



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 03:53 AM UTC

PDB ID : 5JHG / pdb_00005jhg
Title : Crystal structure of the complex between the human RhoA and the DH/PH domain of human ARHGEF11
Authors : Wang, R.; Chen, Q.; Zhang, H.; Yan, Z.; Li, J.; Miao, L.; Wang, F.
Deposited on : 2016-04-21
Resolution : 2.50 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

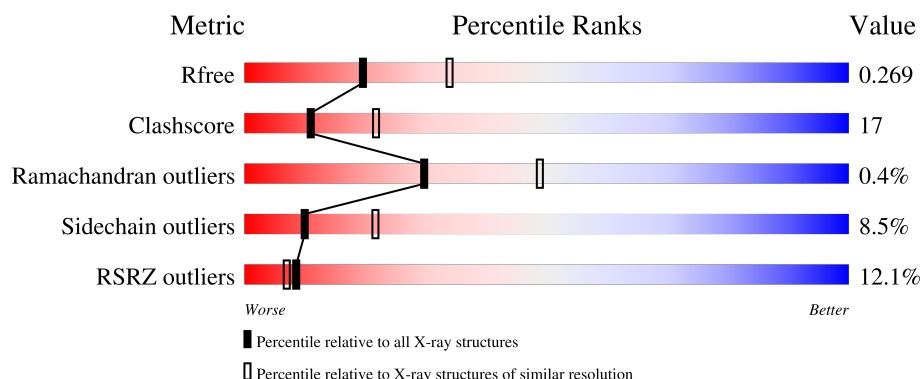
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.50 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	5829 (2.50-2.50)
Clashscore	190562	6492 (2.50-2.50)
Ramachandran outliers	187476	6378 (2.50-2.50)
Sidechain outliers	187428	6380 (2.50-2.50)
RSRZ outliers	180081	5833 (2.50-2.50)

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	369	12% 64% 26% 5% ...
1	E	369	18% 62% 28% 6% ...
2	B	181	4% 69% 25% ...
2	F	181	4% 74% 22% ...

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 8796 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 11.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	356	Total	C	N	O	S	0	0	0
			2916	1843	522	536	15			
1	E	358	Total	C	N	O	S	0	0	0
			2931	1852	525	539	15			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	713	MET	-	expression tag	UNP O15085
E	713	MET	-	expression tag	UNP O15085

- Molecule 2 is a protein called Transforming protein RhoA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	178	Total	C	N	O	S	0	0	0
			1413	894	239	270	10			
2	F	178	Total	C	N	O	S	0	0	0
			1413	894	239	270	10			

- Molecule 3 is GLYCEROL (CCD ID: GOL) (formula: C₃H₈O₃).



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

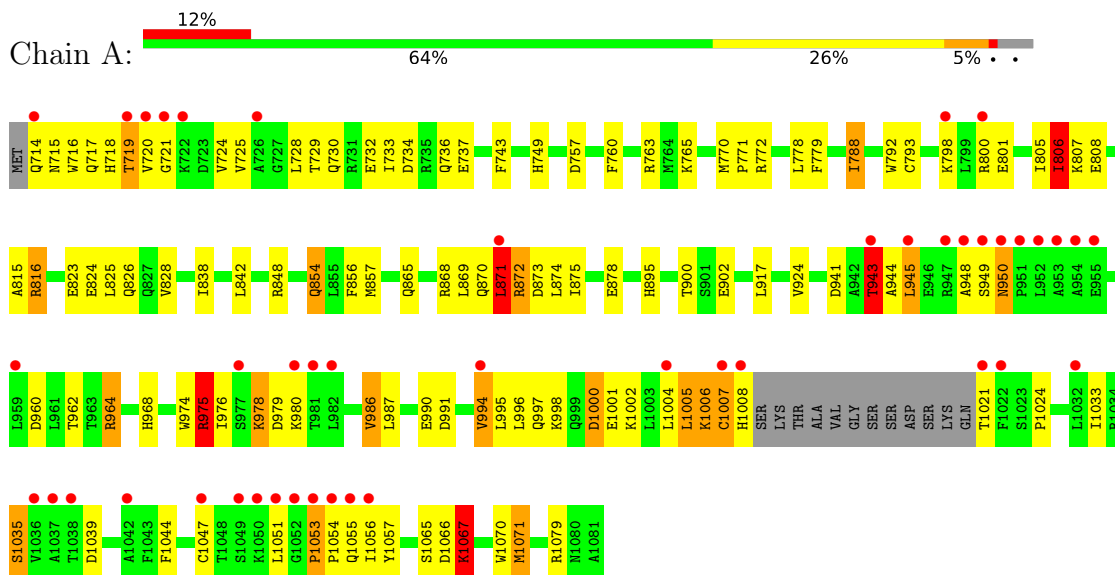
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	41	Total	O	0	0
			41	41		
4	B	23	Total	O	0	0
			23	23		
4	E	26	Total	O	0	0
			26	26		
4	F	9	Total	O	0	0
			9	9		

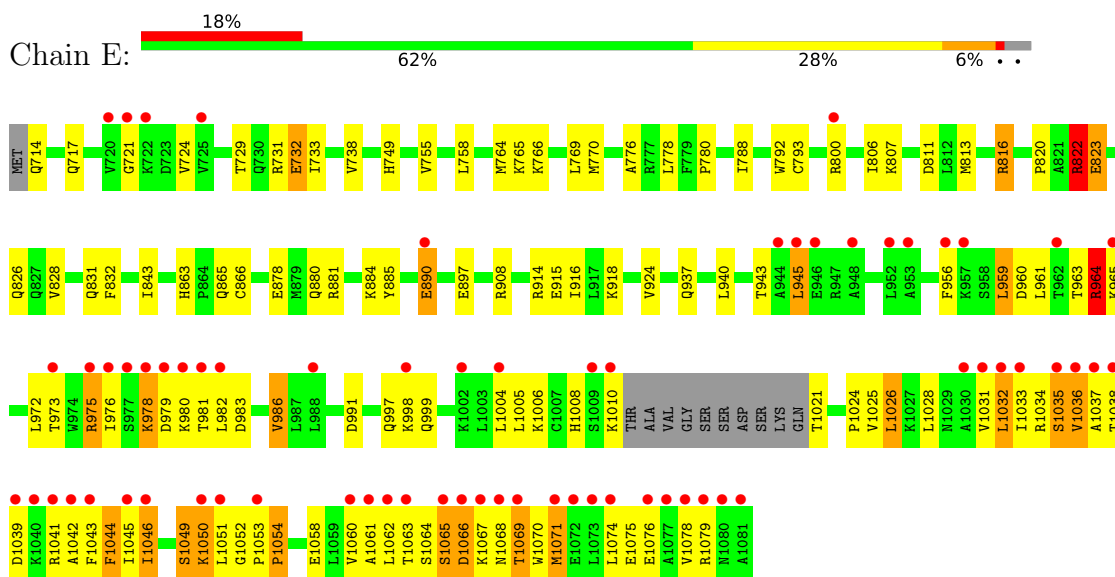
3 Residue-property plots

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

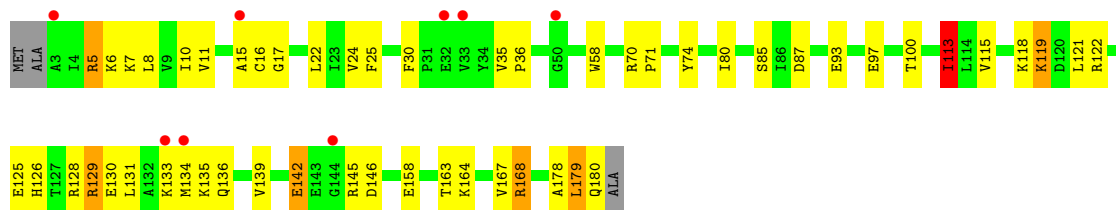
- Molecule 1: Rho guanine nucleotide exchange factor 11



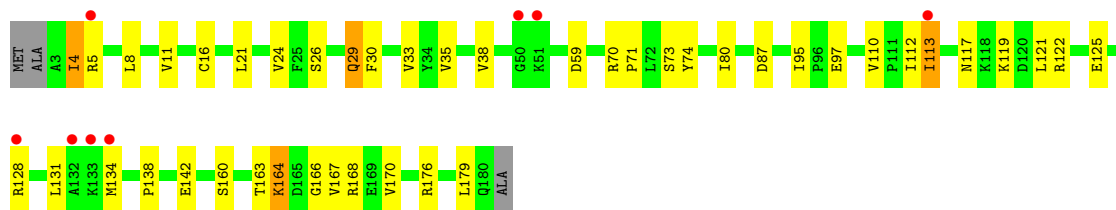
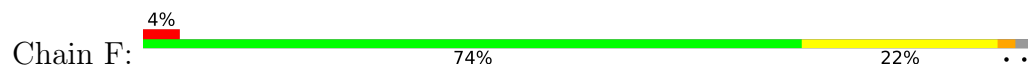
- Molecule 1: Rho guanine nucleotide exchange factor 11



- Molecule 2: Transforming protein RhoA



• Molecule 2: Transforming protein RhoA



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	87.44Å 118.59Å 88.00Å 90.00° 113.00° 90.00°	Depositor
Resolution (Å)	31.13 – 2.50 31.13 – 2.50	Depositor EDS
% Data completeness (in resolution range)	97.0 (31.13-2.50) 97.2 (31.13-2.50)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	23.99 (at 2.51Å)	Xtriage
Refinement program	REFMAC 5.8.0073	Depositor
R, R_{free}	0.221 , 0.270 0.222 , 0.269	Depositor DCC
R_{free} test set	2814 reflections (4.82%)	wwPDB-VP
Wilson B-factor (Å ²)	45.0	Xtriage
Anisotropy	0.096	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 34.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.51$, $\langle L^2 \rangle = 0.35$	Xtriage
Estimated twinning fraction	0.000 for l,-k,h	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	8796	wwPDB-VP
Average B, all atoms (Å ²)	51.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.65% 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: GOL

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	1.46	18/2961 (0.6%)	1.29	28/3985 (0.7%)
1	E	1.37	20/2976 (0.7%)	1.24	15/4004 (0.4%)
2	B	1.29	4/1441 (0.3%)	1.13	4/1949 (0.2%)
2	F	1.30	6/1441 (0.4%)	1.16	3/1949 (0.2%)
All	All	1.38	48/8819 (0.5%)	1.23	50/11887 (0.4%)

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	1
1	E	0	1
All	All	0	2

All (48) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	1006	LYS	CA-C	9.03	1.63	1.52
1	A	807	LYS	CA-C	-8.73	1.48	1.53
1	A	871	LEU	C-N	-7.64	1.23	1.34
1	E	731	ARG	N-CA	-7.64	1.36	1.46
1	E	807	LYS	CA-C	-7.28	1.49	1.53
1	A	807	LYS	N-CA	-6.85	1.40	1.46
1	A	778	LEU	C-O	-6.80	1.15	1.24
2	B	113	ILE	N-CA	-6.79	1.38	1.46
1	E	885	TYR	N-CA	-6.62	1.41	1.46
2	F	110	VAL	CA-C	-6.32	1.47	1.53
2	F	160	SER	C-O	-6.18	1.17	1.24
1	E	813	MET	C-O	-6.17	1.17	1.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	E	732	GLU	C-O	-6.16	1.16	1.24
1	E	820	PRO	C-O	-6.05	1.16	1.24
1	E	733	ILE	C-O	-5.93	1.16	1.24
1	E	831	GLN	C-O	-5.91	1.17	1.24
1	A	770	MET	N-CA	-5.90	1.40	1.46
1	E	778	LEU	C-O	-5.87	1.16	1.24
1	A	1007	CYS	N-CA	5.81	1.52	1.45
1	E	1052	GLY	C-N	5.66	1.40	1.33
1	E	807	LYS	N-CA	-5.65	1.42	1.46
1	A	1033	ILE	C-O	-5.64	1.18	1.24
2	B	7	LYS	CA-C	5.60	1.59	1.52
2	F	112	ILE	N-CA	-5.59	1.39	1.46
1	A	838	ILE	C-O	-5.54	1.17	1.24
1	E	832	PHE	N-CA	-5.53	1.39	1.46
2	F	73	SER	C-O	-5.53	1.16	1.24
2	F	113	ILE	C-O	-5.52	1.18	1.24
1	A	779	PHE	C-O	-5.48	1.18	1.24
1	E	738	VAL	C-O	-5.41	1.18	1.24
2	F	59	ASP	N-CA	5.41	1.52	1.45
1	E	908	ARG	N-CA	-5.35	1.39	1.46
1	E	770	MET	N-CA	-5.32	1.40	1.45
2	B	5	ARG	C-O	-5.28	1.17	1.24
1	E	822	ARG	C-O	-5.27	1.17	1.24
2	B	25	PHE	C-O	-5.24	1.18	1.24
1	A	828	VAL	C-O	-5.20	1.18	1.24
1	E	731	ARG	C-O	-5.18	1.17	1.24
1	A	757	ASP	C-O	-5.17	1.18	1.24
1	A	807	LYS	C-N	5.16	1.40	1.33
1	A	826	GLN	C-O	-5.12	1.18	1.24
1	A	815	ALA	CA-C	5.06	1.59	1.52
1	A	763	ARG	C-O	-5.05	1.18	1.24
1	E	823	GLU	N-CA	-5.04	1.40	1.46
1	E	811	ASP	N-CA	5.03	1.52	1.46
1	E	866	CYS	C-O	5.03	1.30	1.24
1	A	848	ARG	C-O	-5.02	1.17	1.24
1	A	917	LEU	CA-C	-5.00	1.46	1.52

All (50) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	978	LYS	N-CA-C	8.72	122.18	108.67
1	E	1036	VAL	N-CA-C	8.59	119.93	106.88

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	1052	GLY	CA-C-N	-7.62	112.53	120.38
1	E	1052	GLY	C-N-CA	-7.62	112.53	120.38
1	A	719	THR	N-CA-C	7.50	120.85	108.48
1	E	1035	SER	N-CA-C	7.30	121.04	109.50
1	E	1065	SER	N-CA-C	7.02	125.75	110.80
1	A	1051	LEU	CB-CA-C	-6.97	96.54	110.42
1	A	871	LEU	CA-C-O	6.70	128.07	120.90
1	A	948	ALA	N-CA-C	-6.58	99.61	109.94
1	A	718	HIS	CB-CA-C	-6.57	97.89	110.57
1	A	872	ARG	CA-C-N	-6.35	110.12	120.72
1	A	872	ARG	C-N-CA	-6.35	110.12	120.72
1	A	807	LYS	CB-CA-C	-6.32	107.25	116.53
1	A	924	VAL	N-CA-C	-6.21	104.69	110.53
1	A	1051	LEU	N-CA-C	6.07	123.72	110.80
2	F	33	VAL	N-CA-C	6.00	116.78	110.72
1	E	964	ARG	N-CA-C	-5.83	100.69	109.95
1	A	943	THR	CB-CA-C	-5.79	98.56	110.38
1	A	1035	SER	CB-CA-C	-5.77	100.88	112.99
1	A	980	LYS	N-CA-C	-5.76	100.79	109.95
1	E	1069	THR	CB-CA-C	5.74	119.03	109.56
1	E	822	ARG	CA-C-N	-5.72	112.62	120.28
1	E	822	ARG	C-N-CA	-5.72	112.62	120.28
2	B	179	LEU	N-CA-C	5.61	117.47	111.36
2	B	100	THR	CA-C-N	-5.58	112.85	119.05
2	B	100	THR	C-N-CA	-5.58	112.85	119.05
1	E	924	VAL	N-CA-C	-5.53	105.11	110.42
2	F	164	LYS	N-CA-CB	-5.46	107.95	114.17
1	A	978	LYS	CB-CA-C	-5.45	101.68	110.77
1	A	1053	PRO	CA-C-N	-5.39	113.11	119.84
1	A	1053	PRO	C-N-CA	-5.39	113.11	119.84
1	A	1067	LYS	N-CA-C	-5.38	105.50	111.36
1	E	755	VAL	N-CA-C	-5.38	105.48	110.53
1	A	1005	LEU	CA-C-N	5.36	131.81	122.81
1	A	1005	LEU	C-N-CA	5.36	131.81	122.81
1	A	943	THR	N-CA-C	5.35	118.97	112.23
1	A	865	GLN	N-CA-C	5.35	119.29	112.34
1	A	806	ILE	CA-C-N	5.30	128.81	123.13
1	A	806	ILE	C-N-CA	5.30	128.81	123.13
1	E	731	ARG	N-CA-CB	-5.29	102.33	110.20
1	A	771	PRO	CA-C-N	5.27	127.60	120.38
1	A	771	PRO	C-N-CA	5.27	127.60	120.38
1	A	1053	PRO	N-CA-C	5.26	117.12	110.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	1044	PHE	CA-C-N	-5.25	116.68	123.19
1	E	1044	PHE	C-N-CA	-5.25	116.68	123.19
1	E	998	LYS	N-CA-C	-5.22	101.95	110.20
2	F	38	VAL	N-CA-C	5.17	115.41	108.17
1	A	995	LEU	N-CA-C	-5.07	100.97	109.24
2	B	80	ILE	N-CA-C	5.05	115.58	108.36

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	714	GLN	Peptide
1	E	965	LYS	Mainchain

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	2916	0	3003	101	2
1	E	2931	0	3020	136	0
2	B	1413	0	1405	39	0
2	F	1413	0	1405	22	2
3	A	12	0	16	1	0
3	B	6	0	8	2	0
3	E	6	0	8	1	0
4	A	41	0	0	5	0
4	B	23	0	0	0	0
4	E	26	0	0	3	0
4	F	9	0	0	2	0
All	All	8796	0	8865	290	2

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

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:1042:ALA:H	1:E:1067:LYS:CD	1.24	1.45
1:E:1042:ALA:N	1:E:1067:LYS:HD2	1.39	1.33
1:E:1039:ASP:O	1:E:1067:LYS:NZ	1.60	1.32
1:E:1066:ASP:HA	1:E:1069:THR:CG2	1.62	1.29
1:E:1042:ALA:O	1:E:1067:LYS:HE3	1.11	1.25
1:A:715:ASN:O	1:A:719:THR:HG23	1.16	1.24
1:E:1042:ALA:H	1:E:1067:LYS:CE	1.54	1.21
1:A:715:ASN:O	1:A:719:THR:CG2	1.86	1.20
1:E:1066:ASP:C	1:E:1069:THR:HG22	1.67	1.19
1:E:1042:ALA:N	1:E:1067:LYS:CD	2.01	1.14
1:E:1042:ALA:C	1:E:1067:LYS:HE3	1.73	1.12
1:E:1042:ALA:O	1:E:1067:LYS:CE	1.97	1.12
1:E:1041:ARG:C	1:E:1067:LYS:HD2	1.75	1.12
1:A:964:ARG:NH1	1:A:991:ASP:OD2	1.83	1.11
1:E:964:ARG:NH1	1:E:991:ASP:OD2	1.83	1.11
1:E:1065:SER:OG	2:F:97:GLU:O	1.67	1.10
1:E:1066:ASP:CA	1:E:1069:THR:HG22	1.83	1.08
1:E:1066:ASP:CA	1:E:1069:THR:CG2	2.32	1.08
1:E:1066:ASP:O	1:E:1069:THR:HG22	1.49	1.08
1:E:1041:ARG:CA	1:E:1067:LYS:HD2	1.84	1.08
1:E:1066:ASP:O	1:E:1069:THR:CG2	2.02	1.07
1:E:1066:ASP:HA	1:E:1069:THR:HG21	1.34	1.05
1:A:1008:HIS:CD2	1:A:1021:THR:HG22	1.94	1.01
1:E:973:THR:HG22	1:E:983:ASP:OD1	1.60	1.01
1:E:978:LYS:NZ	1:E:979:ASP:OD2	1.93	1.00
1:E:976:ILE:HD12	1:E:980:LYS:HE3	1.44	0.98
1:E:1042:ALA:N	1:E:1067:LYS:CE	2.20	0.98
1:E:937:GLN:NE2	1:E:961:LEU:H	1.60	0.98
1:A:870:GLN:OE1	1:A:872:ARG:NH2	1.98	0.97
1:E:1004:LEU:HD12	1:E:1004:LEU:O	1.66	0.95
1:A:1044:PHE:CD1	1:A:1056:ILE:HG21	2.03	0.94
1:A:872:ARG:NH1	4:A:1201:HOH:O	2.00	0.93
1:A:975:ARG:NH2	1:A:1039:ASP:OD2	2.05	0.90
1:A:1008:HIS:HB2	1:A:1021:THR:CG2	2.00	0.90
1:A:721:GLY:HA2	1:A:724:VAL:HG12	1.54	0.89
1:E:945:LEU:HD23	1:E:956:PHE:O	1.70	0.89
1:E:973:THR:OG1	1:E:1060:VAL:HB	1.73	0.87
1:E:1041:ARG:HA	1:E:1067:LYS:HD2	1.56	0.87
1:E:717:GLN:O	1:E:721:GLY:O	1.92	0.86
1:A:816:ARG:O	1:A:816:ARG:HD3	1.76	0.85
1:E:1070:TRP:O	1:E:1074:LEU:HG	1.77	0.85
1:A:950:ASN:ND2	1:A:950:ASN:O	2.10	0.84

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:890:GLU:OE2	1:E:914:ARG:NH2	2.11	0.83
1:A:1054:PRO:HA	1:E:1034:ARG:HH11	1.45	0.82
1:A:1008:HIS:HD2	1:A:1021:THR:HG22	1.40	0.82
1:A:1008:HIS:HB2	1:A:1021:THR:HB	1.60	0.81
1:E:937:GLN:HE22	1:E:961:LEU:H	1.25	0.80
1:E:964:ARG:HG2	1:E:964:ARG:HH11	1.47	0.79
1:E:1066:ASP:O	1:E:1069:THR:N	2.14	0.79
1:E:964:ARG:NH1	1:E:991:ASP:CG	2.41	0.78
1:A:1008:HIS:HB2	1:A:1021:THR:CB	2.13	0.78
2:F:5:ARG:NE	4:F:201:HOH:O	2.13	0.78
1:E:1042:ALA:N	1:E:1067:LYS:HE3	2.01	0.76
1:E:945:LEU:CD2	1:E:956:PHE:O	2.33	0.76
1:A:964:ARG:HH11	1:A:964:ARG:HG2	1.52	0.75
1:E:816:ARG:O	1:E:816:ARG:HD3	1.85	0.75
1:E:976:ILE:CD1	1:E:980:LYS:HE3	2.16	0.75
1:A:871:LEU:C	1:A:871:LEU:HD13	2.12	0.75
1:E:1042:ALA:CA	1:E:1067:LYS:HE3	2.16	0.74
2:B:168:ARG:HG3	2:B:168:ARG:HH21	1.53	0.74
1:E:1006:LYS:O	1:E:1008:HIS:CD2	2.41	0.73
1:E:1044:PHE:HE1	1:E:1058:GLU:HB2	1.52	0.73
2:B:128:ARG:NH1	2:B:128:ARG:HB2	2.03	0.73
1:E:976:ILE:HD11	1:E:982:LEU:HD12	1.72	0.72
2:B:15:ALA:HA	3:B:201:GOL:O2	1.90	0.71
1:E:1066:ASP:C	1:E:1069:THR:CG2	2.44	0.70
1:E:1041:ARG:HA	1:E:1067:LYS:CD	2.22	0.70
1:A:1044:PHE:CD1	1:A:1056:ILE:CG2	2.74	0.69
1:E:1042:ALA:H	1:E:1067:LYS:HE3	1.50	0.69
1:A:964:ARG:NH1	1:A:991:ASP:CG	2.50	0.69
1:E:884:LYS:NZ	4:E:1201:HOH:O	2.27	0.68
1:A:1008:HIS:CG	1:A:1021:THR:HG22	2.27	0.68
1:E:1043:PHE:CZ	1:E:1074:LEU:HD11	2.29	0.68
1:E:1066:ASP:O	1:E:1069:THR:HG23	1.91	0.68
1:A:871:LEU:HD13	1:A:871:LEU:O	1.95	0.67
1:E:937:GLN:NE2	1:E:961:LEU:N	2.41	0.67
1:E:1006:LYS:O	1:E:1008:HIS:NE2	2.28	0.67
1:A:1006:LYS:O	1:A:1024:PRO:HG3	1.95	0.67
1:A:1008:HIS:CB	1:A:1021:THR:CG2	2.73	0.67
1:E:1028:LEU:O	1:E:1078:VAL:HG23	1.94	0.66
1:E:1033:ILE:C	1:E:1034:ARG:HG2	2.21	0.66
1:A:749:HIS:HD2	4:A:1238:HOH:O	1.79	0.66
2:B:128:ARG:HB2	2:B:128:ARG:HH11	1.59	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:975:ARG:NH2	1:E:1039:ASP:OD2	2.27	0.66
1:E:1049:SER:OG	1:E:1050:LYS:N	2.20	0.65
1:E:822:ARG:HH21	1:E:826:GLN:HE22	1.44	0.65
1:A:1044:PHE:HD1	1:A:1056:ILE:CG2	2.10	0.65
1:E:1041:ARG:HG3	1:E:1041:ARG:O	1.98	0.64
1:A:724:VAL:HG21	1:A:805:ILE:HD11	1.79	0.64
1:A:941:ASP:HB3	1:A:1004:LEU:HD23	1.80	0.64
1:A:716:TRP:O	1:A:720:VAL:O	2.15	0.64
1:A:724:VAL:CG2	1:A:805:ILE:HD11	2.28	0.64
2:F:131:LEU:HD12	2:F:138:PRO:HD3	1.79	0.64
1:A:978:LYS:HE2	1:E:1037:ALA:O	1.98	0.63
1:A:871:LEU:C	1:A:871:LEU:CD1	2.72	0.62
1:E:1044:PHE:HE1	1:E:1058:GLU:CB	2.12	0.62
1:A:943:THR:HG22	1:A:944:ALA:N	2.13	0.62
1:A:721:GLY:HA2	1:A:724:VAL:CG1	2.30	0.62
1:A:798:LYS:O	1:A:801:GLU:HB2	1.99	0.62
1:E:729:THR:HG23	1:E:732:GLU:H	1.63	0.62
1:E:1010:LYS:HE3	1:E:1021:THR:CA	2.29	0.62
1:A:1053:PRO:C	1:A:1055:GLN:H	2.08	0.61
1:A:1008:HIS:HB2	1:A:1021:THR:HG22	1.79	0.61
1:A:716:TRP:HA	1:A:719:THR:OG1	2.00	0.61
1:E:1004:LEU:HD12	1:E:1004:LEU:C	2.25	0.61
1:A:870:GLN:OE1	1:A:872:ARG:CZ	2.50	0.60
1:A:854:GLN:HG3	4:A:1235:HOH:O	2.02	0.60
1:E:973:THR:HG1	1:E:1060:VAL:HB	1.66	0.60
2:F:21:LEU:HD22	2:F:117:ASN:HD21	1.67	0.60
1:A:964:ARG:HH11	1:A:964:ARG:CG	2.16	0.59
2:F:163:THR:O	2:F:164:LYS:HB2	2.02	0.59
1:E:964:ARG:HH12	1:E:991:ASP:CG	2.03	0.59
1:A:724:VAL:O	1:A:724:VAL:HG22	2.02	0.58
2:F:163:THR:O	2:F:164:LYS:CB	2.51	0.58
1:A:871:LEU:O	1:A:874:LEU:HB2	2.03	0.58
1:E:822:ARG:HG2	1:E:916:ILE:HD11	1.85	0.58
1:E:964:ARG:HH11	1:E:964:ARG:CG	2.15	0.57
1:A:1007:CYS:O	1:A:1008:HIS:C	2.46	0.57
1:E:1066:ASP:O	1:E:1070:TRP:N	2.31	0.57
1:E:959:LEU:HD12	1:E:1005:LEU:HD11	1.86	0.57
2:B:113:ILE:HD11	2:B:115:VAL:HG22	1.87	0.56
1:A:816:ARG:HD3	1:A:816:ARG:C	2.29	0.56
1:A:1053:PRO:HB2	1:A:1055:GLN:O	2.06	0.56
1:E:1043:PHE:HE1	1:E:1045:ILE:HD11	1.71	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:736:GLN:NE2	1:A:806:ILE:O	2.32	0.56
1:E:1041:ARG:HG3	1:E:1060:VAL:HG13	1.87	0.55
1:E:1053:PRO:O	1:E:1054:PRO:O	2.25	0.55
2:B:168:ARG:HG3	2:B:168:ARG:NH2	2.20	0.55
1:A:873:ASP:OD1	2:B:58:TRP:HZ2	1.89	0.55
1:E:800:ARG:HG2	4:E:1203:HOH:O	2.07	0.55
2:B:24:VAL:HG12	2:B:30:PHE:HA	1.89	0.55
1:A:760:PHE:CD1	1:A:871:LEU:HD23	2.42	0.54
1:E:960:ASP:OD2	1:E:963:THR:HG23	2.07	0.54
1:E:1010:LYS:HE3	1:E:1021:THR:N	2.22	0.54
2:F:24:VAL:HG12	2:F:30:PHE:HA	1.89	0.54
1:E:1004:LEU:HD13	1:E:1006:LYS:HD3	1.90	0.54
1:A:960:ASP:OD1	1:A:962:THR:HB	2.08	0.54
1:A:1008:HIS:CB	1:A:1021:THR:HG22	2.35	0.54
1:E:1074:LEU:O	1:E:1078:VAL:HG12	2.07	0.54
1:E:880:GLN:O	1:E:884:LYS:HG2	2.09	0.53
1:A:732:GLU:OE2	1:A:736:GLN:HG2	2.09	0.53
1:A:760:PHE:CG	1:A:871:LEU:HD23	2.43	0.53
2:F:4:ILE:HD11	2:F:179:LEU:HD21	1.91	0.52
1:E:1041:ARG:O	1:E:1042:ALA:HB2	2.08	0.52
1:A:715:ASN:O	1:A:719:THR:HG21	1.98	0.52
1:A:968:HIS:HD2	4:A:1233:HOH:O	1.92	0.52
1:A:743:PHE:HB3	1:A:800:ARG:HH21	1.75	0.52
1:A:1053:PRO:C	1:A:1055:GLN:N	2.67	0.52
1:E:1036:VAL:HG12	1:E:1039:ASP:H	1.75	0.51
1:E:816:ARG:HD3	1:E:816:ARG:C	2.34	0.51
1:E:1026:LEU:CD1	1:E:1026:LEU:N	2.73	0.51
2:F:70:ARG:N	2:F:71:PRO:CD	2.74	0.51
1:A:1067:LYS:HE2	1:A:1071:MET:HG3	1.93	0.51
2:F:4:ILE:O	2:F:4:ILE:HG13	2.11	0.50
2:F:122:ARG:O	2:F:128:ARG:NH2	2.43	0.50
1:A:1056:ILE:HG22	1:A:1057:TYR:N	2.26	0.50
1:E:1010:LYS:HE3	1:E:1021:THR:C	2.36	0.50
1:E:1033:ILE:O	1:E:1034:ARG:HG2	2.12	0.50
1:A:1007:CYS:O	1:A:1008:HIS:O	2.29	0.50
1:A:856:PHE:CD1	1:A:856:PHE:C	2.89	0.50
1:A:1065:SER:OG	2:B:97:GLU:O	2.28	0.50
1:E:1043:PHE:CZ	1:E:1074:LEU:CD1	2.95	0.50
2:B:179:LEU:O	2:B:180:GLN:C	2.54	0.49
1:A:1008:HIS:HD2	1:A:1021:THR:CG2	2.20	0.49
1:E:792:TRP:HB2	3:E:1101:GOL:O3	2.12	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:729:THR:HG23	1:A:732:GLU:H	1.76	0.49
1:E:1053:PRO:O	1:E:1054:PRO:C	2.52	0.49
2:F:4:ILE:CD1	2:F:179:LEU:HD21	2.42	0.49
1:E:1067:LYS:C	1:E:1069:THR:N	2.68	0.49
1:E:1067:LYS:O	1:E:1068:ASN:C	2.50	0.49
1:A:1056:ILE:CG2	1:A:1057:TYR:N	2.76	0.49
1:E:881:ARG:O	1:E:884:LYS:HB2	2.13	0.49
1:A:1054:PRO:HA	1:E:1034:ARG:NH1	2.20	0.48
1:E:937:GLN:OE1	1:E:940:LEU:HD23	2.13	0.48
1:E:1043:PHE:CE1	1:E:1074:LEU:CD1	2.96	0.48
1:A:1008:HIS:CD2	1:A:1021:THR:CG2	2.82	0.48
1:E:1042:ALA:CA	1:E:1067:LYS:CE	2.83	0.48
1:A:724:VAL:HG21	1:A:805:ILE:CD1	2.44	0.48
1:E:937:GLN:HE21	1:E:961:LEU:H	1.52	0.48
2:B:24:VAL:HG23	2:B:167:VAL:HG11	1.96	0.48
2:B:119:LYS:C	2:B:121:LEU:H	2.21	0.48
1:A:792:TRP:HD1	3:A:1101:GOL:H11	1.79	0.47
1:E:1025:VAL:C	1:E:1026:LEU:HD12	2.38	0.47
1:E:1031:VAL:O	1:E:1032:LEU:HD13	2.15	0.47
1:A:964:ARG:NH1	1:A:964:ARG:CG	2.73	0.47
2:F:24:VAL:HG23	2:F:167:VAL:HG11	1.97	0.47
1:A:728:LEU:HB2	1:A:733:ILE:HD11	1.97	0.47
1:A:868:ARG:HB3	2:B:5:ARG:HH22	1.79	0.47
1:A:987:LEU:HB2	1:A:994:VAL:HG22	1.96	0.47
2:B:87:ASP:C	2:B:87:ASP:OD1	2.58	0.47
1:A:900:THR:CG2	1:A:902:GLU:HB3	2.45	0.47
1:E:1010:LYS:HG3	1:E:1021:THR:HA	1.96	0.47
1:E:972:LEU:HD23	1:E:1061:ALA:HA	1.95	0.47
1:E:822:ARG:HH21	1:E:826:GLN:NE2	2.11	0.46
2:F:87:ASP:OD1	2:F:87:ASP:C	2.59	0.46
1:A:721:GLY:CA	1:A:724:VAL:HG12	2.36	0.46
2:B:126:HIS:ND1	2:B:126:HIS:C	2.73	0.46
1:A:749:HIS:HE1	1:A:878:GLU:OE1	1.99	0.46
1:A:854:GLN:CG	4:A:1235:HOH:O	2.61	0.46
1:E:964:ARG:NH1	1:E:964:ARG:CG	2.74	0.46
2:B:16:CYS:O	2:B:16:CYS:SG	2.74	0.46
2:F:119:LYS:C	2:F:121:LEU:H	2.24	0.46
1:E:717:GLN:C	1:E:721:GLY:O	2.59	0.46
1:A:1047:CYS:HB2	1:A:1053:PRO:HD2	1.97	0.45
1:A:869:LEU:HB3	1:A:873:ASP:HB2	1.97	0.45
1:A:734:ASP:HB3	1:A:895:HIS:CE1	2.52	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:1044:PHE:CE1	1:E:1058:GLU:CB	2.98	0.45
2:F:8:LEU:HD23	2:F:8:LEU:C	2.42	0.45
1:A:996:LEU:HD23	1:A:1005:LEU:HD13	1.98	0.45
2:B:15:ALA:O	2:B:118:LYS:NZ	2.49	0.45
2:B:135:LYS:HG2	2:B:135:LYS:O	2.17	0.45
1:E:1045:ILE:C	1:E:1046:ILE:HD12	2.42	0.45
1:E:1061:ALA:CB	1:E:1067:LYS:HB2	2.47	0.45
1:A:944:ALA:O	1:A:945:LEU:HD12	2.17	0.45
2:B:129:ARG:O	2:B:130:GLU:C	2.59	0.45
1:E:1066:ASP:O	1:E:1069:THR:CA	2.64	0.45
2:F:29:GLN:HE21	2:F:29:GLN:HB2	1.61	0.44
2:B:133:LYS:C	2:B:135:LYS:H	2.25	0.44
2:B:168:ARG:NH2	2:B:168:ARG:CG	2.77	0.44
1:E:1075:GLU:O	1:E:1079:ARG:HD3	2.17	0.44
1:E:915:GLU:HG3	4:E:1208:HOH:O	2.16	0.44
1:E:945:LEU:HD23	1:E:956:PHE:C	2.39	0.44
2:F:5:ARG:CD	4:F:201:HOH:O	2.63	0.44
2:B:70:ARG:N	2:B:71:PRO:CD	2.80	0.44
2:B:8:LEU:C	2:B:8:LEU:HD23	2.43	0.44
2:B:128:ARG:HH11	2:B:128:ARG:CB	2.26	0.44
1:A:964:ARG:HH11	1:A:991:ASP:CG	2.24	0.44
1:A:941:ASP:OD1	1:A:943:THR:HB	2.18	0.43
1:A:717:GLN:HG3	1:A:737:GLU:OE2	2.19	0.43
1:E:1067:LYS:C	1:E:1069:THR:H	2.25	0.43
1:A:868:ARG:HB3	2:B:5:ARG:NH2	2.33	0.43
1:A:1005:LEU:HD12	1:A:1005:LEU:HA	1.73	0.43
1:E:764:MET:HA	1:E:769:LEU:HD12	2.01	0.43
1:E:788:ILE:HD12	1:E:828:VAL:HG11	2.01	0.43
2:B:131:LEU:O	2:B:136:GLN:N	2.48	0.43
1:E:776:ALA:O	1:E:780:PRO:HA	2.19	0.43
1:E:1042:ALA:H	1:E:1067:LYS:CG	2.14	0.43
2:F:166:GLY:O	2:F:170:VAL:HG23	2.19	0.43
2:B:122:ARG:NH1	2:B:139:VAL:O	2.44	0.43
1:E:1066:ASP:O	1:E:1067:LYS:C	2.61	0.43
1:A:717:GLN:C	1:A:719:THR:H	2.26	0.43
1:E:749:HIS:HE1	1:E:878:GLU:OE1	2.02	0.43
1:A:788:ILE:HD11	1:A:824:GLU:HG2	2.00	0.42
1:E:1041:ARG:O	1:E:1060:VAL:HG13	2.20	0.42
2:B:122:ARG:NH2	2:B:158:GLU:OE1	2.45	0.42
2:F:16:CYS:O	2:F:16:CYS:SG	2.76	0.42
2:B:113:ILE:O	2:B:113:ILE:HG13	2.17	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:724:VAL:HG22	1:A:805:ILE:HD11	2.01	0.42
1:A:816:ARG:HD2	1:A:825:LEU:HD22	2.00	0.42
2:B:10:ILE:HG21	2:B:22:LEU:HD11	2.00	0.42
1:A:721:GLY:O	1:A:725:VAL:HB	2.19	0.42
1:A:856:PHE:CE1	1:A:857:MET:CE	3.02	0.42
1:A:974:TRP:O	1:A:976:ILE:N	2.52	0.42
2:F:71:PRO:HA	2:F:74:TYR:CD2	2.55	0.42
1:A:729:THR:OG1	1:A:730:GLN:N	2.53	0.42
2:B:93:GLU:OE1	2:B:93:GLU:HA	2.19	0.42
2:B:163:THR:O	2:B:164:LYS:HB2	2.20	0.42
2:B:71:PRO:HA	2:B:74:TYR:CD2	2.54	0.42
1:E:943:THR:C	1:E:945:LEU:H	2.27	0.42
1:E:1062:LEU:O	1:E:1063:THR:HG23	2.20	0.42
1:A:950:ASN:HD22	1:A:950:ASN:C	2.26	0.41
1:E:822:ARG:O	1:E:823:GLU:C	2.58	0.41
1:E:1044:PHE:CD1	1:E:1058:GLU:HA	2.55	0.41
2:B:126:HIS:ND1	2:B:126:HIS:O	2.52	0.41
1:E:1041:ARG:O	1:E:1041:ARG:CG	2.64	0.41
1:E:1067:LYS:O	1:E:1069:THR:N	2.53	0.41
2:F:117:ASN:HD22	2:F:117:ASN:HA	1.71	0.41
1:A:943:THR:O	1:A:943:THR:HG23	2.19	0.41
1:E:863:HIS:HD2	1:E:865:GLN:H	1.68	0.41
1:E:991:ASP:OD1	1:E:991:ASP:N	2.47	0.41
1:E:1066:ASP:C	1:E:1069:THR:H	2.22	0.41
1:A:1000:ASP:HB3	1:A:1001:GLU:H	1.58	0.41
1:E:1005:LEU:HD22	1:E:1024:PRO:HG2	2.02	0.41
2:B:17:GLY:CA	3:B:201:GOL:H2	2.51	0.41
1:A:870:GLN:O	1:A:871:LEU:C	2.64	0.41
2:B:142:GLU:O	2:B:146:ASP:OD2	2.38	0.41
2:B:35:VAL:HA	2:B:36:PRO:HD3	1.92	0.41
2:B:85:SER:OG	2:B:118:LYS:HD2	2.21	0.41
1:E:986:VAL:HG22	1:E:1070:TRP:CH2	2.55	0.41
1:E:1004:LEU:C	1:E:1004:LEU:CD1	2.94	0.41
1:E:1031:VAL:HA	1:E:1046:ILE:O	2.20	0.41
1:E:1078:VAL:HG13	1:E:1079:ARG:N	2.36	0.41
2:B:6:LYS:HD2	2:B:178:ALA:HB1	2.03	0.41
1:E:1041:ARG:HG3	1:E:1060:VAL:CG1	2.50	0.40
1:E:822:ARG:NH2	1:E:826:GLN:HE22	2.16	0.40
1:E:976:ILE:CD1	1:E:982:LEU:HD12	2.48	0.40
1:E:1071:MET:HB2	1:E:1071:MET:HE2	1.61	0.40
1:E:1053:PRO:C	1:E:1054:PRO:O	2.65	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:986:VAL:HG22	1:A:1070:TRP:CH2	2.57	0.40
1:A:872:ARG:HA	1:A:875:ILE:HG22	2.03	0.40

All (2) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:823:GLU:OE1	2:F:176:ARG:NH1[1_455]	2.05	0.15
1:A:823:GLU:OE2	2:F:176:ARG:NH1[1_455]	2.10	0.10

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	352/369 (95%)	324 (92%)	26 (7%)	2 (1%)	21	38
1	E	354/369 (96%)	327 (92%)	25 (7%)	2 (1%)	21	38
2	B	176/181 (97%)	167 (95%)	9 (5%)	0	100	100
2	F	176/181 (97%)	169 (96%)	7 (4%)	0	100	100
All	All	1058/1100 (96%)	987 (93%)	67 (6%)	4 (0%)	30	49

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	E	1049	SER
1	A	975	ARG
1	A	979	ASP
1	E	1054	PRO

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	324/335 (97%)	296 (91%)	28 (9%)	10	21
1	E	326/335 (97%)	293 (90%)	33 (10%)	7	15
2	B	156/157 (99%)	147 (94%)	9 (6%)	18	38
2	F	156/157 (99%)	144 (92%)	12 (8%)	12	25
All	All	962/984 (98%)	880 (92%)	82 (8%)	10	22

All (82) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	765	LYS
1	A	772	ARG
1	A	788	ILE
1	A	793	CYS
1	A	806	ILE
1	A	808	GLU
1	A	816	ARG
1	A	842	LEU
1	A	854	GLN
1	A	871	LEU
1	A	943	THR
1	A	945	LEU
1	A	949	SER
1	A	950	ASN
1	A	964	ARG
1	A	975	ARG
1	A	986	VAL
1	A	990	GLU
1	A	994	VAL
1	A	997	GLN
1	A	998	LYS
1	A	1000	ASP
1	A	1002	LYS
1	A	1035	SER

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Mol	Chain	Res	Type
1	A	1066	ASP
1	A	1067	LYS
1	A	1071	MET
1	A	1079	ARG
2	B	11	VAL
2	B	113	ILE
2	B	119	LYS
2	B	125	GLU
2	B	129	ARG
2	B	134	MET
2	B	142	GLU
2	B	145	ARG
2	B	168	ARG
1	E	714	GLN
1	E	724	VAL
1	E	758	LEU
1	E	765	LYS
1	E	766	LYS
1	E	793	CYS
1	E	806	ILE
1	E	816	ARG
1	E	822	ARG
1	E	843	ILE
1	E	890	GLU
1	E	897	GLU
1	E	918	LYS
1	E	945	LEU
1	E	959	LEU
1	E	964	ARG
1	E	975	ARG
1	E	978	LYS
1	E	981	THR
1	E	986	VAL
1	E	997	GLN
1	E	999	GLN
1	E	1026	LEU
1	E	1032	LEU
1	E	1035	SER
1	E	1038	THR
1	E	1046	ILE
1	E	1050	LYS
1	E	1051	LEU

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Mol	Chain	Res	Type
1	E	1064	SER
1	E	1066	ASP
1	E	1071	MET
1	E	1076	GLU
2	F	4	ILE
2	F	11	VAL
2	F	26	SER
2	F	29	GLN
2	F	35	VAL
2	F	80	ILE
2	F	95	ILE
2	F	113	ILE
2	F	125	GLU
2	F	134	MET
2	F	142	GLU
2	F	168	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (31) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	715	ASN
1	A	749	HIS
1	A	827	GLN
1	A	831	GLN
1	A	858	GLN
1	A	880	GLN
1	A	895	HIS
1	A	931	HIS
1	A	950	ASN
1	A	968	HIS
1	A	997	GLN
1	A	1068	ASN
2	B	41	ASN
2	B	123	ASN
1	E	718	HIS
1	E	730	GLN
1	E	749	HIS
1	E	826	GLN
1	E	836	GLN
1	E	880	GLN
1	E	895	HIS
1	E	903	HIS

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Mol	Chain	Res	Type
1	E	926	GLN
1	E	931	HIS
1	E	937	GLN
1	E	997	GLN
1	E	1055	GLN
2	F	29	GLN
2	F	41	ASN
2	F	117	ASN
2	F	123	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

4 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
3	GOL	B	201	-	5,5,5	0.55	0	5,5,5	1.26	0
3	GOL	E	1101	-	5,5,5	0.25	0	5,5,5	0.85	0
3	GOL	A	1102	-	5,5,5	1.15	0	5,5,5	1.40	1 (20%)
3	GOL	A	1101	-	5,5,5	0.53	0	5,5,5	0.87	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	GOL	B	201	-	-	2/4/4/4	-
3	GOL	E	1101	-	-	2/4/4/4	-
3	GOL	A	1102	-	-	2/4/4/4	-
3	GOL	A	1101	-	-	0/4/4/4	-

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	1102	GOL	O3-C3-C2	-2.28	100.10	110.38

There are no chirality outliers.

All (6) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	1102	GOL	O1-C1-C2-C3
3	B	201	GOL	O1-C1-C2-C3
3	A	1102	GOL	O1-C1-C2-O2
3	E	1101	GOL	O2-C2-C3-O3
3	B	201	GOL	O1-C1-C2-O2
3	E	1101	GOL	O1-C1-C2-O2

There are no ring outliers.

3 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	201	GOL	2	0
3	E	1101	GOL	1	0
3	A	1101	GOL	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	356/369 (96%)	0.62	45 (12%) 8 6	22, 47, 99, 135	0
1	E	358/369 (97%)	0.82	68 (18%) 3 2	25, 49, 108, 127	0
2	B	178/181 (98%)	0.37	8 (4%) 38 33	24, 42, 80, 110	0
2	F	178/181 (98%)	0.30	8 (4%) 38 33	25, 44, 80, 100	0
All	All	1070/1100 (97%)	0.59	129 (12%) 8 7	22, 46, 97, 135	0

All (129) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	1051	LEU	5.8
1	A	720	VAL	5.7
1	E	1051	LEU	5.5
1	A	1037	ALA	5.3
1	E	1036	VAL	5.2
1	A	950	ASN	5.1
1	A	1053	PRO	4.9
1	E	952	LEU	4.7
1	A	1054	PRO	4.6
1	A	719	THR	4.6
1	E	1074	LEU	4.5
1	A	982	LEU	4.4
1	E	1069	THR	4.2
1	E	721	GLY	4.1
1	E	1068	ASN	4.0
1	E	1002	LYS	4.0
1	A	1049	SER	4.0
1	E	1042	ALA	4.0
1	A	952	LEU	3.9
1	E	720	VAL	3.9
1	E	1073	LEU	3.8

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Mol	Chain	Res	Type	RSRZ
2	F	134	MET	3.8
1	A	951	PRO	3.7
1	E	1037	ALA	3.7
1	E	1041	ARG	3.7
1	A	953	ALA	3.7
1	A	714	GLN	3.7
1	A	1055	GLN	3.6
1	A	722	LYS	3.6
1	E	1060	VAL	3.6
1	E	1081	ALA	3.5
1	A	981	THR	3.4
1	E	1080	ASN	3.4
1	A	726	ALA	3.3
1	A	871	LEU	3.3
1	E	1010	LYS	3.2
1	A	1050	LYS	3.2
1	E	1004	LEU	3.2
1	E	1076	GLU	3.2
1	E	945	LEU	3.1
2	B	134	MET	3.1
1	A	1038	THR	3.1
1	E	978	LYS	3.1
1	E	1065	SER	3.1
1	A	1047	CYS	3.0
1	E	1009	SER	3.0
2	F	51	LYS	3.0
1	E	1032	LEU	3.0
1	E	975	ARG	2.9
1	E	998	LYS	2.9
1	E	1043	PHE	2.9
1	E	1038	THR	2.9
1	E	976	ILE	2.8
2	B	3	ALA	2.8
1	A	980	LYS	2.8
1	A	1008	HIS	2.8
1	A	943	THR	2.8
1	A	721	GLY	2.7
1	A	1022	PHE	2.8
1	A	954	ALA	2.7
1	E	956	PHE	2.7
2	B	133	LYS	2.7
1	E	946	GLU	2.7

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Mol	Chain	Res	Type	RSRZ
2	F	132	ALA	2.7
2	F	50	GLY	2.7
1	E	722	LYS	2.7
1	E	1045	ILE	2.6
1	E	1071	MET	2.6
1	A	948	ALA	2.6
1	E	944	ALA	2.6
1	A	1021	THR	2.6
2	B	50	GLY	2.6
1	E	890	GLU	2.6
1	E	1062	LEU	2.6
2	B	32	GLU	2.6
1	E	1078	VAL	2.6
1	E	1077	ALA	2.6
1	A	1036	VAL	2.5
1	E	1066	ASP	2.5
1	E	1067	LYS	2.5
1	A	977	SER	2.5
1	A	798	LYS	2.5
1	A	959	LEU	2.5
1	E	1079	ARG	2.5
2	B	33	VAL	2.4
1	E	1053	PRO	2.4
1	E	1063	THR	2.4
1	E	1040	LYS	2.4
1	E	979	ASP	2.4
1	E	1046	ILE	2.4
1	A	945	LEU	2.4
1	E	980	LYS	2.4
1	E	1039	ASP	2.4
1	E	1031	VAL	2.4
1	A	955	GLU	2.4
1	E	1033	ILE	2.3
1	E	957	LYS	2.3
1	E	948	ALA	2.3
1	E	953	ALA	2.3
1	E	988	LEU	2.3
2	F	133	LYS	2.3
1	A	1007	CYS	2.3
1	E	1030	ALA	2.2
1	E	973	THR	2.2
1	E	977	SER	2.2

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Mol	Chain	Res	Type	RSRZ
1	E	1050	LYS	2.2
1	A	947	ARG	2.2
1	A	994	VAL	2.2
1	E	981	THR	2.2
1	E	965	LYS	2.2
1	A	949	SER	2.2
1	E	800	ARG	2.2
1	E	1061	ALA	2.1
1	E	1072	GLU	2.1
2	F	5	ARG	2.1
2	B	15	ALA	2.1
1	E	982	LEU	2.1
1	A	1056	ILE	2.1
2	F	113	ILE	2.1
2	F	128	ARG	2.1
1	E	1035	SER	2.1
1	A	1042	ALA	2.1
1	E	962	THR	2.1
1	E	725	VAL	2.0
1	A	1032	LEU	2.0
1	A	1052	GLY	2.0
2	B	144	GLY	2.0
1	A	800	ARG	2.0
1	A	1004	LEU	2.0

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

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

6.3 Carbohydrates [i](#)

There are no 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($\text{\AA}^2$)	Q<0.9
3	GOL	B	201	6/6	0.83	0.15	42,50,57,66	0
3	GOL	A	1102	6/6	0.89	0.13	29,32,34,35	0
3	GOL	E	1101	6/6	0.90	0.12	40,49,50,57	0
3	GOL	A	1101	6/6	0.96	0.07	39,41,45,46	0

6.5 Other polymers [i](#)

There are no such residues in this entry.