.56
2:B:85:SER:HB3	2:B:88:SER:HB3	1.88	0.55
2:F:96:PRO:CB	2:F:150:ARG:NH2	2.69	0.55
1:E:975:ASN:HA	2:F:69:LEU:HD21	1.87	0.55
1:G:1021:ILE:O	1:G:1022:HIS:CB	2.54	0.55
1:A:1031:ASN:O	1:A:1035:THR:HG22	2.07	0.55
1:A:842:HIS:O	1:A:843:ILE:C	2.43	0.55
1:E:864:ILE:HG23	1:E:868:LEU:HD12	1.89	0.55
1:E:1041:LEU:O	1:E:1047:LEU:HD12	2.07	0.55
2:F:105:HIS:HD2	2:F:106:PHE:CE1	2.24	0.55
2:B:157:MET:HE1	2:B:173:MET:SD	2.47	0.55
1:E:789:GLN:NE2	1:E:861:ILE:O	2.38	0.55
2:B:10:ILE:HD13	2:B:18:LYS:HB3	1.88	0.55
1:A:1042:LEU:HD11	1:A:1130:MET:HG3	1.89	0.54
1:G:924:LEU:HD22	1:G:928:ASP:HB2	1.88	0.54
1:G:868:LEU:HD22	1:G:944:LEU:HD21	1.89	0.54
2:D:82:MET:SD	2:D:95:ILE:HG23	2.48	0.54
2:H:127:THR:O	2:H:129:ARG:N	2.40	0.54
1:E:881:LYS:O	1:E:885:ALA:HB2	2.06	0.54
2:H:71:PRO:HA	2:H:74:TYR:CD2	2.42	0.54
1:G:833:SER:HB3	1:G:890:ASN:ND2	2.22	0.54
1:A:865:GLY:N	1:A:956:GLU:OE1	2.38	0.54
2:F:151:ILE:O	2:F:151:ILE:HG22	2.08	0.54
1:E:795:LEU:HA	1:E:943:LEU:CD1	2.37	0.54
2:H:157:MET:HG2	2:H:170:VAL:HG22	1.89	0.54
2:B:86:ILE:HD12	2:B:122:ARG:NH2	2.23	0.54
1:C:823:LEU:HD11	1:C:908:PHE:CE1	2.43	0.54
1:A:935:GLN:OE1	2:B:41:ASN:ND2	2.41	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:979:LYS:O	1:G:983:ASN:OD1	2.26	0.54
1:G:1023:GLU:HA	1:G:1040:THR:O	2.08	0.53
2:B:74:TYR:HB3	2:B:107:CYS:SG	2.48	0.53
1:G:1094:ASN:OD1	1:G:1094:ASN:N	2.42	0.53
2:F:166:GLY:O	2:F:170:VAL:HG23	2.08	0.53
2:B:71:PRO:HA	2:B:74:TYR:CD2	2.42	0.53
1:G:1096:ALA:HB1	1:G:1111:GLU:HG3	1.89	0.53
1:G:962:LYS:O	1:G:965:ASP:N	2.40	0.53
2:D:83:CYS:HB2	2:D:115:VAL:O	2.09	0.53
1:G:1042:LEU:HD21	1:G:1130:MET:CG	2.34	0.53
1:A:902:GLN:HE21	1:A:909:GLN:HG2	1.72	0.53
2:D:71:PRO:HA	2:D:74:TYR:CD2	2.44	0.53
1:G:939:LYS:NZ	2:H:61:ALA:HB3	2.24	0.53
1:A:884:ALA:O	1:A:885:ALA:C	2.46	0.52
2:D:10:ILE:CG2	2:D:22:LEU:HD11	2.40	0.52
1:E:823:LEU:HD23	1:E:901:ARG:NH1	2.24	0.52
2:D:27:LYS:O	2:D:29:GLN:N	2.42	0.52
1:G:984:LYS:HA	1:G:984:LYS:HE2	1.90	0.52
1:G:939:LYS:HZ3	2:H:61:ALA:HB3	1.73	0.52
1:E:1027:VAL:CG2	1:E:1115:GLN:HE21	2.22	0.52
1:A:884:ALA:O	1:A:887:PHE:N	2.41	0.52
1:A:978:VAL:O	1:A:982:GLU:HG2	2.09	0.52
1:E:782:LYS:HB3	1:E:783:PRO:HD2	1.91	0.52
1:E:1018:ARG:CZ	1:E:1046:ILE:HD12	2.39	0.52
2:B:82:MET:HE2	2:B:103:VAL:HG21	1.90	0.52
1:C:799:GLU:HA	1:C:936:ARG:HH21	1.75	0.52
1:G:798:THR:CG2	1:G:936:ARG:NH1	2.73	0.52
2:B:100:THR:HG22	2:B:104:LYS:HD2	1.91	0.52
1:E:808:VAL:HG12	1:E:809:LEU:N	2.23	0.52
1:G:1120:LYS:HG3	1:G:1121:THR:N	2.24	0.52
1:G:841:LEU:HD21	1:G:880:LEU:HD13	1.90	0.52
2:D:107:CYS:HB3	2:D:110:VAL:HG21	1.92	0.52
1:E:844:GLY:O	1:E:848:GLN:HG3	2.10	0.52
2:D:95:ILE:HG22	2:D:151:ILE:HG21	1.93	0.52
1:E:1095:LYS:CE	1:E:1117:VAL:HG22	2.39	0.52
1:G:1124:GLN:O	1:G:1128:CYS:SG	2.61	0.51
1:E:813:PHE:CD1	1:E:926:LEU:HD13	2.45	0.51
1:E:834:ASN:O	1:E:837:ASP:N	2.39	0.51
1:E:974:VAL:O	1:E:978:VAL:HG23	2.09	0.51
1:G:1098:PHE:HA	1:G:1110:TYR:O	2.11	0.51
1:A:838:ILE:O	1:A:839:LEU:C	2.49	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:829:ARG:O	1:G:833:SER:HA	2.10	0.51
2:B:10:ILE:CG2	2:B:22:LEU:HD11	2.40	0.51
2:D:10:ILE:HG21	2:D:22:LEU:HD11	1.92	0.51
2:H:24:VAL:O	2:H:28:ASP:HA	2.11	0.51
2:H:7:LYS:N	2:H:78:ASP:OD2	2.43	0.51
2:D:21:LEU:CD1	2:D:167:VAL:HG13	2.41	0.51
1:C:773:VAL:CG1	1:C:777:VAL:HB	2.41	0.51
1:A:839:LEU:HD11	1:A:843:ILE:HD11	1.93	0.51
2:B:86:ILE:HD11	2:B:116:GLY:HA3	1.91	0.51
1:A:891:GLN:NE2	2:B:72:LEU:HB3	2.22	0.51
1:C:916:GLU:OE2	1:C:925:GLN:HB3	2.11	0.51
1:A:985:GLN:O	1:A:985:GLN:HG3	2.11	0.51
1:C:841:LEU:HD21	1:C:880:LEU:HD13	1.92	0.51
1:G:809:LEU:HD23	1:G:835:LEU:HD13	1.93	0.51
1:A:814:TYR:O	1:A:814:TYR:CD2	2.64	0.50
2:B:83:CYS:HB3	2:B:115:VAL:HB	1.93	0.50
1:E:1028:TRP:HB2	1:E:1038:LEU:HD12	1.93	0.50
1:E:1038:LEU:HD11	1:E:1049:LEU:HD22	1.94	0.50
1:E:1123:TRP:O	1:E:1127:ILE:HG13	2.11	0.50
1:A:929:ILE:O	1:A:932:THR:CG2	2.45	0.50
1:A:969:GLN:HA	1:A:972:ASN:HD22	1.76	0.50
2:D:47:GLU:OE2	2:D:50:GLY:HA2	2.11	0.50
1:E:809:LEU:HD13	1:E:929:ILE:CG2	2.42	0.50
1:A:774:SER:HB3	1:A:777:VAL:HG23	1.92	0.50
2:B:154:PHE:CD1	2:B:177:ALA:HB2	2.46	0.50
2:D:8:LEU:HD21	2:D:81:LEU:CD1	2.38	0.50
1:E:856:ASN:ND2	1:E:861:ILE:HA	2.26	0.50
1:G:1027:VAL:HG12	1:G:1028:TRP:N	2.27	0.50
1:A:946:ASN:O	1:A:947:ILE:C	2.49	0.50
2:B:10:ILE:HG21	2:B:22:LEU:HD11	1.92	0.50
2:B:99:TRP:O	2:B:103:VAL:HG23	2.11	0.50
1:E:1097:LEU:HD11	1:E:1124:GLN:HB2	1.92	0.50
1:A:1061:CYS:HB3	1:A:1078:PRO:HD3	1.93	0.50
2:B:70:ARG:N	2:B:71:PRO:CD	2.74	0.50
1:C:1038:LEU:CD1	1:C:1049:LEU:HD13	2.42	0.50
1:G:798:THR:HG22	1:G:936:ARG:NH1	2.27	0.50
2:H:157:MET:CG	2:H:170:VAL:HG22	2.42	0.50
1:A:1019:LYS:HB2	1:A:1044:GLU:CD	2.32	0.49
1:A:999:LEU:HD21	1:A:1010:LEU:HB3	1.94	0.49
1:C:922:ARG:C	1:C:923:ARG:HG3	2.32	0.49
1:C:799:GLU:HA	1:C:936:ARG:NH2	2.27	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:836:GLU:O	1:A:837:ASP:C	2.50	0.49
1:A:936:ARG:O	1:A:937:LEU:C	2.50	0.49
2:H:146:ASP:HA	2:H:149:ASN:HB2	1.95	0.49
1:E:1029:LYS:NZ	1:E:1113:VAL:HG21	2.27	0.49
1:E:809:LEU:HD23	1:E:835:LEU:HD13	1.94	0.49
1:G:848:GLN:O	1:G:851:ALA:HB3	2.11	0.49
2:B:74:TYR:N	2:B:75:PRO:HD3	2.26	0.49
1:E:1046:ILE:HG12	1:E:1081:LYS:HG3	1.93	0.49
1:G:940:TYR:O	1:G:941:PRO:C	2.49	0.49
1:E:890:ASN:O	1:E:891:GLN:C	2.50	0.49
1:E:841:LEU:CD2	1:E:880:LEU:HD13	2.42	0.49
2:H:127:THR:O	2:H:130:GLU:N	2.45	0.49
1:A:773:VAL:HG12	1:A:777:VAL:HB	1.94	0.49
2:B:96:PRO:HG3	2:B:147:MET:SD	2.52	0.49
1:C:947:ILE:O	1:C:951:THR:OG1	2.30	0.49
1:A:930:ILE:N	1:A:931:PRO:CD	2.76	0.49
2:B:40:GLU:O	2:B:41:ASN:C	2.49	0.49
2:B:8:LEU:HD21	2:B:81:LEU:HG	1.94	0.49
1:E:865:GLY:N	1:E:956:GLU:OE2	2.46	0.49
2:H:81:LEU:HD22	2:H:115:VAL:CG2	2.42	0.49
2:H:8:LEU:HD21	2:H:81:LEU:HD12	1.95	0.49
1:A:935:GLN:O	1:A:938:THR:CG2	2.60	0.49
2:B:100:THR:N	2:B:101:PRO:CD	2.76	0.49
1:E:991:GLN:HE22	1:E:994:LEU:HD22	1.78	0.48
2:F:102:GLU:O	2:F:106:PHE:CD2	2.66	0.48
1:G:984:LYS:NZ	1:G:1016:THR:HG22	2.28	0.48
1:A:916:GLU:OE2	1:A:925:GLN:HB3	2.12	0.48
2:B:157:MET:HE2	2:B:173:MET:SD	2.53	0.48
2:B:19:THR:O	2:B:22:LEU:HB2	2.14	0.48
1:E:823:LEU:HD21	1:E:908:PHE:CE1	2.47	0.48
2:H:81:LEU:HD22	2:H:115:VAL:HG22	1.95	0.48
1:C:822:ILE:HG22	1:C:823:LEU:HD23	1.95	0.48
1:C:945:ASP:O	1:C:948:ALA:N	2.45	0.48
1:C:955:THR:HB	1:E:811:GLN:CD	2.34	0.48
2:D:95:ILE:HG21	2:D:114:LEU:HD13	1.95	0.48
2:D:92:LEU:HD11	2:D:147:MET:HG2	1.95	0.48
1:A:785:GLU:O	1:A:789:GLN:HG2	2.14	0.48
1:E:897:MET:O	1:E:901:ARG:HG2	2.14	0.48
2:F:102:GLU:O	2:F:102:GLU:HG3	2.13	0.48
2:H:127:THR:O	2:H:128:ARG:C	2.51	0.48
1:C:848:GLN:O	1:C:851:ALA:HB3	2.13	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:1040:THR:HG22	1:E:1047:LEU:HD11	1.94	0.48
1:G:1038:LEU:HD22	1:G:1050:LEU:O	2.14	0.48
1:A:779:LEU:HA	1:A:779:LEU:HD12	1.78	0.48
2:B:59:ASP:OD1	2:B:61:ALA:N	2.45	0.48
1:G:1093:ASP:OD2	1:G:1096:ALA:N	2.46	0.48
2:D:12:GLY:O	2:D:13:ASP:O	2.32	0.48
1:C:999:LEU:HD22	1:C:1011:ARG:HG2	1.96	0.47
2:F:157:MET:HG2	2:F:170:VAL:HG22	1.95	0.47
1:G:799:GLU:OE2	1:G:940:TYR:OH	2.20	0.47
1:C:801:ALA:O	1:C:804:ARG:HB3	2.14	0.47
1:E:974:VAL:HG12	2:F:69:LEU:HD21	1.96	0.47
2:F:100:THR:OG1	2:F:151:ILE:HD13	2.14	0.47
1:G:984:LYS:HZ1	1:G:1016:THR:CB	2.27	0.47
2:B:42:TYR:CD2	2:B:42:TYR:C	2.88	0.47
1:C:1002:SER:HB2	1:C:1004:TYR:CE2	2.49	0.47
1:C:775:ARG:HD3	1:C:779:LEU:HD13	1.96	0.47
1:C:852:VAL:HA	1:C:855:ARG:HD3	1.96	0.47
1:G:957:ARG:HD2	1:G:961:LYS:NZ	2.29	0.47
2:F:7:LYS:HG3	2:F:58:TRP:CD1	2.50	0.47
1:G:839:LEU:HG	1:G:843:ILE:CD1	2.44	0.47
2:B:112:ILE:O	2:B:154:PHE:HB3	2.15	0.47
1:C:1084:THR:HB	1:C:1102:MET:HB2	1.97	0.47
1:C:854:LYS:NZ	1:C:854:LYS:HB2	2.29	0.47
1:A:791:VAL:O	1:A:794:GLU:N	2.48	0.47
1:E:1090:VAL:O	1:E:1090:VAL:HG12	2.15	0.47
1:A:1036:ILE:HG22	1:A:1037:ASP:N	2.30	0.47
2:B:86:ILE:O	2:B:86:ILE:CG2	2.62	0.47
1:C:841:LEU:CD2	1:C:880:LEU:HD13	2.44	0.47
1:A:801:ALA:O	1:A:804:ARG:HB3	2.15	0.47
2:D:8:LEU:C	2:D:8:LEU:HD23	2.34	0.47
1:E:932:THR:HG22	1:E:935:GLN:OE1	2.15	0.47
1:E:993:ARG:NE	1:E:1055:ASP:O	2.47	0.47
1:A:944:LEU:HD23	1:A:944:LEU:N	2.30	0.47
1:E:1038:LEU:O	1:E:1052:LYS:NZ	2.44	0.47
1:E:943:LEU:O	1:E:947:ILE:HG13	2.15	0.47
1:G:1021:ILE:HB	1:G:1042:LEU:HG	1.97	0.47
1:G:934:MET:CE	2:H:63:GLN:NE2	2.78	0.47
1:A:774:SER:CB	1:A:777:VAL:HG23	2.46	0.47
1:E:993:ARG:HB3	1:E:1056:ARG:HG2	1.97	0.47
1:G:844:GLY:O	1:G:848:GLN:HG3	2.15	0.47
2:H:114:LEU:HB3	2:H:156:TYR:HD1	1.80	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1126:LEU:O	1:A:1130:MET:HG2	2.16	0.46
1:A:881:LYS:HB2	1:A:973:PHE:CD2	2.50	0.46
2:B:180:GLN:O	2:B:181:ALA:HB3	2.15	0.46
1:C:1053:GLN:O	1:C:1054:ASP:C	2.53	0.46
1:G:813:PHE:CD1	1:G:926:LEU:HD13	2.50	0.46
1:G:911:PHE:CD2	1:G:912:VAL:N	2.82	0.46
1:E:856:ASN:ND2	1:E:862:ASP:H	2.13	0.46
1:E:1128:CYS:O	1:E:1132:ALA:N	2.47	0.46
1:E:799:GLU:OE2	1:E:940:TYR:OH	2.26	0.46
1:G:987:LEU:HD22	1:G:1015:LEU:HB3	1.97	0.46
1:C:1000:LYS:C	1:C:1002:SER:N	2.68	0.46
1:E:1055:ASP:N	1:E:1055:ASP:OD1	2.48	0.46
1:A:898:ILE:HD13	1:A:926:LEU:HG	1.98	0.46
1:C:856:ASN:HD22	1:C:862:ASP:HB2	1.81	0.46
1:A:838:ILE:O	1:A:841:LEU:N	2.49	0.46
1:C:1124:GLN:O	1:C:1128:CYS:HB2	2.16	0.46
1:C:852:VAL:HG22	1:C:855:ARG:NH1	2.31	0.46
2:B:22:LEU:HD22	2:B:57:LEU:HB3	1.98	0.46
1:E:949:LYS:HE3	1:E:950:TYR:CZ	2.51	0.46
2:F:159:CYS:HA	2:F:165:ASP:O	2.15	0.46
1:G:1018:ARG:HB2	1:G:1044:GLU:HB3	1.97	0.46
1:G:973:PHE:O	1:G:976:GLN:HB3	2.15	0.46
2:F:112:ILE:O	2:F:154:PHE:N	2.49	0.46
1:C:1041:LEU:O	1:C:1047:LEU:HD12	2.16	0.46
1:C:940:TYR:HB2	1:C:941:PRO:HD3	1.97	0.45
1:C:989:ASP:HA	1:C:992:ARG:HE	1.80	0.45
1:C:787:LYS:O	1:C:791:VAL:HG23	2.16	0.45
1:C:891:GLN:HB3	1:C:892:PRO:HD3	1.98	0.45
2:D:126:HIS:HA	2:D:129:ARG:HD2	1.97	0.45
2:F:65:ASP:HB2	2:F:66:TYR:CE2	2.51	0.45
2:F:70:ARG:N	2:F:71:PRO:CD	2.79	0.45
2:B:116:GLY:O	2:B:158:GLU:HA	2.16	0.45
1:E:912:VAL:O	1:E:915:ALA:HB3	2.16	0.45
1:E:791:VAL:HG11	1:E:946:ASN:HB2	1.97	0.45
1:G:1100:ILE:HG22	1:G:1101:SER:N	2.31	0.45
2:D:95:ILE:N	2:D:96:PRO:CD	2.79	0.45
1:G:938:THR:HG21	2:H:63:GLN:CG	2.46	0.45
2:D:80:ILE:HD12	2:D:103:VAL:HG22	1.97	0.45
1:E:770:GLN:HE22	2:F:33:VAL:HG12	1.81	0.45
1:E:809:LEU:HD13	1:E:929:ILE:HG22	1.97	0.45
1:E:856:ASN:OD1	1:E:856:ASN:N	2.48	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:7:LYS:HB3	2:F:76:ASP:O	2.16	0.45
2:D:118:LYS:HB3	2:D:121:LEU:HD12	1.98	0.45
1:G:847:GLU:HA	1:G:847:GLU:OE2	2.16	0.45
1:E:782:LYS:HB3	1:E:783:PRO:CD	2.47	0.45
1:E:934:MET:C	1:E:934:MET:SD	2.94	0.45
1:G:806:LEU:HB3	1:G:839:LEU:CD1	2.44	0.45
1:G:984:LYS:HZ3	1:G:1016:THR:HG22	1.81	0.45
1:A:1022:HIS:HB2	1:A:1126:LEU:HD13	1.98	0.45
2:B:122:ARG:O	2:B:122:ARG:HG2	2.16	0.45
2:D:102:GLU:O	2:D:105:HIS:HB3	2.17	0.45
2:D:82:MET:O	2:D:83:CYS:HB3	2.16	0.45
1:G:823:LEU:HB3	1:G:827:GLU:HB2	1.98	0.45
1:A:865:GLY:O	1:A:866:GLU:C	2.54	0.45
1:C:822:ILE:HG22	1:C:823:LEU:CD2	2.46	0.45
2:D:175:THR:O	2:D:179:LEU:HG	2.16	0.45
1:E:1111:GLU:C	1:E:1112:LEU:HG	2.38	0.45
1:E:834:ASN:O	1:E:835:LEU:C	2.54	0.45
1:G:813:PHE:CG	1:G:926:LEU:HD13	2.52	0.45
1:A:939:LYS:O	1:A:943:LEU:HD12	2.16	0.44
2:B:147:MET:O	2:B:151:ILE:HG23	2.17	0.44
1:C:918:ASN:OD1	1:C:918:ASN:C	2.56	0.44
1:E:991:GLN:HE22	1:E:994:LEU:CD2	2.30	0.44
1:A:846:ASN:HD21	1:A:850:LYS:HE3	1.81	0.44
2:B:140:LYS:O	2:B:143:GLU:HB2	2.17	0.44
1:C:773:VAL:HG12	1:C:774:SER:O	2.17	0.44
2:D:129:ARG:O	2:D:132:ALA:N	2.50	0.44
1:E:788:ARG:O	1:E:791:VAL:N	2.50	0.44
1:G:1095:LYS:O	1:G:1120:LYS:HB2	2.18	0.44
1:G:839:LEU:HG	1:G:843:ILE:HD11	1.99	0.44
2:H:95:ILE:HB	2:H:96:PRO:HD3	1.99	0.44
1:E:856:ASN:HD22	1:E:862:ASP:H	1.66	0.44
1:G:814:TYR:C	1:G:814:TYR:CD2	2.90	0.44
2:H:108:PRO:O	2:H:110:VAL:HG23	2.18	0.44
1:C:778:LEU:HD22	1:C:786:ILE:HD11	2.00	0.44
1:G:776:GLU:OE2	1:G:776:GLU:N	2.50	0.44
1:A:945:ASP:OD2	1:A:968:ARG:NH2	2.51	0.44
1:C:1051:GLN:O	1:C:1058:VAL:N	2.50	0.44
1:C:940:TYR:N	1:C:941:PRO:CD	2.81	0.44
1:C:956:GLU:O	1:C:957:ARG:C	2.56	0.44
1:C:1028:TRP:HD1	1:C:1111:GLU:O	2.00	0.44
2:D:146:ASP:O	2:D:149:ASN:N	2.51	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:82:MET:O	2:F:114:LEU:HD12	2.17	0.44
2:F:142:GLU:O	2:F:143:GLU:C	2.56	0.44
1:A:791:VAL:HG11	1:A:947:ILE:HG13	2.00	0.44
2:D:25:PHE:CD1	2:D:171:PHE:CD2	3.06	0.44
1:E:831:ILE:HG13	1:E:897:MET:HG2	1.99	0.44
2:F:151:ILE:O	2:F:151:ILE:CG2	2.66	0.44
1:G:983:ASN:ND2	1:G:1020:MET:O	2.51	0.44
1:A:885:ALA:HB1	1:A:977:ALA:CB	2.48	0.43
1:A:910:THR:HG22	1:A:911:PHE:N	2.33	0.43
2:D:126:HIS:ND1	2:D:126:HIS:O	2.50	0.43
1:G:1024:GLY:O	1:G:1039:TYR:HA	2.18	0.43
1:G:895:LEU:HD21	1:G:927:LYS:HA	1.99	0.43
1:G:938:THR:HG21	2:H:63:GLN:HG3	1.99	0.43
1:A:1116:THR:O	1:A:1117:VAL:C	2.56	0.43
2:B:154:PHE:CE1	2:B:177:ALA:HB2	2.53	0.43
2:B:86:ILE:HG12	2:B:117:ASN:O	2.17	0.43
2:B:8:LEU:C	2:B:8:LEU:HD23	2.39	0.43
1:E:931:PRO:O	1:E:934:MET:N	2.51	0.43
2:B:12:GLY:O	2:B:13:ASP:C	2.57	0.43
1:C:782:LYS:NZ	1:E:922:ARG:HH12	2.17	0.43
2:D:95:ILE:HB	2:D:96:PRO:HD3	2.00	0.43
1:E:1027:VAL:HG22	1:E:1115:GLN:HE21	1.82	0.43
1:E:974:VAL:HG12	1:E:975:ASN:N	2.32	0.43
2:F:27:LYS:O	2:F:28:ASP:C	2.57	0.43
2:F:49:ASP:N	2:F:49:ASP:OD2	2.51	0.43
2:B:129:ARG:HB3	2:B:129:ARG:HE	1.69	0.43
1:E:831:ILE:HG22	1:E:832:PHE:N	2.32	0.43
1:G:778:LEU:HD22	1:G:786:ILE:HD11	1.99	0.43
1:G:868:LEU:HD21	1:G:944:LEU:HD11	2.01	0.43
2:B:162:LYS:C	2:B:163:THR:HG23	2.39	0.43
2:H:103:VAL:CG1	2:H:112:ILE:HD11	2.48	0.43
2:B:118:LYS:CG	2:B:161:ALA:HB2	2.48	0.43
1:C:828:LEU:HA	1:C:828:LEU:HD23	1.85	0.43
1:E:991:GLN:HE21	1:E:991:GLN:HA	1.82	0.43
1:G:836:GLU:OE1	1:G:840:GLN:HG2	2.19	0.43
2:H:169:GLU:N	2:H:169:GLU:OE1	2.50	0.43
1:A:922:ARG:C	1:A:923:ARG:HG3	2.38	0.43
1:C:770:GLN:HE21	1:C:786:ILE:HG21	1.84	0.43
2:D:74:TYR:N	2:D:75:PRO:CD	2.81	0.43
1:G:945:ASP:OD2	1:G:968:ARG:NH2	2.51	0.43
2:H:74:TYR:HB3	2:H:107:CYS:SG	2.58	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:6:LYS:HD2	2:H:178:ALA:HB1	2.00	0.43
2:B:68:ARG:HD2	2:B:68:ARG:HA	1.85	0.43
2:D:82:MET:HG2	2:D:95:ILE:HD12	2.00	0.43
2:H:129:ARG:O	2:H:132:ALA:N	2.51	0.43
1:A:936:ARG:O	1:A:938:THR:N	2.52	0.43
1:C:809:LEU:HD13	1:C:929:ILE:CG2	2.49	0.43
1:E:1014:ASP:O	1:E:1015:LEU:C	2.57	0.43
2:H:74:TYR:N	2:H:75:PRO:HD2	2.33	0.43
1:A:799:GLU:O	1:A:803:VAL:HG23	2.19	0.43
2:D:157:MET:CG	2:D:170:VAL:HG22	2.49	0.43
1:E:886:THR:OG1	1:E:887:PHE:N	2.52	0.43
2:F:95:ILE:N	2:F:96:PRO:CD	2.81	0.43
1:G:1097:LEU:CD1	1:G:1124:GLN:HB2	2.49	0.43
2:B:142:GLU:O	2:B:143:GLU:C	2.57	0.42
1:C:833:SER:HB3	1:C:890:ASN:ND2	2.34	0.42
2:F:47:GLU:HG3	2:F:52:GLN:HE22	1.84	0.42
1:G:1090:VAL:HG21	1:G:1096:ALA:HB3	2.00	0.42
1:A:953:TRP:HA	1:A:954:PRO:HD2	1.89	0.42
1:A:962:LYS:O	1:A:963:ALA:C	2.57	0.42
2:B:127:THR:O	2:B:128:ARG:C	2.57	0.42
1:A:1031:ASN:HB3	1:A:1034:LYS:HB2	2.01	0.42
1:C:1085:VAL:HG12	1:C:1086:LEU:N	2.34	0.42
1:E:891:GLN:NE2	2:F:72:LEU:O	2.51	0.42
1:C:1089:GLN:HE21	1:C:1120:LYS:NZ	2.17	0.42
1:C:924:LEU:HB3	1:C:928:ASP:HB2	2.02	0.42
1:G:1022:HIS:CG	1:G:1023:GLU:N	2.86	0.42
2:F:34:TYR:CE2	2:F:36:PRO:HA	2.55	0.42
1:A:971:LEU:O	1:A:972:ASN:C	2.56	0.42
2:D:22:LEU:O	2:D:26:SER:OG	2.28	0.42
2:D:83:CYS:HB3	2:D:115:VAL:HB	2.01	0.42
1:E:932:THR:HA	1:E:935:GLN:HB2	2.01	0.42
1:E:942:LEU:HD23	1:E:942:LEU:N	2.35	0.42
1:G:1042:LEU:HD11	1:G:1130:MET:HG3	2.02	0.42
1:G:940:TYR:HB2	1:G:941:PRO:HD3	2.02	0.42
1:C:1092:THR:O	1:C:1092:THR:HG22	2.20	0.42
1:E:902:GLN:HE22	1:E:912:VAL:HG11	1.82	0.42
1:A:946:ASN:O	1:A:949:LYS:N	2.53	0.42
1:C:997:SER:C	1:C:999:LEU:H	2.22	0.42
2:D:86:ILE:HG22	2:D:86:ILE:O	2.19	0.42
1:E:1087:VAL:CG1	1:E:1097:LEU:HD22	2.49	0.42
1:G:962:LYS:O	1:G:963:ALA:C	2.57	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:799:GLU:CA	1:C:936:ARG:NH2	2.83	0.42
1:C:968:ARG:HD3	2:D:66:TYR:OH	2.20	0.42
1:E:1039:TYR:O	1:E:1050:LEU:HB2	2.20	0.42
1:G:947:ILE:HG22	1:G:960:VAL:HG11	2.02	0.42
1:A:845:LEU:HD11	1:A:871:TRP:HB3	2.02	0.41
1:C:1026:LEU:HD21	1:C:1123:TRP:NE1	2.34	0.41
2:D:58:TRP:CD1	2:D:58:TRP:N	2.88	0.41
2:D:87:ASP:C	2:D:87:ASP:OD1	2.59	0.41
1:E:1123:TRP:O	1:E:1127:ILE:CG1	2.68	0.41
1:A:1000:LYS:NZ	1:A:1000:LYS:HB3	2.35	0.41
1:A:791:VAL:O	1:A:792:ILE:C	2.55	0.41
1:A:891:GLN:HB3	1:A:892:PRO:HD3	2.01	0.41
1:A:968:ARG:O	1:A:971:LEU:N	2.53	0.41
2:B:82:MET:HG2	2:B:95:ILE:CD1	2.46	0.41
1:C:980:GLU:O	1:C:984:LYS:HB2	2.20	0.41
1:E:813:PHE:O	1:E:814:TYR:C	2.59	0.41
2:H:63:GLN:HB3	2:H:70:ARG:HB2	2.02	0.41
1:A:808:VAL:O	1:A:812:VAL:HB	2.21	0.41
1:C:789:GLN:NE2	1:C:860:VAL:CG1	2.83	0.41
1:C:809:LEU:HD13	1:C:929:ILE:HG21	2.02	0.41
1:G:823:LEU:HD13	1:G:831:ILE:HD12	2.02	0.41
1:C:1060:ARG:HG2	1:C:1061:CYS:N	2.36	0.41
1:C:953:TRP:HA	1:C:954:PRO:HD3	1.87	0.41
1:E:834:ASN:O	1:E:836:GLU:N	2.53	0.41
1:G:1080:ILE:O	1:G:1081:LYS:C	2.59	0.41
1:G:849:MET:C	1:G:851:ALA:H	2.23	0.41
1:A:1004:TYR:CD1	1:A:1006:ASN:HB3	2.56	0.41
1:A:1026:LEU:HD23	1:A:1026:LEU:HA	1.93	0.41
1:A:798:THR:CG2	1:A:936:ARG:NH1	2.84	0.41
2:B:21:LEU:HD12	2:B:21:LEU:O	2.21	0.41
1:G:824:SER:HB2	1:G:825:PRO:HD2	2.03	0.41
2:H:70:ARG:N	2:H:71:PRO:HD2	2.36	0.41
1:E:1124:GLN:O	1:E:1125:ASP:C	2.58	0.41
1:E:796:PHE:CD1	1:E:849:MET:HG2	2.56	0.41
2:B:172:GLU:O	2:B:176:ARG:HG3	2.21	0.41
1:E:845:LEU:HD12	1:E:845:LEU:HA	1.86	0.41
1:G:781:LEU:HD22	1:G:785:GLU:HG2	2.03	0.41
1:G:831:ILE:CG1	1:G:897:MET:HG2	2.48	0.41
2:B:53:VAL:HG12	2:B:54:GLU:N	2.36	0.41
1:E:812:VAL:HG12	1:E:812:VAL:O	2.20	0.41
2:F:133:LYS:C	2:F:135:LYS:H	2.24	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:809:LEU:HD13	1:G:929:ILE:HG22	2.03	0.41
1:E:917:SER:O	1:E:918:ASN:C	2.59	0.41
1:G:1087:VAL:HA	1:G:1098:PHE:O	2.21	0.41
1:G:1089:GLN:HB2	1:G:1124:GLN:HE22	1.86	0.41
1:G:895:LEU:CD2	1:G:927:LYS:HB2	2.50	0.41
2:B:134:MET:O	2:B:135:LYS:HB2	2.20	0.40
1:E:841:LEU:HD12	1:E:879:LYS:NZ	2.36	0.40
2:H:8:LEU:HD23	2:H:9:VAL:N	2.36	0.40
2:B:25:PHE:O	2:B:25:PHE:CD1	2.74	0.40
1:E:794:GLU:OE1	2:F:38:VAL:HG23	2.21	0.40
1:E:979:LYS:HA	2:F:68:ARG:NH1	2.36	0.40
1:G:881:LYS:HD3	1:G:973:PHE:CG	2.56	0.40
1:G:925:GLN:N	1:G:928:ASP:OD1	2.51	0.40
1:G:937:LEU:HA	1:G:937:LEU:HD12	1.92	0.40
1:G:975:ASN:HA	2:H:69:LEU:HD21	2.04	0.40
1:A:768:ASN:OD1	1:A:768:ASN:N	2.54	0.40
1:A:905:ASP:HB3	1:A:908:PHE:HB3	2.02	0.40
2:B:17:GLY:HA2	3:B:401:PO4:P	2.62	0.40
2:D:83:CYS:CB	2:D:115:VAL:O	2.69	0.40
1:E:1049:LEU:HD12	1:E:1078:PRO:HA	2.04	0.40
1:E:913:GLN:C	1:E:915:ALA:H	2.25	0.40
1:G:966:HIS:HA	1:G:969:GLN:HG3	2.03	0.40
1:A:794:GLU:HA	1:A:797:TYR:CE2	2.56	0.40
1:A:936:ARG:C	1:A:938:THR:N	2.73	0.40
2:B:20:CYS:O	2:B:23:ILE:HB	2.22	0.40
1:C:1050:LEU:CD2	1:C:1059:LEU:HD13	2.51	0.40
1:E:940:TYR:HB2	1:E:941:PRO:HD3	2.03	0.40
2:H:121:LEU:HD22	2:H:127:THR:CG2	2.47	0.40
2:H:21:LEU:CD1	2:H:167:VAL:HG13	2.51	0.40

There are no symmetry-related clashes.

## 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	358/385 (93%)	306 (86%)	40 (11%)	12 (3%)	4	29
1	C	358/385 (93%)	309 (86%)	40 (11%)	9 (2%)	6	38
1	E	326/385 (85%)	276 (85%)	41 (13%)	9 (3%)	6	34
1	G	304/385 (79%)	255 (84%)	41 (14%)	8 (3%)	6	37
2	B	178/196 (91%)	152 (85%)	24 (14%)	2 (1%)	17	58
2	D	178/196 (91%)	149 (84%)	21 (12%)	8 (4%)	3	21
2	F	177/196 (90%)	147 (83%)	24 (14%)	6 (3%)	4	29
2	H	177/196 (90%)	146 (82%)	26 (15%)	5 (3%)	6	34
All	All	2056/2324 (88%)	1740 (85%)	257 (12%)	59 (3%)	5	33

All (59) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	768	ASN
2	B	13	ASP
1	C	836	GLU
1	C	1001	LEU
1	C	1054	ASP
2	D	13	ASP
2	D	28	ASP
2	D	67	ASP
1	G	1022	HIS
2	H	128	ARG
2	B	29	GLN
1	C	826	SER
1	C	1005	PRO
2	D	16	CYS
2	D	86	ILE
1	E	862	ASP
2	F	16	CYS
2	F	28	ASP
1	G	855	ARG
1	G	862	ASP
2	H	154	PHE
1	A	833	SER
1	A	858	THR
1	A	866	GLU
1	A	947	ILE
1	A	1001	LEU
2	D	129	ARG

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Mol	Chain	Res	Type
1	E	981	ALA
2	F	17	GLY
2	F	118	LYS
1	A	862	ASP
1	A	937	LEU
1	A	1005	PRO
1	C	822	ILE
2	D	93	GLU
1	E	783	PRO
2	F	13	ASP
1	G	774	SER
2	H	98	LYS
1	A	954	PRO
1	A	1118	SER
1	C	828	LEU
1	E	835	LEU
1	E	891	GLN
1	G	783	PRO
1	G	903	LYS
1	G	1081	LYS
1	A	851	ALA
1	C	862	ASP
1	G	954	PRO
2	H	152	GLY
1	E	782	LYS
1	E	1117	VAL
1	E	831	ILE
1	C	919	PRO
1	E	864	ILE
2	D	31	PRO
2	F	33	VAL
2	H	151	ILE

### 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	336/354 (95%)	284 (84%)	52 (16%)	3	14
1	C	336/354 (95%)	313 (93%)	23 (7%)	18	55
1	E	313/354 (88%)	274 (88%)	39 (12%)	5	24
1	G	290/354 (82%)	258 (89%)	32 (11%)	7	31
2	B	156/169 (92%)	145 (93%)	11 (7%)	17	54
2	D	156/169 (92%)	146 (94%)	10 (6%)	20	59
2	F	156/169 (92%)	143 (92%)	13 (8%)	13	46
2	H	156/169 (92%)	149 (96%)	7 (4%)	32	70
All	All	1899/2092 (91%)	1712 (90%)	187 (10%)	9	36

All (187) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	771	GLN
1	A	773	VAL
1	A	774	SER
1	A	788	ARG
1	A	797	TYR
1	A	800	ARG
1	A	820	GLU
1	A	829	ARG
1	A	830	LYS
1	A	835	LEU
1	A	846	ASN
1	A	848	GLN
1	A	856	ASN
1	A	864	ILE
1	A	873	SER
1	A	880	LEU
1	A	897	MET
1	A	899	LYS
1	A	903	LYS
1	A	906	SER
1	A	910	THR
1	A	914	ASP
1	A	923	ARG
1	A	926	LEU
1	A	938	THR
1	A	944	LEU
1	A	952	GLU

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Mol	Chain	Res	Type
1	A	982	GLU
1	A	995	ASP
1	A	1000	LYS
1	A	1004	TYR
1	A	1007	VAL
1	A	1016	THR
1	A	1018	ARG
1	A	1019	LYS
1	A	1032	ARG
1	A	1035	THR
1	A	1052	LYS
1	A	1053	GLN
1	A	1054	ASP
1	A	1055	ASP
1	A	1060	ARG
1	A	1075	THR
1	A	1077	SER
1	A	1083	SER
1	A	1092	THR
1	A	1102	MET
1	A	1108	GLN
1	A	1120	LYS
1	A	1122	VAL
1	A	1128	CYS
1	A	1134	VAL
2	B	4	ILE
2	B	8	LEU
2	B	18	LYS
2	B	21	LEU
2	B	33	VAL
2	B	54	GLU
2	B	60	THR
2	B	85	SER
2	B	98	LYS
2	B	119	LYS
2	B	126	HIS
1	C	775	ARG
1	C	778	LEU
1	C	786	ILE
1	C	787	LYS
1	C	793	ASN
1	C	817	VAL

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Mol	Chain	Res	Type
1	C	826	SER
1	C	839	LEU
1	C	856	ASN
1	C	859	SER
1	C	914	ASP
1	C	943	LEU
1	C	975	ASN
1	C	1016	THR
1	C	1032	ARG
1	C	1075	THR
1	C	1093	ASP
1	C	1102	MET
1	C	1104	ASP
1	C	1105	ASN
1	C	1113	VAL
1	C	1120	LYS
1	C	1128	CYS
2	D	8	LEU
2	D	16	CYS
2	D	49	ASP
2	D	102	GLU
2	D	103	VAL
2	D	117	ASN
2	D	126	HIS
2	D	143	GLU
2	D	145	ARG
2	D	173	MET
1	E	768	ASN
1	E	773	VAL
1	E	774	SER
1	E	775	ARG
1	E	776	GLU
1	E	787	LYS
1	E	804	ARG
1	E	823	LEU
1	E	854	LYS
1	E	856	ASN
1	E	859	SER
1	E	862	ASP
1	E	864	ILE
1	E	868	LEU
1	E	877	GLU

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Mol	Chain	Res	Type
1	E	909	GLN
1	E	911	PHE
1	E	922	ARG
1	E	934	MET
1	E	938	THR
1	E	944	LEU
1	E	949	LYS
1	E	987	LEU
1	E	991	GLN
1	E	995	ASP
1	E	996	THR
1	E	1008	GLU
1	E	1030	VAL
1	E	1033	ASP
1	E	1037	ASP
1	E	1039	TYR
1	E	1052	LYS
1	E	1055	ASP
1	E	1077	SER
1	E	1080	ILE
1	E	1089	GLN
1	E	1120	LYS
1	E	1127	ILE
1	E	1129	ARG
2	F	11	VAL
2	F	21	LEU
2	F	38	VAL
2	F	49	ASP
2	F	53	VAL
2	F	55	LEU
2	F	73	SER
2	F	78	ASP
2	F	85	SER
2	F	102	GLU
2	F	137	GLU
2	F	173	MET
2	F	175	THR
1	G	776	GLU
1	G	778	LEU
1	G	797	TYR
1	G	800	ARG
1	G	805	THR

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Mol	Chain	Res	Type
1	G	806	LEU
1	G	815	GLN
1	G	817	VAL
1	G	830	LYS
1	G	837	ASP
1	G	841	LEU
1	G	846	ASN
1	G	856	ASN
1	G	863	GLN
1	G	867	ASP
1	G	886	THR
1	G	891	GLN
1	G	893	PHE
1	G	909	GLN
1	G	911	PHE
1	G	932	THR
1	G	934	MET
1	G	937	LEU
1	G	971	LEU
1	G	984	LYS
1	G	993	ARG
1	G	1041	LEU
1	G	1049	LEU
1	G	1055	ASP
1	G	1094	ASN
1	G	1120	LYS
1	G	1121	THR
2	H	26	SER
2	H	33	VAL
2	H	49	ASP
2	H	83	CYS
2	H	125	GLU
2	H	143	GLU
2	H	175	THR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (39) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	815	GLN
1	A	846	ASN
1	A	848	GLN
1	A	856	ASN

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Mol	Chain	Res	Type
1	A	891	GLN
1	A	902	GLN
1	A	935	GLN
1	A	969	GLN
1	A	972	ASN
1	A	1022	HIS
1	A	1089	GLN
1	A	1115	GLN
2	B	41	ASN
2	B	117	ASN
1	C	770	GLN
1	C	793	ASN
1	C	848	GLN
1	C	856	ASN
1	C	925	GLN
1	C	1012	ASN
1	C	1089	GLN
1	E	768	ASN
1	E	771	GLN
1	E	882	HIS
1	E	902	GLN
1	E	925	GLN
1	E	935	GLN
1	E	972	ASN
1	E	991	GLN
1	E	1031	ASN
1	E	1115	GLN
2	F	105	HIS
2	F	109	ASN
1	G	891	GLN
1	G	902	GLN
1	G	925	GLN
1	G	935	GLN
1	G	991	GLN
1	G	1124	GLN

### 5.3.3 RNA ⓘ

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	$\# Z  > 2$
3	PO4	B	401	-	4,4,4	0.80	0	6,6,6	0.23	0
3	PO4	D	402	-	4,4,4	0.79	0	6,6,6	0.33	0
3	PO4	F	403	-	4,4,4	0.79	0	6,6,6	0.34	0
3	PO4	H	404	-	4,4,4	0.67	0	6,6,6	0.54	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
3	PO4	B	401	-	-	0/0/0/0	0/0/0/0
3	PO4	D	402	-	-	0/0/0/0	0/0/0/0
3	PO4	F	403	-	-	0/0/0/0	0/0/0/0
3	PO4	H	404	-	-	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.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	401	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<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	362/385 (94%)	-0.19	3 (0%) 86 78	15, 38, 57, 82	0
1	C	362/385 (94%)	0.02	10 (2%) 53 40	22, 42, 55, 61	0
1	E	336/385 (87%)	0.23	26 (7%) 14 8	14, 51, 67, 74	0
1	G	314/385 (81%)	0.36	31 (9%) 8 5	26, 48, 59, 63	0
2	B	180/196 (91%)	-0.35	0 100 100	15, 34, 51, 66	0
2	D	180/196 (91%)	-0.20	0 100 100	23, 43, 56, 63	0
2	F	179/196 (91%)	0.29	7 (3%) 40 27	39, 53, 62, 65	0
2	H	179/196 (91%)	0.36	13 (7%) 16 10	36, 46, 53, 55	0
All	All	2092/2324 (90%)	0.07	90 (4%) 36 24	14, 45, 60, 82	0

All (90) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	G	1082	LEU	7.9
1	G	1113	VAL	6.0
1	G	1027	VAL	5.8
1	G	1114	ALA	5.4
1	G	994	LEU	5.2
1	G	1079	VAL	5.1
1	G	1026	LEU	5.0
1	E	1090	VAL	4.9
1	E	1013	LEU	4.6
1	G	1051	GLN	4.3
1	G	1112	LEU	4.3
2	H	156	TYR	4.2
2	F	121	LEU	4.2
1	G	1057	LEU	4.2
1	G	1058	VAL	3.9
1	E	1026	LEU	3.9

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Mol	Chain	Res	Type	RSRZ
2	F	114	LEU	3.9
1	C	1013	LEU	3.8
1	E	1050	LEU	3.8
1	G	1052	LYS	3.7
2	H	49	ASP	3.7
1	C	1006	ASN	3.6
1	G	992	ARG	3.6
1	E	1057	LEU	3.6
1	E	1116	THR	3.5
1	E	1112	LEU	3.5
1	E	1049	LEU	3.4
1	G	1049	LEU	3.4
1	E	1029	LYS	3.3
2	H	154	PHE	3.3
1	G	1111	GLU	3.3
1	C	908	PHE	3.3
1	C	1034	LYS	3.2
2	F	53	VAL	3.2
2	H	139	VAL	3.2
1	E	1115	GLN	3.1
1	G	1045	ASP	3.1
1	G	1018	ARG	3.0
1	E	1039	TYR	3.0
1	E	1080	ILE	2.9
1	E	1037	ASP	2.9
1	E	1027	VAL	2.8
2	H	137	GLU	2.8
2	H	138	PRO	2.8
1	E	1079	VAL	2.8
2	H	80	ILE	2.8
1	E	1038	LEU	2.7
1	G	1050	LEU	2.7
2	H	135	LYS	2.7
1	G	1087	VAL	2.7
2	H	121	LEU	2.7
1	G	987	LEU	2.7
1	G	1109	ILE	2.7
1	E	1030	VAL	2.6
1	G	1080	ILE	2.6
2	H	122	ARG	2.6
1	E	1088	ARG	2.6
1	A	1059	LEU	2.6

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Mol	Chain	Res	Type	RSRZ
1	C	1107	ALA	2.5
1	G	1097	LEU	2.5
2	H	153	ALA	2.5
1	C	1001	LEU	2.5
1	G	1083	SER	2.5
1	G	1098	PHE	2.4
1	C	1050	LEU	2.4
1	E	1028	TRP	2.4
1	A	1013	LEU	2.4
1	G	1015	LEU	2.4
1	E	1114	ALA	2.4
1	C	1082	LEU	2.3
2	F	139	VAL	2.3
1	G	1039	TYR	2.3
1	G	903	LYS	2.3
1	A	1097	LEU	2.2
1	G	1081	LYS	2.2
1	E	1085	VAL	2.2
1	E	1111	GLU	2.2
2	F	89	PRO	2.2
1	G	1048	VAL	2.2
2	H	171	PHE	2.2
2	F	137	GLU	2.2
1	E	1010	LEU	2.2
1	E	1109	ILE	2.1
2	F	171	PHE	2.1
2	H	86	ILE	2.1
1	E	766	PRO	2.1
1	C	1049	LEU	2.1
1	E	1033	ASP	2.1
1	C	1080	ILE	2.1
1	G	828	LEU	2.1

## 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
3	PO4	B	401	5/5	0.84	0.35	3.47	169,169,169,170	0
3	PO4	F	403	5/5	0.89	0.34	3.12	124,124,125,125	0
3	PO4	H	404	5/5	0.68	0.39	2.98	123,123,123,123	0
3	PO4	D	402	5/5	0.90	0.20	0.54	135,135,135,135	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.