



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 07:18 AM UTC

PDB ID : 1X86 / pdb_00001x86
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

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:

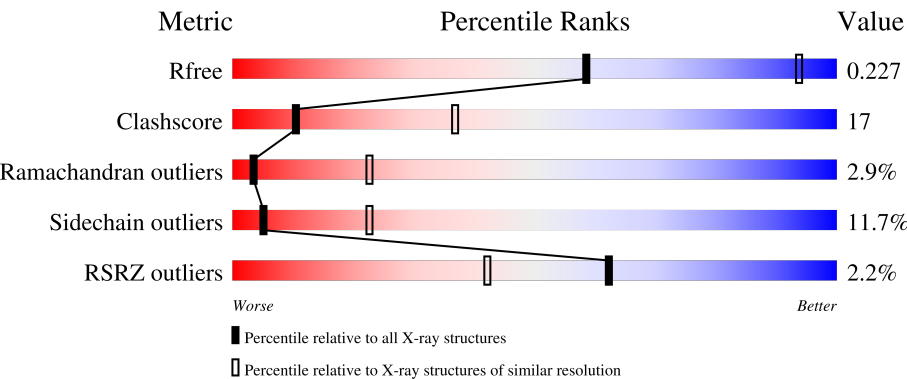
MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry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

1 Overall quality at a glance i

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}	180053	1768 (3.24-3.20)
Clashscore	190562	1879 (3.24-3.20)
Ramachandran outliers	187476	1844 (3.24-3.20)
Sidechain outliers	187428	1843 (3.24-3.20)
RSRZ outliers	180081	1768 (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 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	385	47%38%9%6%
1	C	385	% 57%32%5%6%
1	E	385	9% 45%34%8%13%
1	G	385	% 43%32%7%18%
2	B	196	47%35%10%8%

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Mol	Chain	Length	Quality of chain
2	D	196	56%31%5%8%
2	F	196	% 57%27%7%9%
2	H	196	% 63%27%9%

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 mutation	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 mutation	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 mutation	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 mutation	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

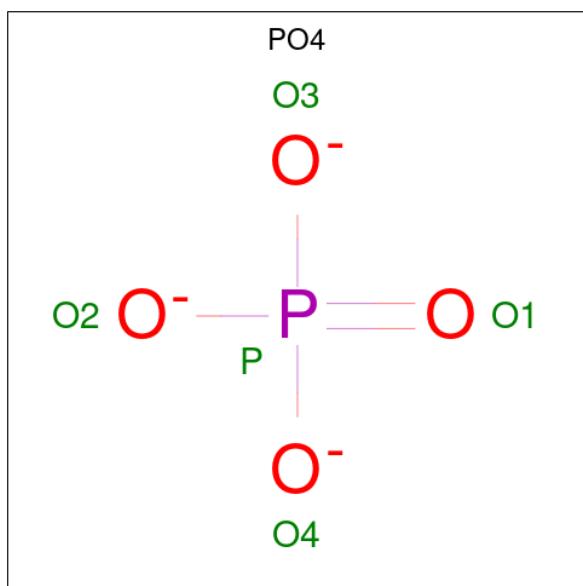
- Molecule 2 is a protein called Transforming protein RhoA.

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			

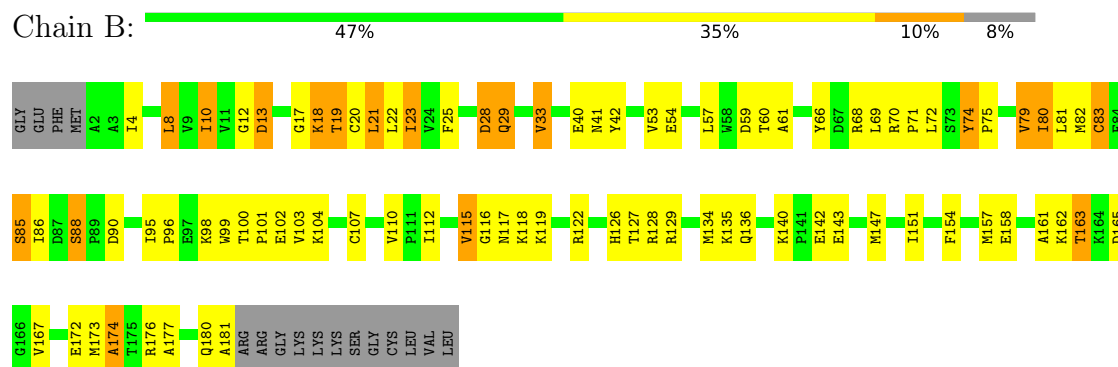
There are 12 discrepancies between the modelled and reference sequences:

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

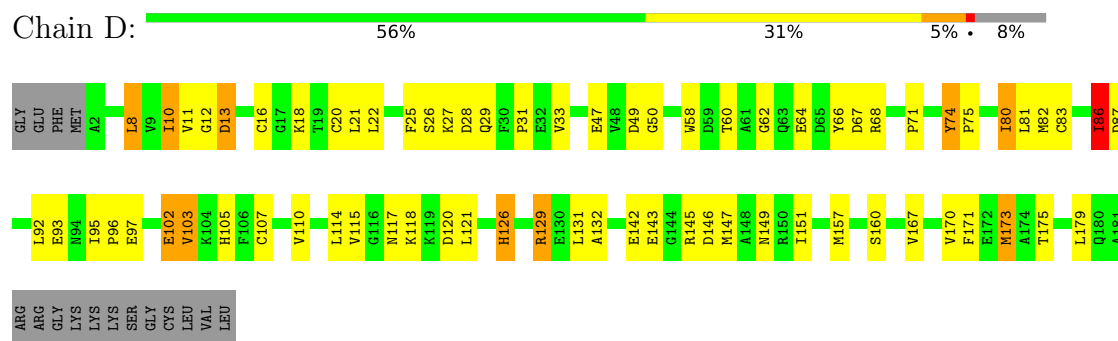
- Molecule 3 is PHOSPHATE ION (CCD ID: PO4) (formula: O₄P).



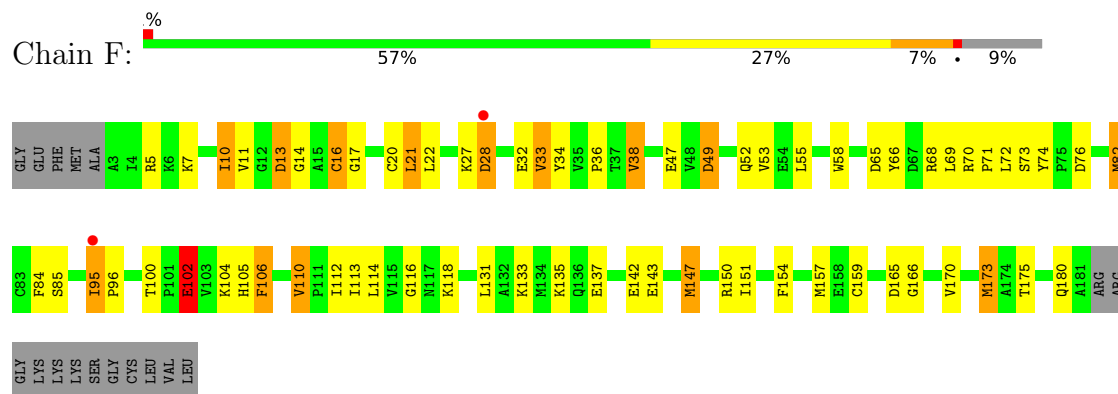
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	B	1	Total	O	P	0	0
			5	4	1		
3	D	1	Total	O	P	0	0
			5	4	1		
3	F	1	Total	O	P	0	0
			5	4	1		
3	H	1	Total	O	P	0	0
			5	4	1		



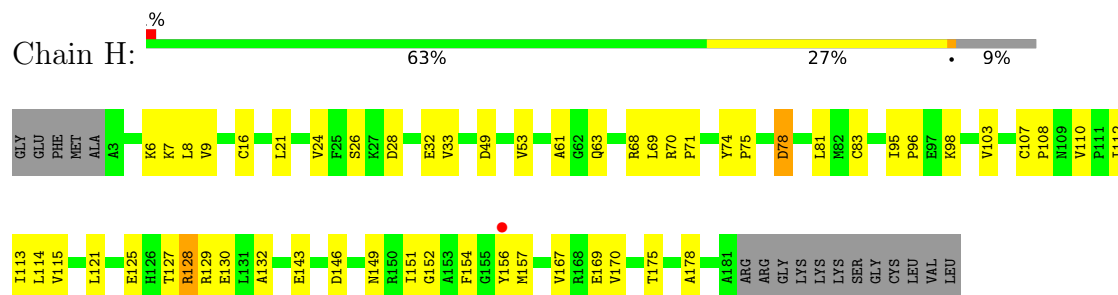
• Molecule 2: Transforming protein RhoA



• Molecule 2: Transforming protein RhoA



• Molecule 2: Transforming protein RhoA



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	296.42Å 95.24Å 157.34Å 90.00° 94.19° 90.00°	Depositor
Resolution (Å)	15.00 – 3.22 15.00 – 3.22	Depositor EDS
% Data completeness (in resolution range)	90.4 (15.00-3.22) 88.9 (15.00-3.22)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	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	3282 reflections (5.05%)	wwPDB-VP
Wilson B-factor (Å ²)	86.6	Xtriage
Anisotropy	0.423	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.23 , 65.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.44$, $\langle L^2 \rangle = 0.27$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	16981	wwPDB-VP
Average B, all atoms (Å ²)	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.*

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 [i](#)

5.1 Standard geometry [i](#)

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	1.17	4/3010 (0.1%)	1.25	15/4060 (0.4%)
1	C	0.79	0/3010	1.00	5/4060 (0.1%)
1	E	0.86	1/2806 (0.0%)	0.97	4/3779 (0.1%)
1	G	0.94	9/2622 (0.3%)	1.01	6/3532 (0.2%)
2	B	1.28	4/1451 (0.3%)	1.37	13/1963 (0.7%)
2	D	0.88	0/1451	1.02	4/1963 (0.2%)
2	F	0.88	4/1446 (0.3%)	0.97	6/1956 (0.3%)
2	H	0.62	0/1446	0.86	1/1956 (0.1%)
All	All	0.95	22/17242 (0.1%)	1.07	54/23269 (0.2%)

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

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

All (22) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	G	982	GLU	CD-OE2	11.22	1.46	1.25
1	G	1108	GLN	CD-NE2	10.21	1.54	1.33
2	F	102	GLU	C-O	-9.53	1.11	1.24
2	F	147	MET	SD-CE	8.20	2.00	1.79
1	G	980	GLU	CD-OE2	7.74	1.40	1.25
1	G	890	ASN	C-O	7.20	1.33	1.23
1	E	1058	VAL	C-O	7.04	1.37	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	F	82	MET	CG-SD	6.66	1.97	1.80
2	B	28	ASP	CA-C	-6.24	1.47	1.53
2	B	80	ILE	CA-C	-5.80	1.45	1.52
1	A	843	ILE	CA-CB	-5.60	1.46	1.54
1	G	834	ASN	CG-ND2	5.55	1.45	1.33
2	F	104	LYS	C-O	5.55	1.30	1.24
1	G	809	LEU	C-O	5.51	1.30	1.24
2	B	80	ILE	C-O	-5.49	1.18	1.24
1	A	875	PRO	CA-C	-5.46	1.46	1.52
2	B	163	THR	CA-CB	-5.29	1.47	1.54
1	G	980	GLU	CD-OE1	5.23	1.35	1.25
1	A	863	GLN	CA-C	5.22	1.59	1.52
1	G	1040	THR	CA-CB	5.13	1.62	1.53
1	A	771	GLN	CG-CD	5.10	1.64	1.52
1	G	983	ASN	CG-ND2	5.09	1.44	1.33

All (54) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	83	CYS	N-CA-C	9.28	122.96	109.14
1	A	940	TYR	CA-C-N	-8.57	111.30	120.47
1	A	940	TYR	C-N-CA	-8.57	111.30	120.47
1	A	791	VAL	CB-CA-C	-7.45	102.26	111.87
2	B	165	ASP	N-CA-C	7.32	120.35	109.59
2	B	23	ILE	CB-CA-C	-7.02	103.03	111.81
2	B	174	ALA	N-CA-C	-6.78	103.97	111.36
1	G	1050	LEU	N-CA-C	6.51	120.31	109.95
2	B	19	THR	N-CA-C	-6.26	104.08	111.03
1	A	861	ILE	N-CA-C	-6.04	98.87	107.98
2	F	102	GLU	O-C-N	6.03	130.51	122.43
1	A	808	VAL	N-CA-C	-5.96	104.70	110.42
2	B	74	TYR	CA-C-N	-5.85	113.91	119.76
2	B	74	TYR	C-N-CA	-5.85	113.91	119.76
1	A	777	VAL	CB-CA-C	-5.84	104.41	111.88
1	A	981	ALA	N-CA-C	5.83	118.42	111.71
1	G	942	LEU	N-CA-C	5.83	117.30	111.07
1	E	933	GLN	N-CA-C	-5.79	104.88	111.14
1	G	1039	TYR	N-CA-C	-5.78	101.44	110.17
1	C	953	TRP	CA-C-N	5.73	124.93	118.97
1	C	953	TRP	C-N-CA	5.73	124.93	118.97
1	A	832	PHE	N-CA-C	5.72	119.99	112.89
2	B	88	SER	CA-C-N	-5.67	113.98	119.87

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	88	SER	C-N-CA	-5.67	113.98	119.87
1	C	1024	GLY	CA-C-N	5.59	125.92	119.93
1	C	1024	GLY	C-N-CA	5.59	125.92	119.93
1	G	1108	GLN	OE1-CD-NE2	5.59	128.19	122.60
2	D	74	TYR	CA-C-N	-5.55	113.98	119.92
2	D	74	TYR	C-N-CA	-5.55	113.98	119.92
1	E	918	ASN	CA-C-N	5.54	126.76	119.84
1	E	918	ASN	C-N-CA	5.54	126.76	119.84
1	A	818	SER	N-CA-C	-5.53	105.15	111.07
1	A	792	ILE	N-CA-C	-5.43	104.66	110.36
1	A	1061	CYS	N-CA-C	5.41	116.74	107.28
2	D	142	GLU	N-CA-C	-5.39	105.06	111.69
2	F	106	PHE	N-CA-C	5.34	118.95	112.23
2	B	163	THR	N-CA-C	5.32	115.57	108.23
1	A	979	LYS	N-CA-C	-5.30	104.93	111.40
1	A	1058	VAL	N-CA-C	5.28	115.91	108.36
1	A	869	LEU	N-CA-C	-5.28	105.61	111.36
2	F	110	VAL	CA-C-N	5.20	126.34	119.84
2	F	110	VAL	C-N-CA	5.20	126.34	119.84
1	A	863	GLN	N-CA-C	5.20	118.33	110.64
2	B	33	VAL	N-CA-C	5.16	120.08	109.34
2	B	79	VAL	CB-CA-C	-5.15	104.64	111.80
2	D	74	TYR	N-CA-C	5.13	121.16	109.81
1	E	860	VAL	CB-CA-C	-5.13	104.73	111.25
2	H	16	CYS	N-CA-C	5.11	116.85	111.28
1	C	1122	VAL	CB-CA-C	-5.09	105.37	112.04
1	G	918	ASN	CA-C-N	5.05	125.32	119.47
1	G	918	ASN	C-N-CA	5.05	125.32	119.47
2	F	95	ILE	CA-C-N	-5.01	115.11	120.47
2	F	95	ILE	C-N-CA	-5.01	115.11	120.47
2	B	115	VAL	CB-CA-C	-5.00	103.09	111.29

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	95	0
1	C	2964	0	3047	83	0
1	E	2767	0	2861	115	0
1	G	2584	0	2671	109	0
2	B	1423	0	1415	72	0
2	D	1423	0	1415	52	0
2	F	1418	0	1410	39	0
2	H	1418	0	1410	40	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	580	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 17.

All (580) 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:814:TYR:C	1:A:814:TYR:CD2	2.62	0.77
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:902:GLN:NE2	1:E:912:VAL:HG11	2.01	0.76
2:D:8:LEU:HD23	2:D:8:LEU:O	1.89	0.73
2:H:121:LEU:HD22	2:H:127:THR:HG21	1.70	0.73
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
1:C:1020:MET:HE3	1:C:1023:GLU:HB3	1.72	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:C:1000:LYS:C	1:C:1002:SER:H	2.01	0.68
1:G:831:ILE:HG12	1:G:897:MET:HG2	1.74	0.68
1:A:974:VAL:O	1:A:978:VAL:HG23	1.93	0.68
1:G:837:ASP:OD1	1:G:837:ASP:N	2.26	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
2:B:157:MET:HE2	2:B:173:MET:SD	2.37	0.65
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: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:984:LYS:HZ1	1:G:1016:THR:HB	1.63	0.63
1:A:987:LEU:HD22	1:A:1015:LEU:HB3	1.79	0.63
1:G:1021:ILE:O	1:G:1021:ILE:HG22	1.98	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:A:854:LYS:O	1:A:855:ARG:C	2.40	0.62
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:768:ASN:HD21	1:E:771:GLN:HB2	1.65	0.62
2:D:126:HIS:ND1	2:D:126:HIS:C	2.57	0.61
1:A:1025:PRO:HG2	1:A:1115:GLN:HE22	1.65	0.61
2:B:82:MET:HE2	2:B:103:VAL:HG21	1.82	0.61
1:A:993:ARG:HH12	1:A:1057:LEU:HD21	1.65	0.61
1:C:1004:TYR:O	1:C:1006:ASN:N	2.34	0.61
1:G:891:GLN:C	1:G:891:GLN:HE21	2.08	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
1:A:842:HIS:O	1:A:843:ILE:C	2.43	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: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
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
1:A:884:ALA:O	1:A:885:ALA:C	2.46	0.57
2:B:86:ILE:HG22	2:B:86:ILE:O	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:1043:LEU:N	1:C:1043:LEU:HD23	2.20	0.57
1:A:869:LEU:HD23	1:A:963:ALA:HB2	1.87	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
1:A:1097:LEU:HD11	1:A:1124:GLN:N	2.21	0.56
2:B:28:ASP:O	2:B:29:GLN:HB2	2.05	0.56
2:B:118:LYS:HA	2:B:161:ALA:HB2	1.86	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: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:A:838:ILE:O	1:A:839:LEU:C	2.49	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:E:830:LYS:HG2	1:E:897:MET:HE3	1.87	0.55
1:A:1031:ASN:O	1:A:1035:THR:HG22	2.07	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
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
1:A:1019:LYS:HB2	1:A:1044:GLU:CD	2.32	0.54
1:C:922:ARG:C	1:C:923:ARG:HG3	2.32	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:A:836:GLU:O	1:A:837:ASP:C	2.50	0.54
1:A:936:ARG:O	1:A:937:LEU:C	2.50	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
1:E:890:ASN:O	1:E:891:GLN:C	2.50	0.54
2:F:151:ILE:HG22	2:F:151:ILE:O	2.08	0.54
1:G:940:TYR:O	1:G:941:PRO:C	2.49	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
2:B:40:GLU:O	2:B:41:ASN:C	2.49	0.54
1:G:979:LYS:O	1:G:983:ASN:OD1	2.26	0.54
1:A:946:ASN:O	1:A:947:ILE:C	2.49	0.53
1:G:984:LYS:HZ1	1:G:1016:THR:CB	2.21	0.53
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:E:897:MET:HA	1:E:897:MET:HE2	1.90	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:962:LYS:O	1:G:965:ASP:N	2.40	0.53
1:G:1096:ALA:HB1	1:G:1111:GLU:HG3	1.89	0.53
1:C:955:THR:HB	1:E:811:GLN:CD	2.34	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
2:H:127:THR:O	2:H:128:ARG:C	2.51	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
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:HE2	1:G:984:LYS:HA	1.90	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
2:B:42:TYR:C	2:B:42:TYR:CD2	2.88	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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:841:LEU:HD21	1:G:880:LEU:HD13	1.90	0.52
1:G:1120:LYS:HG3	1:G:1121:THR:N	2.24	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
2:D:8:LEU:HD23	2:D:8:LEU:C	2.34	0.51
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:C:1053:GLN:O	1:C:1054:ASP:C	2.53	0.51
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
1:C:1000:LYS:C	1:C:1002:SER:N	2.68	0.51
2:D:10:ILE:HG21	2:D:22:LEU:HD11	1.92	0.51
2:H:7:LYS:N	2:H:78:ASP:OD2	2.43	0.51
2:H:24:VAL:O	2:H:28:ASP:HA	2.11	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
1:A:891:GLN:NE2	2:B:72:LEU:HB3	2.22	0.51
2:B:86:ILE:HD11	2:B:116:GLY:HA3	1.91	0.51
1:C:916:GLU:OE2	1:C:925:GLN:HB3	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
2:D:22:LEU:O	2:D:26:SER:OG	2.28	0.50
1:A:814:TYR:CD2	1:A:814:TYR:O	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:E:934:MET:SD	1:E:934:MET:C	2.94	0.50
1:A:774:SER:HB3	1:A:777:VAL:HG23	1.92	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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:G:934:MET:HE1	2:H:63:GLN:NE2	2.27	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:999:LEU:HD21	1:A:1010:LEU:HB3	1.94	0.49
1:C:799:GLU:HA	1:C:936:ARG:NH2	2.27	0.49
2:H:146:ASP:HA	2:H:149:ASN:HB2	1.95	0.49
1:E:809:LEU:HD23	1:E:835:LEU:HD13	1.94	0.49
1:E:1029:LYS:NZ	1:E:1113:VAL:HG21	2.27	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:E:1111:GLU:C	1:E:1112:LEU:HG	2.38	0.49
1:A:1021:ILE:HG21	1:A:1130:MET:HE3	1.95	0.49
1:E:834:ASN:O	1:E:835:LEU:C	2.54	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
1:A:985:GLN:HG3	1:A:985:GLN:O	2.11	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: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
1:G:814:TYR:CD2	1:G:814:TYR:C	2.90	0.49
2:H:8:LEU:HD21	2:H:81:LEU:HD12	1.95	0.49
2:H:81:LEU:HD22	2:H:115:VAL:CG2	2.42	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:A:865:GLY:O	1:A:866:GLU:C	2.54	0.49
1:C:956:GLU:O	1:C:957:ARG:C	2.56	0.48
1:E:991:GLN:HE22	1:E:994:LEU:HD22	1.78	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:19:THR:O	2:B:22:LEU:HB2	2.14	0.48
1:C:918:ASN:C	1:C:918:ASN:OD1	2.56	0.48
1:E:823:LEU:HD21	1:E:908:PHE:CE1	2.47	0.48
2:F:142:GLU:O	2:F:143:GLU:C	2.56	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
2:D:92:LEU:HD11	2:D:147:MET:HG2	1.95	0.48
2:D:95:ILE:HG21	2:D:114:LEU:HD13	1.95	0.48
1:G:984:LYS:HZ1	1:G:1016:THR:CG2	2.25	0.48
1:A:785:GLU:O	1:A:789:GLN:HG2	2.14	0.48
2:B:8:LEU:C	2:B:8:LEU:HD23	2.39	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:B:12:GLY:O	2:B:13:ASP:C	2.57	0.48
1:C:848:GLN:O	1:C:851:ALA:HB3	2.13	0.48
2:D:157:MET:CE	2:D:173:MET:HE2	2.44	0.48
2:F:27:LYS:O	2:F:28:ASP:C	2.57	0.48
1:A:1116:THR:O	1:A:1117:VAL:C	2.56	0.48
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
2:B:162:LYS:C	2:B:163:THR:HG23	2.39	0.48
1:A:779:LEU:HD12	1:A:779:LEU:HA	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:A:922:ARG:C	1:A:923:ARG:HG3	2.38	0.47
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: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
1:E:1014:ASP:O	1:E:1015:LEU:C	2.57	0.47
2:F:100:THR:OG1	2:F:151:ILE:HD13	2.14	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:C:1002:SER:HB2	1:C:1004:TYR:CE2	2.49	0.47
1:G:957:ARG:HD2	1:G:961:LYS:NZ	2.29	0.47
2:B:142:GLU:O	2:B:143:GLU:C	2.57	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:782:LYS:HZ1	1:E:922:ARG:HH12	1.61	0.47
1:C:997:SER:C	1:C:999:LEU:H	2.22	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
1:A:962:LYS:O	1:A:963:ALA:C	2.57	0.47
2:B:112:ILE:O	2:B:154:PHE:HB3	2.15	0.47
2:B:127:THR:O	2:B:128:ARG:C	2.57	0.47
1:C:854:LYS:HB2	1:C:854:LYS:NZ	2.29	0.47
1:C:1084:THR:HB	1:C:1102:MET:HB2	1.97	0.47
1:A:791:VAL:O	1:A:794:GLU:N	2.48	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:E:1090:VAL:HG12	1:E:1090:VAL:O	2.15	0.47
1:A:801:ALA:O	1:A:804:ARG:HB3	2.15	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:943:LEU:O	1:E:947:ILE:HG13	2.15	0.47
1:E:1038:LEU:O	1:E:1052:LYS:NZ	2.44	0.47
1:G:934:MET:CE	2:H:63:GLN:NE2	2.78	0.47
1:G:1021:ILE:HB	1:G:1042:LEU:HG	1.97	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
1:G:962:LYS:O	1:G:963:ALA:C	2.57	0.46
2:H:114:LEU:HB3	2:H:156:TYR:HD1	1.80	0.46
1:A:881:LYS:HB2	1:A:973:PHE:CD2	2.50	0.46
1:A:1126:LEU:O	1:A:1130:MET:HG2	2.16	0.46
2:B:180:GLN:O	2:B:181:ALA:HB3	2.15	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
2:D:87:ASP:OD1	2:D:87:ASP:C	2.59	0.46
2:D:157:MET:HE2	2:D:173:MET:HE2	1.98	0.46
1:E:856:ASN:ND2	1:E:862:ASP:H	2.13	0.46
1:A:791:VAL:O	1:A:792:ILE:C	2.55	0.46
1:E:799:GLU:OE2	1:E:940:TYR:OH	2.26	0.46
1:E:1128:CYS:O	1:E:1132:ALA:N	2.47	0.46
1:G:987:LEU:HD22	1:G:1015:LEU:HB3	1.97	0.46
1:E:813:PHE:O	1:E:814:TYR:C	2.59	0.46
1:E:1055:ASP:OD1	1:E:1055:ASP:N	2.48	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:852:VAL:HG22	1:C:855:ARG:NH1	2.31	0.46
1:C:1124:GLN:O	1:C:1128:CYS:HB2	2.16	0.46
1:G:1020:MET:HE3	1:G:1022:HIS:O	2.16	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:849:MET:C	1:G:851:ALA:H	2.23	0.46
1:G:973:PHE:O	1:G:976:GLN:HB3	2.15	0.46
1:G:1018:ARG:HB2	1:G:1044:GLU:HB3	1.97	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:E:1124:GLN:O	1:E:1125:ASP:C	2.58	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:F:133:LYS:C	2:F:135:LYS:H	2.24	0.45
2:B:116:GLY:O	2:B:158:GLU:HA	2.16	0.45
1:E:791:VAL:HG11	1:E:946:ASN:HB2	1.97	0.45
1:E:912:VAL:O	1:E:915:ALA:HB3	2.16	0.45
1:E:917:SER:O	1:E:918:ASN:C	2.59	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:913:GLN:C	1:E:915:ALA:H	2.25	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
2:F:7:LYS:HB3	2:F:76:ASP:O	2.16	0.45
1:A:936:ARG:C	1:A:938:THR:N	2.73	0.45
2:D:118:LYS:HB3	2:D:121:LEU:HD12	1.98	0.45
1:G:847:GLU:OE2	1:G:847:GLU:HA	2.16	0.45
1:E:782:LYS:HB3	1:E:783:PRO:CD	2.47	0.45
1:G:806:LEU:HB3	1:G:839:LEU:CD1	2.44	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
1:G:823:LEU:HB3	1:G:827:GLU:HB2	1.98	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: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:E:991:GLN:HE22	1:E:994:LEU:CD2	2.30	0.44
1:E:1020:MET:HE2	1:E:1041:LEU:HB3	1.99	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:E:865:GLY:O	1:E:866:GLU:C	2.59	0.44
2:F:147:MET:HE1	2:F:150:ARG:NH1	2.33	0.44
1:G:839:LEU:HG	1:G:843:ILE:HD11	1.99	0.44
1:G:1095:LYS:O	1:G:1120:LYS:HB2	2.18	0.44
2:H:8:LEU:HD23	2:H:8:LEU:C	2.42	0.44
2:H:95:ILE:HB	2:H:96:PRO:HD3	1.99	0.44
1:A:971:LEU:O	1:A:972:ASN:C	2.56	0.44
1:C:771:GLN:C	1:C:772:LEU:HD23	2.42	0.44
1:E:856:ASN:HD22	1:E:862:ASP:H	1.66	0.44
1:G:1080:ILE:O	1:G:1081:LYS:C	2.59	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
2:D:82:MET:O	2:D:83:CYS:HB3	2.16	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:940:TYR:N	1:C:941:PRO:CD	2.81	0.44
1:C:945:ASP:O	1:C:946:ASN:C	2.61	0.44
1:C:1051:GLN:O	1:C:1058:VAL:N	2.50	0.44
1:E:1117:VAL:O	1:E:1118:SER:C	2.61	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
2:F:82:MET:O	2:F:114:LEU:HD12	2.17	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:20:CYS:O	2:F:21:LEU:C	2.59	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:794:GLU:O	1:A:795:LEU:C	2.59	0.43
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: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:G:1024:GLY:O	1:G:1039:TYR:HA	2.18	0.43
2:B:86:ILE:HG12	2:B:117:ASN:O	2.17	0.43
2:B:154:PHE:CE1	2:B:177:ALA:HB2	2.53	0.43
1:E:931:PRO:O	1:E:934:MET:N	2.51	0.43
2:B:90:ASP:CG	2:B:136:GLN:HE22	2.26	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
2:F:49:ASP:OD2	2:F:49:ASP:N	2.51	0.43
2:B:129:ARG:HE	2:B:129:ARG:HB3	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
1:G:1100:ILE:O	1:G:1101:SER:OG	2.36	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:HD23	1:C:828:LEU:HA	1.85	0.43
1:E:799:GLU:CD	1:E:940:TYR:HH	2.25	0.43
1:E:991:GLN:HA	1:E:991:GLN:HE21	1.82	0.43
1:G:797:TYR:CD1	1:G:797:TYR:C	2.97	0.43
1:G:836:GLU:OE1	1:G:840:GLN:HG2	2.19	0.43
2:H:169:GLU:OE1	2:H:169:GLU:N	2.50	0.43
1:A:1130:MET:O	1:A:1131:ALA:C	2.60	0.43
2:B:74:TYR:OH	2:B:102:GLU:OE2	2.28	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:6:LYS:HD2	2:H:178:ALA:HB1	2.00	0.43
2:H:74:TYR:HB3	2:H:107:CYS:SG	2.58	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:F:113:ILE:HD12	2:F:173:MET:HE2	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:974:VAL:HG12	1:E:975:ASN:N	2.32	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
1:E:888:CYS:C	1:E:890:ASN:N	2.76	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:134:MET:HE2	2:B:134:MET:HA	2.01	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:1000:LYS:O	1:A:1001:LEU:C	2.62	0.42
1:A:1123:TRP:O	1:A:1124:GLN:C	2.59	0.42
1:G:799:GLU:OE2	1:G:940:TYR:OH	2.20	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
2:F:13:ASP:O	2:F:14:GLY:C	2.61	0.42
1:C:777:VAL:O	1:C:778:LEU:C	2.62	0.42
1:E:891:GLN:NE2	2:F:72:LEU:O	2.51	0.42
2:B:12:GLY:C	2:B:13:ASP:O	2.62	0.42
1:C:924:LEU:HB3	1:C:928:ASP:HB2	2.02	0.42
1:C:1089:GLN:HE21	1:C:1120:LYS:NZ	2.17	0.42
1:G:1022:HIS:CG	1:G:1023:GLU:N	2.86	0.42
2:D:18:LYS:NZ	2:D:60:THR:O	2.51	0.42
2:F:34:TYR:CE2	2:F:36:PRO:HA	2.55	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:N	1:E:942:LEU:HD23	2.35	0.42
1:G:849:MET:C	1:G:851:ALA:N	2.77	0.42
1:G:940:TYR:HB2	1:G:941:PRO:HD3	2.02	0.42
1:G:1042:LEU:HD11	1:G:1130:MET:HG3	2.02	0.42
1:C:1092:THR:HG22	1:C:1092:THR:O	2.20	0.42
2:D:20:CYS:O	2:D:21:LEU:C	2.63	0.42
1:E:902:GLN:HE22	1:E:912:VAL:HG11	1.82	0.42
1:E:960:VAL:O	1:E:961:LYS:C	2.63	0.42
1:A:849:MET:O	1:A:850:LYS:C	2.62	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:946:ASN:O	1:A:949:LYS:N	2.53	0.42
2:D:86:ILE:O	2:D:86:ILE:HG22	2.19	0.42
1:E:1087:VAL:CG1	1:E:1097:LEU:HD22	2.49	0.42
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:797:TYR:C	1:G:797:TYR:HD1	2.28	0.42
1:G:939:LYS:HZ3	2:H:61:ALA:HB3	1.85	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
1:E:1123:TRP:O	1:E:1127:ILE:CG1	2.68	0.41
1:A:1000:LYS:HB3	1:A:1000:LYS:NZ	2.35	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:E:874:GLY:O	1:E:875:PRO:C	2.63	0.41
1:A:797:TYR:CD1	1:A:797:TYR:C	2.98	0.41
1:C:980:GLU:O	1:C:984:LYS:HB2	2.20	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:A:1119:GLU:O	1:A:1120:LYS:C	2.63	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:C:1101:SER:C	1:C:1102:MET:HG2	2.46	0.41
1:G:823:LEU:HD13	1:G:831:ILE:HD12	2.02	0.41
1:C:953:TRP:HA	1:C:954:PRO:HD3	1.87	0.41
1:C:1060:ARG:HG2	1:C:1061:CYS:N	2.36	0.41
1:E:834:ASN:O	1:E:836:GLU:N	2.53	0.41
1:A:798:THR:CG2	1:A:936:ARG:NH1	2.84	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
2:B:21:LEU:O	2:B:21:LEU:HD12	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:796:PHE:CD1	1:E:849:MET:HG2	2.56	0.41
1:G:1123:TRP:O	1:G:1124:GLN:C	2.64	0.41
2:B:53:VAL:HG12	2:B:54:GLU:N	2.36	0.41
2:B:172:GLU:O	2:B:176:ARG:HG3	2.21	0.41
1:E:812:VAL:HG12	1:E:812:VAL:O	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:845:LEU:HD12	1:E:845:LEU:HA	1.86	0.41
1:E:888:CYS:C	1:E:890:ASN:H	2.29	0.41
1:G:781:LEU:HD22	1:G:785:GLU:HG2	2.03	0.41
1:G:809:LEU:HD13	1:G:929:ILE:HG22	2.03	0.41
1:G:831:ILE:CG1	1:G:897:MET:HG2	2.48	0.41
1:G:1053:GLN:O	1:G:1054:ASP:C	2.63	0.41
1:G:895:LEU:CD2	1:G:927:LYS:HB2	2.50	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
2:B:134:MET:O	2:B:135:LYS:HB2	2.20	0.40
2:D:146:ASP:O	2:D:147:MET:C	2.64	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:HD12	1:G:937:LEU:HA	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: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
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:21:LEU:CD1	2:H:167:VAL:HG13	2.51	0.40
2:H:121:LEU:HD22	2:H:127:THR:CG2	2.47	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%)	3	19
1	C	358/385 (93%)	309 (86%)	40 (11%)	9 (2%)	4	25
1	E	326/385 (85%)	276 (85%)	41 (13%)	9 (3%)	4	23
1	G	304/385 (79%)	255 (84%)	41 (14%)	8 (3%)	4	25
2	B	178/196 (91%)	152 (85%)	24 (14%)	2 (1%)	11	42
2	D	178/196 (91%)	149 (84%)	21 (12%)	8 (4%)	2	14
2	F	177/196 (90%)	147 (83%)	24 (14%)	6 (3%)	3	19
2	H	177/196 (90%)	146 (82%)	26 (15%)	5 (3%)	4	23
All	All	2056/2324 (88%)	1740 (85%)	257 (12%)	59 (3%)	3	23

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

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Mol	Chain	Res	Type
1	A	866	GLU
1	A	947	ILE
1	A	1001	LEU
2	D	129	ARG
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%)	279 (83%)	57 (17%)	2	10
1	C	336/354 (95%)	305 (91%)	31 (9%)	8	32
1	E	313/354 (88%)	268 (86%)	45 (14%)	3	15
1	G	290/354 (82%)	254 (88%)	36 (12%)	4	21
2	B	156/169 (92%)	144 (92%)	12 (8%)	12	40
2	D	156/169 (92%)	141 (90%)	15 (10%)	8	31
2	F	156/169 (92%)	139 (89%)	17 (11%)	6	25
2	H	156/169 (92%)	146 (94%)	10 (6%)	16	46
All	All	1899/2092 (91%)	1676 (88%)	223 (12%)	5	23

All (223) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	771	GLN
1	A	772	LEU
1	A	773	VAL
1	A	774	SER
1	A	786	ILE
1	A	800	ARG
1	A	815	GLN
1	A	820	GLU
1	A	829	ARG
1	A	835	LEU
1	A	845	LEU
1	A	846	ASN
1	A	848	GLN
1	A	856	ASN
1	A	864	ILE
1	A	870	THR
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	923	ARG
1	A	926	LEU

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Mol	Chain	Res	Type
1	A	938	THR
1	A	944	LEU
1	A	952	GLU
1	A	955	THR
1	A	982	GLU
1	A	995	ASP
1	A	1000	LYS
1	A	1004	TYR
1	A	1007	VAL
1	A	1013	LEU
1	A	1016	THR
1	A	1018	ARG
1	A	1019	LYS
1	A	1027	VAL
1	A	1035	THR
1	A	1042	LEU
1	A	1046	ILE
1	A	1052	LYS
1	A	1053	GLN
1	A	1054	ASP
1	A	1060	ARG
1	A	1075	THR
1	A	1077	SER
1	A	1083	SER
1	A	1085	VAL
1	A	1087	VAL
1	A	1092	THR
1	A	1102	MET
1	A	1108	GLN
1	A	1113	VAL
1	A	1120	LYS
1	A	1122	VAL
1	A	1134	VAL
2	B	4	ILE
2	B	8	LEU
2	B	10	ILE
2	B	18	LYS
2	B	21	LEU
2	B	33	VAL
2	B	60	THR
2	B	85	SER
2	B	98	LYS

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Mol	Chain	Res	Type
2	B	119	LYS
2	B	126	HIS
2	B	167	VAL
1	C	775	ARG
1	C	778	LEU
1	C	786	ILE
1	C	787	LYS
1	C	791	VAL
1	C	793	ASN
1	C	800	ARG
1	C	817	VAL
1	C	826	SER
1	C	839	LEU
1	C	845	LEU
1	C	854	LYS
1	C	856	ASN
1	C	859	SER
1	C	881	LYS
1	C	914	ASP
1	C	918	ASN
1	C	922	ARG
1	C	943	LEU
1	C	952	GLU
1	C	975	ASN
1	C	1010	LEU
1	C	1016	THR
1	C	1043	LEU
1	C	1075	THR
1	C	1093	ASP
1	C	1102	MET
1	C	1104	ASP
1	C	1113	VAL
1	C	1120	LYS
1	C	1128	CYS
2	D	8	LEU
2	D	10	ILE
2	D	11	VAL
2	D	33	VAL
2	D	49	ASP
2	D	80	ILE
2	D	86	ILE
2	D	97	GLU

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Mol	Chain	Res	Type
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	775	ARG
1	E	776	GLU
1	E	787	LYS
1	E	804	ARG
1	E	808	VAL
1	E	815	GLN
1	E	823	LEU
1	E	833	SER
1	E	850	LYS
1	E	854	LYS
1	E	856	ASN
1	E	859	SER
1	E	861	ILE
1	E	864	ILE
1	E	866	GLU
1	E	868	LEU
1	E	877	GLU
1	E	909	GLN
1	E	911	PHE
1	E	922	ARG
1	E	934	MET
1	E	937	LEU
1	E	938	THR
1	E	942	LEU
1	E	943	LEU
1	E	944	LEU
1	E	949	LYS
1	E	951	THR
1	E	987	LEU
1	E	991	GLN
1	E	995	ASP
1	E	996	THR
1	E	1008	GLU

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Mol	Chain	Res	Type
1	E	1030	VAL
1	E	1033	ASP
1	E	1034	LYS
1	E	1052	LYS
1	E	1055	ASP
1	E	1077	SER
1	E	1080	ILE
1	E	1089	GLN
1	E	1127	ILE
1	E	1128	CYS
2	F	10	ILE
2	F	11	VAL
2	F	21	LEU
2	F	32	GLU
2	F	38	VAL
2	F	49	ASP
2	F	53	VAL
2	F	55	LEU
2	F	73	SER
2	F	85	SER
2	F	102	GLU
2	F	110	VAL
2	F	131	LEU
2	F	137	GLU
2	F	173	MET
2	F	175	THR
2	F	180	GLN
1	G	776	GLU
1	G	778	LEU
1	G	797	TYR
1	G	800	ARG
1	G	805	THR
1	G	806	LEU
1	G	815	GLN
1	G	817	VAL
1	G	823	LEU
1	G	837	ASP
1	G	841	LEU
1	G	846	ASN
1	G	856	ASN
1	G	861	ILE
1	G	863	GLN

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Mol	Chain	Res	Type
1	G	867	ASP
1	G	886	THR
1	G	891	GLN
1	G	909	GLN
1	G	911	PHE
1	G	930	ILE
1	G	932	THR
1	G	934	MET
1	G	937	LEU
1	G	947	ILE
1	G	971	LEU
1	G	984	LYS
1	G	993	ARG
1	G	1041	LEU
1	G	1043	LEU
1	G	1049	LEU
1	G	1094	ASN
1	G	1113	VAL
1	G	1119	GLU
1	G	1120	LYS
1	G	1121	THR
2	H	26	SER
2	H	32	GLU
2	H	33	VAL
2	H	49	ASP
2	H	53	VAL
2	H	78	ASP
2	H	83	CYS
2	H	125	GLU
2	H	143	GLU
2	H	175	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (45) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	815	GLN
1	A	846	ASN
1	A	848	GLN
1	A	891	GLN
1	A	902	GLN
1	A	933	GLN
1	A	935	GLN

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Mol	Chain	Res	Type
1	A	969	GLN
1	A	972	ASN
1	A	1022	HIS
1	A	1062	HIS
1	A	1115	GLN
2	B	41	ASN
2	B	117	ASN
2	B	136	GLN
1	C	770	GLN
1	C	793	ASN
1	C	848	GLN
1	C	856	ASN
1	C	909	GLN
1	C	1089	GLN
2	D	123	ASN
2	D	136	GLN
1	E	768	ASN
1	E	770	GLN
1	E	771	GLN
1	E	882	HIS
1	E	902	GLN
1	E	925	GLN
1	E	972	ASN
1	E	991	GLN
1	E	1115	GLN
2	F	105	HIS
2	F	109	ASN
1	G	771	GLN
1	G	891	GLN
1	G	902	GLN
1	G	925	GLN
1	G	935	GLN
1	G	991	GLN
1	G	1124	GLN
2	H	52	GLN
2	H	126	HIS
2	H	136	GLN
2	H	180	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 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	$\# Z > 2$
3	PO4	H	404	-	4,4,4	0.86	0	6,6,6	0.64	0
3	PO4	B	401	-	4,4,4	0.98	0	6,6,6	0.27	0
3	PO4	D	402	-	4,4,4	0.97	0	6,6,6	0.39	0
3	PO4	F	403	-	4,4,4	0.98	0	6,6,6	0.40	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 [i](#)

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, 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	362/385 (94%)	-0.56	1 (0%) 90 81	15, 38, 57, 82	0
1	C	362/385 (94%)	-0.52	3 (0%) 82 67	22, 42, 55, 61	0
1	E	336/385 (87%)	0.67	35 (10%) 11 8	14, 51, 67, 74	0
1	G	314/385 (81%)	-0.11	3 (0%) 79 62	26, 48, 59, 63	0
2	B	180/196 (91%)	-0.85	0 100 100	15, 34, 51, 66	0
2	D	180/196 (91%)	-0.63	0 100 100	23, 43, 56, 63	0
2	F	179/196 (91%)	0.27	2 (1%) 78 60	39, 53, 62, 65	0
2	H	179/196 (91%)	-0.18	1 (0%) 85 73	36, 46, 53, 55	0
All	All	2092/2324 (90%)	-0.22	45 (2%) 62 42	14, 45, 60, 82	0

All (45) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	E	875	PRO	4.8
1	E	955	THR	4.6
1	E	973	PHE	3.9
2	F	95	ILE	3.4
1	E	866	GLU	3.4
1	C	1006	ASN	3.3
1	E	969	GLN	3.2
1	E	1013	LEU	3.1
1	E	914	ASP	3.1
1	E	1037	ASP	3.0
1	E	966	HIS	2.9
1	C	1001	LEU	2.8
1	E	963	ALA	2.8
1	E	1030	VAL	2.8
1	E	972	ASN	2.8
1	E	868	LEU	2.8

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Mol	Chain	Res	Type	RSRZ
1	E	886	THR	2.7
1	E	962	LYS	2.7
1	E	1116	THR	2.7
2	H	156	TYR	2.7
1	C	1106	GLY	2.6
1	E	888	CYS	2.6
1	E	971	LEU	2.6
1	G	1082	LEU	2.6
1	E	873	SER	2.5
1	E	880	LEU	2.5
1	E	864	ILE	2.4
1	E	833	SER	2.4
1	G	1055	ASP	2.3
1	G	1025	PRO	2.3
1	E	974	VAL	2.3
1	E	854	LYS	2.3
1	E	984	LYS	2.3
1	E	1119	GLU	2.2
1	E	872	PHE	2.2
1	E	842	HIS	2.2
1	E	1101	SER	2.2
1	E	803	VAL	2.2
1	A	1104	ASP	2.1
1	E	1035	THR	2.1
1	E	953	TRP	2.1
1	E	814	TYR	2.1
1	E	1090	VAL	2.0
1	E	858	THR	2.0
2	F	28	ASP	2.0

6.2 Non-standard residues in protein, DNA, RNA chains ⓘ

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

6.3 Carbohydrates ⓘ

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
3	PO4	H	404	5/5	0.68	0.11	123,123,123,123	0
3	PO4	F	403	5/5	0.73	0.16	124,124,125,125	0
3	PO4	B	401	5/5	0.88	0.13	169,169,169,170	0
3	PO4	D	402	5/5	0.93	0.07	135,135,135,135	0

6.5 Other polymers [i](#)

There are no such residues in this entry.