



Full wwPDB X-ray Structure Validation Report ⓘ

Jun 22, 2026 – 05:28 pm BST

PDB ID : 28NB / pdb_000028nb
Title : crystal structure of Dpo31, of a tail-spike protein with depolymerase activity identified in a marine podovirus
Authors : Czjzek, M.; Sirigu, S.; Roret, T.; Baudoux, A.C.; Legrand, P.
Deposited on : 2026-02-09
Resolution : 3.30 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	:	1.8.4, CSD as541be (2020)
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

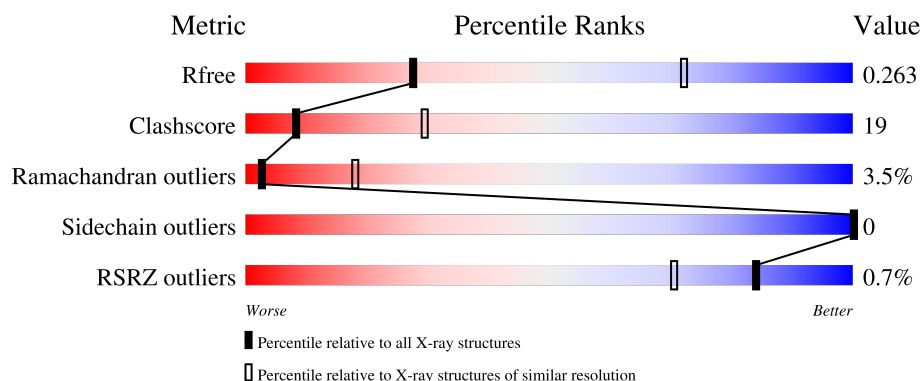
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.30 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	1169 (3.32-3.28)
Clashscore	190562	1209 (3.32-3.28)
Ramachandran outliers	187476	1188 (3.32-3.28)
Sidechain outliers	187428	1187 (3.32-3.28)
RSRZ outliers	180081	1169 (3.32-3.28)

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	173	<div> <div>58%</div> <div>36%</div> <div>..</div> </div>
1	B	173	<div> <div>%</div> <div>61%</div> <div>31%</div> <div>.. 5%</div> </div>
1	C	173	<div> <div>55%</div> <div>39%</div> <div>• 6%</div> </div>
1	D	173	<div> <div>%</div> <div>52%</div> <div>40%</div> <div>.. 5%</div> </div>
1	E	173	<div> <div>%</div> <div>58%</div> <div>36%</div> <div>• 5%</div> </div>

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Mol	Chain	Length	Quality of chain
1	F	173	<div><div><div></div><div></div><div></div></div><div>%</div><div><div></div><div></div><div></div></div><div>59%34%• 6%</div></div>
1	G	173	<div><div><div></div><div></div><div></div></div><div></div><div><div></div><div></div><div></div></div><div>57%36%• 5%</div></div>
1	H	173	<div><div><div></div><div></div><div></div></div><div>%</div><div><div></div><div></div><div></div></div><div>57%35%• 6%</div></div>
1	I	173	<div><div><div></div><div></div><div></div></div><div>2%</div><div><div></div><div></div><div></div></div><div>57%33%• • 6%</div></div>

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 10941 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 chaperon domain D4 for tailspike protein Dpo31.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	167	Total	C	N	O	S	0	0	0
			1243	775	218	245	5			
1	B	164	Total	C	N	O	S	0	0	0
			1204	747	211	241	5			
1	C	163	Total	C	N	O	S	0	0	0
			1198	744	210	239	5			
1	D	164	Total	C	N	O	S	0	0	0
			1202	746	211	240	5			
1	E	164	Total	C	N	O	S	0	0	0
			1204	747	211	241	5			
1	F	163	Total	C	N	O	S	0	0	0
			1198	744	210	239	5			
1	G	164	Total	C	N	O	S	0	0	0
			1202	746	211	240	5			
1	H	163	Total	C	N	O	S	0	0	0
			1198	744	210	239	5			
1	I	163	Total	C	N	O	S	0	0	0
			1198	744	210	239	5			

- Molecule 2 is ACETATE ION (CCD ID: ACT) (formula: C₂H₃O₂).



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

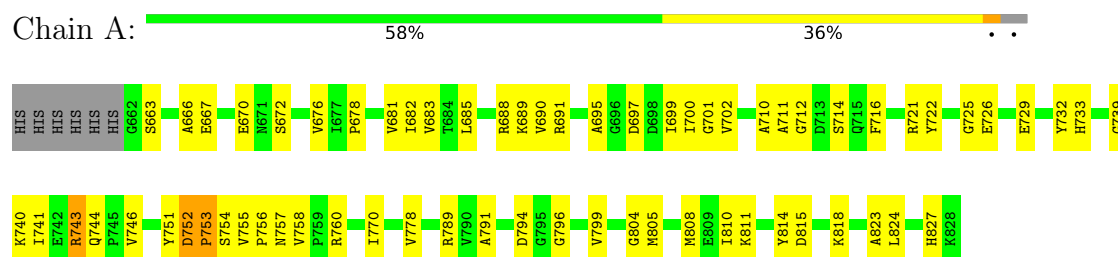
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	7	Total	O	0	0
			7	7		
3	B	10	Total	O	0	0
			10	10		
3	C	11	Total	O	0	0
			11	11		
3	D	13	Total	O	0	0
			13	13		
3	E	9	Total	O	0	0
			9	9		
3	F	11	Total	O	0	0
			11	11		
3	G	16	Total	O	0	0
			16	16		
3	H	6	Total	O	0	0
			6	6		
3	I	7	Total	O	0	0
			7	7		

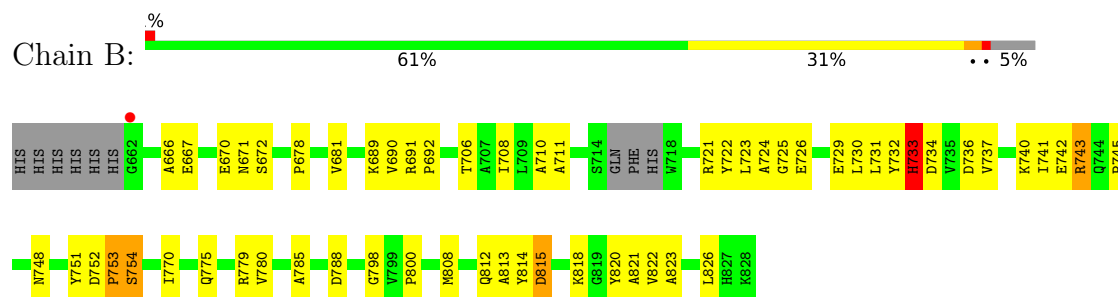
3 Residue-property plots

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.

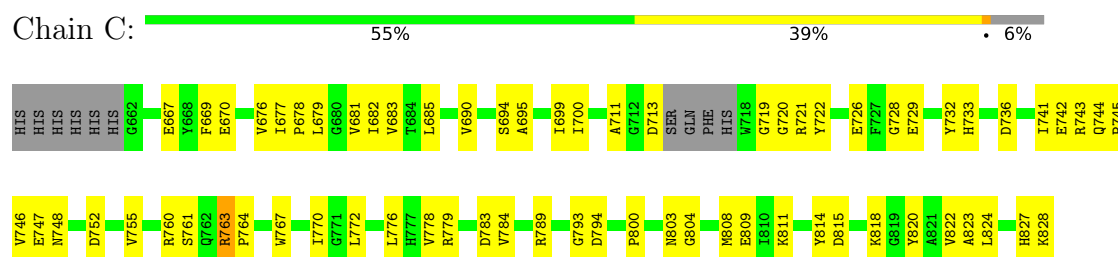
- Molecule 1: chaperon domain D4 for tailspike protein Dpo31



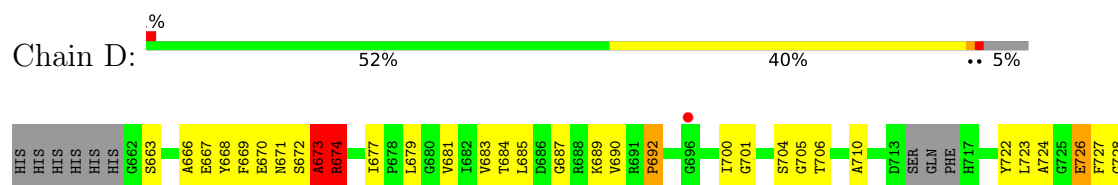
- Molecule 1: chaperon domain D4 for tailspike protein Dpo31

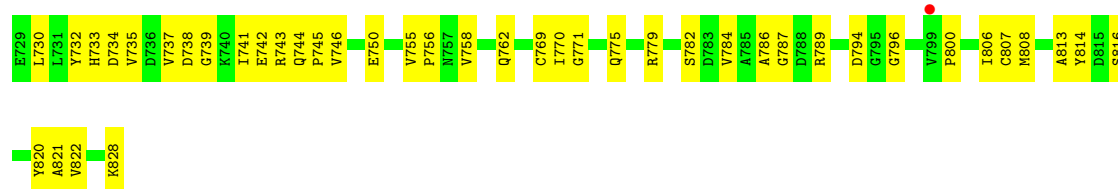


- Molecule 1: chaperon domain D4 for tailspike protein Dpo31

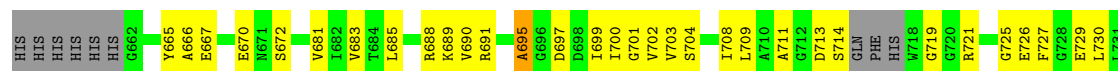


- Molecule 1: chaperon domain D4 for tailspike protein Dpo31





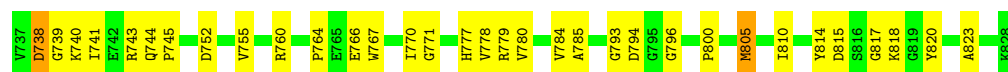
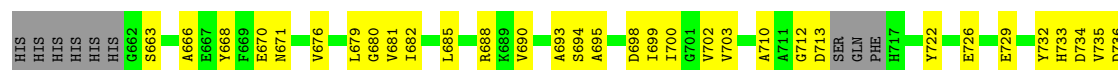
- Molecule 1: chaperon domain D4 for tailspike protein Dpo31



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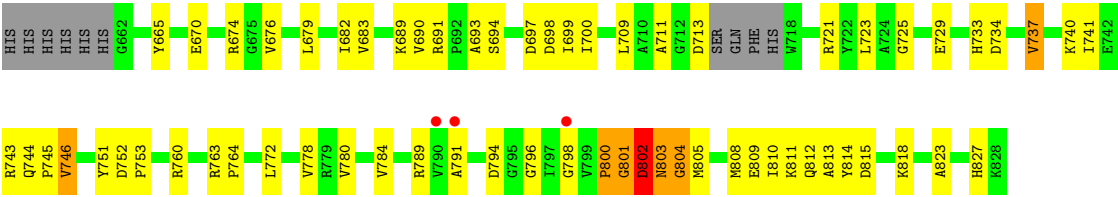
- Molecule 1: chaperon domain D4 for tailspike protein Dpo31



- Molecule 1: chaperon domain D4 for tailspike protein Dpo31



- Molecule 1: chaperon domain D4 for tailspike protein Dpo31



4 Data and refinement statistics

Property	Value	Source
Space group	P 32 2 1	Depositor
Cell constants a, b, c, α , β , γ	69.74Å 69.74Å 533.35Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	47.33 – 3.30 47.33 – 3.30	Depositor EDS
% Data completeness (in resolution range)	100.0 (47.33-3.30) 100.0 (47.33-3.30)	Depositor EDS
R_{merge}	0.52	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	350.52 (at 3.33Å)	Xtriage
Refinement program	PHENIX 1.14_3260, PHENIX 1.14_3260	Depositor
R, R_{free}	0.247 , 0.259 0.246 , 0.263	Depositor DCC
R_{free} test set	1207 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å ²)	64.7	Xtriage
Anisotropy	0.479	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 99.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.32$, $\langle L^2 \rangle = 0.15$	Xtriage
Estimated twinning fraction	0.159 for -h,-k,l	Xtriage
F_o, F_c correlation	0.85	EDS
Total number of atoms	10941	wwPDB-VP
Average B, all atoms (Å ²)	67.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.89% 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: ACT

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	0.21	0/1269	0.54	2/1721 (0.1%)
1	B	0.26	0/1225	0.60	5/1659 (0.3%)
1	C	0.20	0/1219	0.50	0/1651
1	D	0.38	2/1223 (0.2%)	0.67	4/1656 (0.2%)
1	E	0.16	0/1225	0.47	0/1659
1	F	0.17	0/1219	0.47	0/1651
1	G	0.22	0/1223	0.57	0/1656
1	H	0.17	0/1219	0.46	0/1651
1	I	0.54	4/1219 (0.3%)	1.04	10/1651 (0.6%)
All	All	0.28	6/11041 (0.1%)	0.61	21/14955 (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	D	0	1
1	H	0	1
1	I	0	3
All	All	0	5

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	674	ARG	CG-CD	8.08	1.76	1.52
1	I	803	ASN	N-CA	7.69	1.60	1.46
1	I	802	ASP	CB-CG	-7.53	1.33	1.52
1	I	803	ASN	CA-CB	5.84	1.65	1.53
1	I	802	ASP	C-N	5.39	1.40	1.33
1	D	674	ARG	CB-CG	5.26	1.68	1.52

All (21) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	I	802	ASP	CA-C-N	16.76	151.86	121.70
1	I	802	ASP	C-N-CA	16.76	151.86	121.70
1	I	804	GLY	N-CA-C	15.64	126.06	111.67
1	I	801	GLY	N-CA-C	-12.19	92.80	110.60
1	D	674	ARG	CG-CD-NE	8.57	130.85	112.00
1	I	803	ASN	N-CA-CB	7.95	124.02	110.50
1	D	674	ARG	CD-NE-CZ	7.70	135.17	124.40
1	D	673	ALA	CA-C-N	7.32	135.52	121.54
1	D	673	ALA	C-N-CA	7.32	135.52	121.54
1	I	803	ASN	CB-CA-C	-7.02	96.76	110.10
1	I	803	ASN	CA-CB-CG	6.98	119.58	112.60
1	I	801	GLY	CA-C-O	-6.29	115.14	121.30
1	I	802	ASP	OD1-CG-OD2	6.17	137.71	122.90
1	I	802	ASP	N-CA-C	5.58	117.17	111.14
1	A	753	PRO	N-CA-C	5.46	123.72	112.47
1	B	740	LYS	CD-CE-NZ	-5.34	94.81	111.90
1	B	733	HIS	CA-C-N	5.20	131.47	121.54
1	B	733	HIS	C-N-CA	5.20	131.47	121.54
1	B	743	ARG	CB-CG-CD	5.10	123.03	111.30
1	A	752	ASP	CB-CA-C	5.06	116.82	109.08
1	B	754	SER	CB-CA-C	-5.03	101.97	111.97

There are no chirality outliers.

All (5) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	D	674	ARG	Sidechain
1	H	664	ASP	Peptide
1	I	800	PRO	Peptide
1	I	801	GLY	Peptide
1	I	802	ASP	Peptide

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1243	0	1193	54	2
1	B	1204	0	1160	55	1
1	C	1198	0	1155	48	1
1	D	1202	0	1156	56	2
1	E	1204	0	1160	46	0
1	F	1198	0	1155	43	0
1	G	1202	0	1156	51	2
1	H	1198	0	1155	52	1
1	I	1198	0	1155	46	1
2	A	4	0	3	0	0
3	A	7	0	0	1	0
3	B	10	0	0	0	0
3	C	11	0	0	1	0
3	D	13	0	0	0	0
3	E	9	0	0	0	0
3	F	11	0	0	1	0
3	G	16	0	0	0	0
3	H	6	0	0	0	0
3	I	7	0	0	0	0
All	All	10941	0	10448	408	5

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 19.

All (408) 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:D:674:ARG:CD	1:D:674:ARG:CG	1.76	1.58
1:I:802:ASP:OD1	1:I:803:ASN:ND2	1.74	1.21
1:B:734:ASP:H	1:B:743:ARG:HG3	1.21	1.03
1:A:827:HIS:NE2	1:C:828:LYS:NZ	2.08	1.01
1:D:742:GLU:HB3	1:H:674:ARG:HD2	1.47	0.96
1:F:667:GLU:HG2	1:F:711:ALA:HB3	1.59	0.85
1:D:663:SER:HB2	1:E:711:ALA:HB1	1.58	0.85
1:I:733:HIS:HD2	1:I:746:VAL:HG22	1.41	0.84
1:E:815:ASP:HB3	1:E:818:LYS:HG3	1.59	0.84
1:E:714:SER:HB3	1:E:719:GLY:HA2	1.57	0.83
1:G:740:LYS:HG2	1:G:741:ILE:H	1.44	0.83
1:F:742:GLU:HG3	1:H:802:ASP:HB2	1.61	0.82
1:B:732:TYR:O	1:B:733:HIS:ND1	2.12	0.81
1:F:672:SER:HB3	1:F:689:LYS:HB3	1.65	0.78
1:B:734:ASP:H	1:B:743:ARG:CG	1.97	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:721:ARG:HA	1:F:751:TYR:HB2	1.66	0.77
1:A:691:ARG:NH2	1:A:697:ASP:OD2	2.17	0.76
1:H:758:VAL:HG12	1:H:759:PRO:HD2	1.68	0.74
1:D:814:TYR:HB2	1:D:821:ALA:HB2	1.68	0.74
1:H:683:VAL:HG21	1:H:770:ILE:HD12	1.69	0.74
1:A:667:GLU:HG2	1:A:711:ALA:HB3	1.69	0.74
1:D:723:LEU:HB3	1:D:746:VAL:HG23	1.69	0.73
1:H:685:LEU:HG	1:H:700:ILE:HD13	1.70	0.73
1:D:737:VAL:HG21	1:H:674:ARG:HH22	1.52	0.73
1:G:713:ASP:HA	1:G:760:ARG:H	1.52	0.73
1:A:755:VAL:HG22	1:A:756:PRO:HD2	1.69	0.73
1:C:667:GLU:HG2	1:C:711:ALA:HB3	1.69	0.73
1:B:779:ARG:O	1:B:798:GLY:N	2.20	0.73
1:H:667:GLU:HG3	1:H:711:ALA:HB3	1.69	0.73
1:E:667:GLU:HG3	1:E:711:ALA:HB3	1.71	0.73
1:B:667:GLU:HG2	1:B:711:ALA:HB3	1.70	0.72
1:B:733:HIS:HA	1:B:743:ARG:HG2	1.70	0.72
1:E:702:VAL:HB	1:E:776:LEU:HD13	1.70	0.71
1:D:755:VAL:HG22	1:D:756:PRO:HD2	1.72	0.71
1:A:672:SER:HA	1:A:689:LYS:HE3	1.71	0.71
1:F:663:SER:HA	1:F:706:THR:HG22	1.73	0.70
1:A:699:ILE:HG21	1:A:805:MET:HE2	1.74	0.70
1:B:690:VAL:HG11	1:B:770:ILE:HG13	1.73	0.70
1:D:681:VAL:HG22	1:D:796:GLY:HA3	1.71	0.70
1:D:737:VAL:HG11	1:H:674:ARG:NH1	2.07	0.69
1:E:685:LEU:HG	1:E:700:ILE:HD13	1.73	0.69
1:H:672:SER:HA	1:H:689:LYS:HD3	1.74	0.68
1:B:730:LEU:HD12	1:B:745:PRO:HB3	1.75	0.68
1:A:663:SER:HB2	1:B:711:ALA:HB1	1.75	0.68
1:B:752:ASP:C	1:B:754:SER:H	2.01	0.68
1:B:734:ASP:N	1:B:743:ARG:HG3	2.04	0.67
1:C:736:ASP:OD1	1:C:741:ILE:HG12	1.95	0.67
1:C:683:VAL:HG21	1:C:770:ILE:HD12	1.77	0.66
1:H:690:VAL:HG11	1:H:770:ILE:HG13	1.77	0.66
1:G:784:VAL:HG22	1:G:800:PRO:HD3	1.78	0.66
1:C:789:ARG:HH11	1:C:804:GLY:H	1.42	0.66
1:I:733:HIS:CD2	1:I:746:VAL:HG22	2.26	0.65
1:C:811:LYS:HD2	1:C:824:LEU:HB2	1.80	0.64
1:E:713:ASP:HA	1:E:760:ARG:HB2	1.79	0.64
1:A:789:ARG:HD3	1:A:804:GLY:H	1.63	0.63
1:D:677:ILE:HG22	1:D:681:VAL:HG11	1.79	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:721:ARG:HA	1:H:748:ASN:HB3	1.81	0.63
1:B:800:PRO:HB3	1:G:740:LYS:HD3	1.79	0.63
1:H:735:VAL:HG12	1:H:736:ASP:H	1.62	0.63
1:D:679:LEU:HD22	1:E:727:PHE:HB2	1.81	0.62
1:C:694:SER:HB3	1:C:794:ASP:HA	1.79	0.62
1:E:735:VAL:HG21	1:E:744:GLN:HB2	1.80	0.62
1:C:752:ASP:HB3	1:C:755:VAL:HB	1.80	0.62
1:A:725:GLY:HA3	1:A:729:GLU:HG3	1.81	0.62
1:B:691:ARG:HD2	1:I:721:ARG:CZ	2.31	0.61
1:D:743:ARG:C	1:H:674:ARG:HD3	2.25	0.61
1:F:676:VAL:HG22	1:F:764:PRO:HB2	1.81	0.61
1:C:760:ARG:HG3	1:C:763:ARG:CZ	2.29	0.61
1:B:808:MET:HE3	1:B:826:LEU:HB2	1.80	0.61
1:D:822:VAL:HG21	1:E:726:GLU:HG2	1.83	0.61
1:A:760:ARG:HH11	1:A:760:ARG:HG3	1.66	0.60
1:G:712:GLY:HA3	1:G:760:ARG:HD2	1.83	0.60
1:G:732:TYR:HA	1:G:745:PRO:HA	1.84	0.60
1:B:678:PRO:HD2	1:B:681:VAL:HG21	1.81	0.60
1:C:772:LEU:O	1:C:827:HIS:ND1	2.35	0.60
1:H:678:PRO:HD2	1:H:681:VAL:HG21	1.81	0.60
1:D:724:ALA:HA	1:D:730:LEU:HA	1.83	0.60
1:I:810:ILE:HD12	1:I:823:ALA:HB2	1.83	0.60
1:A:685:LEU:HG	1:A:700:ILE:HD13	1.84	0.59
1:B:788:ASP:HB3	1:G:740:LYS:HE3	1.83	0.59
1:I:734:ASP:HB3	1:I:741:ILE:HG23	1.85	0.59
1:C:678:PRO:HD2	1:C:681:VAL:HG21	1.85	0.59
1:G:688:ARG:HA	1:I:808:MET:HB3	1.84	0.59
1:F:743:ARG:NH1	3:F:202:HOH:O	2.36	0.58
1:G:681:VAL:HG13	1:G:796:GLY:HA3	1.84	0.58
1:I:772:LEU:O	1:I:827:HIS:ND1	2.36	0.58
1:E:732:TYR:HA	1:E:745:PRO:HA	1.85	0.58
1:H:679:LEU:O	1:H:779:ARG:NE	2.28	0.58
1:H:674:ARG:HG2	1:H:675:GLY:H	1.68	0.58
1:B:670:GLU:O	1:B:690:VAL:N	2.37	0.58
1:B:785:ALA:H	1:G:740:LYS:HE2	1.68	0.58
1:F:725:GLY:HA3	1:F:729:GLU:HG3	1.85	0.58
1:F:735:VAL:HG21	1:F:744:GLN:HB2	1.86	0.58
1:H:818:LYS:HB3	1:H:820:TYR:CE2	2.39	0.57
1:B:754:SER:O	1:B:754:SER:OG	2.13	0.57
1:B:820:TYR:OH	1:C:726:GLU:OE2	2.23	0.57
1:H:706:THR:HG21	1:H:777:HIS:HD1	1.69	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:688:ARG:HA	1:C:808:MET:HB3	1.85	0.57
1:E:744:GLN:HG2	1:E:745:PRO:HD2	1.87	0.57
1:B:736:ASP:HA	1:B:741:ILE:HD12	1.87	0.57
1:C:677:ILE:HD12	1:C:690:VAL:HG23	1.87	0.57
1:G:685:LEU:HG	1:G:700:ILE:HG21	1.86	0.56
1:H:708:ILE:HG13	1:I:711:ALA:HB1	1.87	0.56
1:I:812:GLN:NE2	1:I:813:ALA:O	2.34	0.56
1:B:813:ALA:O	1:B:815:ASP:N	2.37	0.56
1:E:713:ASP:OD1	1:E:713:ASP:N	2.39	0.56
1:C:815:ASP:HB3	1:C:818:LYS:HG3	1.88	0.56
1:H:663:SER:HB3	1:I:711:ALA:HB1	1.87	0.56
1:E:691:ARG:NH1	1:E:697:ASP:OD2	2.39	0.56
1:A:811:LYS:HD3	1:A:824:LEU:HB2	1.89	0.55
1:B:785:ALA:N	1:G:740:LYS:HG3	2.21	0.55
1:D:667:GLU:HB2	1:D:669:PHE:HE1	1.69	0.55
1:F:737:VAL:O	1:F:740:LYS:HB2	2.06	0.55
1:A:740:LYS:HG2	1:A:741:ILE:H	1.71	0.55
1:C:679:LEU:O	1:C:779:ARG:NH2	2.38	0.55
1:B:818:LYS:HB3	1:B:820:TYR:CE2	2.41	0.55
1:G:702:VAL:HG21	1:G:778:VAL:HG22	1.87	0.55
1:I:683:VAL:HG23	1:I:700:ILE:HG13	1.89	0.55
1:A:721:ARG:NH2	3:A:301:HOH:O	2.30	0.55
1:D:722:TYR:HB3	1:D:746:VAL:O	2.07	0.55
1:B:752:ASP:C	1:B:754:SER:N	2.64	0.54
1:G:738:ASP:OD1	1:G:738:ASP:O	2.26	0.54
1:E:725:GLY:N	1:E:729:GLU:O	2.41	0.54
1:F:734:ASP:HB2	1:F:741:ILE:HG23	1.90	0.54
1:A:700:ILE:O	1:C:828:LYS:NZ	2.41	0.54
1:F:686:ASP:HB3	1:F:689:LYS:HB2	1.90	0.54
1:E:775:GLN:HB3	1:E:824:LEU:HD11	1.89	0.54
1:E:802:ASP:N	1:E:802:ASP:OD1	2.39	0.54
1:G:690:VAL:HG11	1:G:770:ILE:HG13	1.89	0.54
1:D:787:GLY:N	1:D:807:CYS:O	2.38	0.53
1:G:695:ALA:HB2	1:G:793:GLY:HA2	1.90	0.53
1:I:670:GLU:HB3	1:I:689:LYS:HG2	1.89	0.53
1:D:786:ALA:HA	1:D:807:CYS:HB3	1.90	0.53
1:F:773:VAL:HG23	1:F:828:LYS:HA	1.91	0.53
1:D:722:TYR:CG	1:D:745:PRO:HB2	2.43	0.53
1:A:721:ARG:HG3	1:A:751:TYR:CD2	2.44	0.53
1:E:733:HIS:N	1:E:744:GLN:O	2.34	0.53
1:A:726:GLU:O	1:C:822:VAL:HG11	2.09	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:815:ASP:O	1:E:817:GLY:N	2.43	0.52
1:D:679:LEU:HD21	1:D:705:GLY:H	1.73	0.52
1:D:784:VAL:HG22	1:D:800:PRO:HD3	1.90	0.52
1:F:809:GLU:HG2	1:F:810:ILE:H	1.74	0.52
1:G:726:GLU:OE2	1:I:818:LYS:NZ	2.36	0.52
1:G:698:ASP:OD1	1:G:699:ILE:N	2.43	0.52
1:H:748:ASN:O	1:H:751:TYR:HD2	1.93	0.52
1:C:763:ARG:HD2	1:C:767:TRP:CD1	2.45	0.52
1:I:760:ARG:H	1:I:760:ARG:HD3	1.73	0.52
1:B:820:TYR:HE1	1:B:822:VAL:HG23	1.74	0.52
1:G:740:LYS:HG2	1:G:741:ILE:N	2.19	0.52
1:E:683:VAL:HG21	1:E:770:ILE:HD12	1.91	0.52
1:H:674:ARG:HG3	1:H:674:ARG:HH11	1.75	0.52
1:B:737:VAL:HG11	1:B:742:GLU:OE1	2.09	0.51
1:G:752:ASP:O	1:G:755:VAL:HG12	2.10	0.51
1:H:790:VAL:HG13	1:H:798:GLY:HA3	1.93	0.51
1:A:682:ILE:HG12	1:A:702:VAL:HG22	1.92	0.51
1:I:682:ILE:HB	1:I:693:ALA:HB2	1.91	0.51
1:I:760:ARG:HA	1:I:763:ARG:HG3	1.93	0.51
1:B:672:SER:HA	1:B:689:LYS:HD3	1.92	0.51
1:G:680:GLY:HA3	1:G:779:ARG:HG3	1.92	0.51
1:H:762:GLN:C	1:H:764:PRO:HD3	2.35	0.51
1:I:691:ARG:NH2	1:I:694:SER:OG	2.43	0.51
1:I:737:VAL:HG23	1:I:740:LYS:HB2	1.93	0.51
1:B:721:ARG:HG2	1:B:751:TYR:CD1	2.46	0.51
1:D:669:PHE:HB2	1:D:770:ILE:HD13	1.93	0.51
1:F:735:VAL:CG2	1:F:744:GLN:HB2	2.40	0.51
1:G:815:ASP:O	1:G:817:GLY:N	2.37	0.51
1:H:706:THR:HG21	1:H:777:HIS:ND1	2.26	0.51
1:G:733:HIS:O	1:G:744:GLN:N	2.44	0.50
1:D:671:ASN:C	1:D:673:ALA:H	2.19	0.50
1:G:666:ALA:HA	1:G:771:GLY:HA2	1.93	0.50
1:H:776:LEU:HD12	1:H:778:VAL:HG22	1.93	0.50
1:I:744:GLN:HG2	1:I:745:PRO:HD2	1.93	0.50
1:E:672:SER:HB3	1:E:689:LYS:HB2	1.93	0.50
1:A:695:ALA:N	1:A:794:ASP:OD1	2.39	0.50
1:B:785:ALA:H	1:G:740:LYS:HG3	1.75	0.50
1:G:671:ASN:N	1:G:766:GLU:O	2.41	0.50
1:I:733:HIS:O	1:I:744:GLN:N	2.39	0.50
1:A:741:ILE:HD12	1:A:741:ILE:O	2.11	0.50
1:C:690:VAL:HG11	1:C:770:ILE:HG13	1.93	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:684:THR:HG22	1:D:692:PRO:O	2.12	0.50
1:D:742:GLU:OE2	1:H:674:ARG:NH1	2.44	0.50
1:E:695:ALA:N	1:E:793:GLY:O	2.45	0.50
1:I:693:ALA:HB3	1:I:796:GLY:HA2	1.94	0.50
1:A:721:ARG:NH1	1:A:722:TYR:OH	2.45	0.50
1:D:666:ALA:HB2	1:D:771:GLY:HA2	1.94	0.50
1:C:682:ILE:HG23	1:C:699:ILE:HG23	1.94	0.49
1:D:663:SER:HA	1:D:706:THR:HB	1.93	0.49
1:H:664:ASP:OD2	1:H:776:LEU:HB3	2.12	0.49
1:F:664:ASP:HB3	1:F:776:LEU:HG	1.93	0.49
1:A:678:PRO:HD2	1:A:681:VAL:HG21	1.94	0.49
1:B:681:VAL:HG11	1:B:692:PRO:HB3	1.94	0.49
1:G:663:SER:HB2	1:H:711:ALA:HB1	1.94	0.49
1:D:737:VAL:HG11	1:H:674:ARG:HH12	1.73	0.49
1:F:679:LEU:HA	1:F:703:VAL:HB	1.94	0.49
1:C:783:ASP:HB2	1:C:800:PRO:HG3	1.94	0.49
1:E:789:ARG:HD2	1:E:805:MET:O	2.13	0.49
1:B:737:VAL:HG21	1:B:742:GLU:CD	2.38	0.49
1:F:760:ARG:HD2	1:F:767:TRP:CD2	2.48	0.49
1:A:729:GLU:OE2	1:C:679:LEU:HD12	2.12	0.48
1:C:760:ARG:O	1:C:763:ARG:HB2	2.13	0.48
1:F:722:TYR:HB3	1:F:730:LEU:HD21	1.96	0.48
1:F:734:ASP:OD1	1:F:734:ASP:N	2.42	0.48
1:H:763:ARG:NH1	1:H:767:TRP:HE1	2.11	0.48
1:B:731:LEU:O	1:B:745:PRO:HA	2.14	0.48
1:E:729:GLU:O	1:E:729:GLU:HG2	2.12	0.48
1:E:737:VAL:HG23	1:E:740:LYS:HG3	1.95	0.48
1:F:807:CYS:SG	1:F:808:MET:N	2.87	0.48
1:A:714:SER:H	1:A:760:ARG:HG2	1.78	0.48
1:D:733:HIS:HD2	1:D:734:ASP:N	2.12	0.48
1:E:681:VAL:O	1:E:703:VAL:HG23	2.13	0.48
1:G:702:VAL:HG23	1:G:805:MET:HE1	1.96	0.48
1:H:682:ILE:HA	1:H:702:VAL:HG22	1.96	0.48
1:C:713:ASP:OD1	1:C:761:SER:N	2.47	0.47
1:C:803:ASN:ND2	3:C:201:HOH:O	2.46	0.47
1:D:679:LEU:CD2	1:D:704:SER:HA	2.44	0.47
1:F:721:ARG:CA	1:F:751:TYR:HB2	2.39	0.47
1:G:682:ILE:HG22	1:G:693:ALA:HB2	1.96	0.47
1:A:688:ARG:NH1	1:C:809:GLU:OE1	2.48	0.47
1:A:702:VAL:HG21	1:A:778:VAL:HG22	1.95	0.47
1:C:676:VAL:HG22	1:C:764:PRO:HB2	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:814:TYR:HA	1:G:820:TYR:O	2.15	0.47
1:A:681:VAL:HG13	1:A:796:GLY:HA3	1.97	0.47
1:C:670:GLU:O	1:C:690:VAL:HG22	2.14	0.47
1:C:722:TYR:HA	1:C:747:GLU:HA	1.97	0.47
1:B:751:TYR:O	1:B:753:PRO:HD3	2.15	0.47
1:G:680:GLY:HA2	1:G:777:HIS:O	2.14	0.47
1:G:734:ASP:OD1	1:G:743:ARG:HG3	2.13	0.47
1:B:691:ARG:HB2	1:I:721:ARG:NH2	2.30	0.47
1:I:665:TYR:CE1	1:I:709:LEU:HD23	2.50	0.47
1:I:670:GLU:O	1:I:690:VAL:N	2.45	0.47
1:C:685:LEU:HG	1:C:700:ILE:HD13	1.97	0.46
1:A:670:GLU:OE2	1:A:688:ARG:NH2	2.45	0.46
1:E:721:ARG:HG3	1:E:751:TYR:CD1	2.50	0.46
1:D:685:LEU:HG	1:D:700:ILE:HG21	1.97	0.46
1:E:818:LYS:HB3	1:E:820:TYR:CE2	2.51	0.46
1:F:720:GLY:O	1:F:748:ASN:ND2	2.49	0.46
1:A:725:GLY:N	1:A:729:GLU:O	2.47	0.46
1:A:712:GLY:HA2	1:A:716:PHE:CE1	2.50	0.46
1:E:690:VAL:HG11	1:E:770:ILE:HG13	1.98	0.46
1:B:812:GLN:O	1:B:821:ALA:HB1	2.16	0.46
1:F:694:SER:O	1:F:697:ASP:HB2	2.16	0.46
1:D:679:LEU:HD22	1:E:727:PHE:CB	2.43	0.46
1:H:674:ARG:CG	1:H:765:GLU:HB3	2.45	0.46
1:H:677:ILE:HG23	1:H:692:PRO:HG3	1.96	0.46
1:A:755:VAL:CG2	1:A:756:PRO:HD2	2.44	0.46
1:B:733:HIS:HA	1:B:743:ARG:CG	2.42	0.46
1:D:726:GLU:HG3	1:D:727:PHE:H	1.80	0.46
1:A:732:TYR:HB3	1:A:743:ARG:HG2	1.96	0.46
1:A:752:ASP:OD1	1:A:753:PRO:HD2	2.16	0.46
1:H:694:SER:O	1:H:697:ASP:HB2	2.15	0.46
1:I:725:GLY:N	1:I:729:GLU:O	2.48	0.46
1:A:688:ARG:HD3	1:C:809:GLU:OE2	2.16	0.46
1:C:694:SER:HA	1:C:793:GLY:O	2.15	0.46
1:G:729:GLU:OE2	1:I:679:LEU:HD12	2.15	0.46
1:H:674:ARG:HG2	1:H:765:GLU:HB3	1.98	0.46
1:A:714:SER:N	1:A:760:ARG:HG2	2.30	0.45
1:I:789:ARG:HH11	1:I:804:GLY:CA	2.28	0.45
1:E:746:VAL:HG22	1:E:747:GLU:H	1.81	0.45
1:D:701:GLY:HA3	1:D:771:GLY:O	2.17	0.45
1:E:812:GLN:HB3	1:E:822:VAL:HB	1.99	0.45
1:B:724:ALA:HA	1:B:729:GLU:O	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:713:ASP:OD1	1:I:760:ARG:N	2.50	0.45
1:G:734:ASP:HA	1:G:743:ARG:HA	1.99	0.45
1:G:818:LYS:HB3	1:G:820:TYR:CE2	2.52	0.45
1:A:760:ARG:HG3	1:A:760:ARG:NH1	2.30	0.45
1:B:732:TYR:HE1	1:B:745:PRO:HD3	1.82	0.45
1:H:722:TYR:HD1	1:H:745:PRO:HB2	1.82	0.45
1:I:791:ALA:O	1:I:798:GLY:HA2	2.16	0.45
1:D:758:VAL:HG13	1:D:762:GLN:OE1	2.16	0.44
1:G:695:ALA:N	1:G:794:ASP:OD1	2.50	0.44
1:A:810:ILE:HD13	1:A:823:ALA:HB2	1.99	0.44
1:G:679:LEU:HD12	1:G:679:LEU:H	1.82	0.44
1:G:810:ILE:HD13	1:G:823:ALA:HB2	1.97	0.44
1:A:691:ARG:HH11	1:A:691:ARG:HG3	1.82	0.44
1:D:735:VAL:O	1:D:741:ILE:HA	2.16	0.44
1:E:670:GLU:OE2	1:E:688:ARG:NH2	2.51	0.44
1:E:809:GLU:OE2	1:F:688:ARG:HD3	2.18	0.44
1:I:729:GLU:O	1:I:729:GLU:HG2	2.16	0.44
1:A:690:VAL:HG11	1:A:770:ILE:HG13	1.99	0.44
1:B:670:GLU:HG3	1:B:671:ASN:N	2.33	0.44
1:E:681:VAL:HG13	1:E:796:GLY:HA3	1.98	0.44
1:H:729:GLU:O	1:H:730:LEU:C	2.60	0.44
1:I:734:ASP:OD1	1:I:743:ARG:HG3	2.17	0.44
1:C:763:ARG:N	1:C:764:PRO:HD3	2.33	0.44
1:G:780:VAL:HB	1:G:784:VAL:HG21	2.00	0.44
1:B:788:ASP:HB3	1:G:740:LYS:CE	2.46	0.44
1:C:776:LEU:O	1:C:778:VAL:HG23	2.18	0.44
1:D:683:VAL:CG1	1:D:690:VAL:HB	2.47	0.44
1:C:719:GLY:O	1:C:721:ARG:N	2.51	0.44
1:E:700:ILE:HG13	1:E:701:GLY:N	2.30	0.44
1:A:682:ILE:HG23	1:A:699:ILE:HG23	1.99	0.44
1:B:721:ARG:HG2	1:B:751:TYR:CE1	2.52	0.44
1:B:729:GLU:H	1:B:729:GLU:HG2	1.55	0.44
1:D:779:ARG:HD3	1:D:820:TYR:HB3	1.99	0.44
1:E:726:GLU:N	1:E:729:GLU:OE2	2.50	0.44
1:F:818:LYS:HB2	1:F:818:LYS:HE3	1.89	0.44
1:H:780:VAL:HG23	1:H:821:ALA:HB3	1.99	0.44
1:G:785:ALA:HA	1:G:810:ILE:HG13	1.99	0.44
1:G:679:LEU:HA	1:G:703:VAL:HB	2.00	0.43
1:I:809:GLU:CD	1:I:811:LYS:HE3	2.43	0.43
1:A:714:SER:H	1:A:760:ARG:H	1.64	0.43
1:B:723:LEU:HG	1:B:748:ASN:HA	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:669:PHE:O	1:C:767:TRP:HA	2.18	0.43
1:E:803:ASN:OD1	1:E:803:ASN:N	2.52	0.43
1:I:723:LEU:HD23	1:I:723:LEU:HA	1.89	0.43
1:A:690:VAL:HG12	1:A:700:ILE:HD11	1.99	0.43
1:E:666:ALA:HA	1:E:771:GLY:HA2	2.00	0.43
1:B:706:THR:HG22	1:C:728:GLY:O	2.18	0.43
1:F:757:ASN:O	1:F:757:ASN:ND2	2.46	0.43
1:C:721:ARG:O	1:C:747:GLU:HG3	2.18	0.43
1:D:727:PHE:HD1	1:D:727:PHE:O	2.02	0.43
1:F:723:LEU:HG	1:F:748:ASN:HB2	2.00	0.43
1:B:729:GLU:O	1:B:730:LEU:HD22	2.19	0.43
1:B:752:ASP:O	1:B:754:SER:N	2.50	0.43
1:F:725:GLY:N	1:F:729:GLU:O	2.52	0.43
1:G:733:HIS:HB2	1:G:745:PRO:C	2.44	0.43
1:H:729:GLU:O	1:H:729:GLU:HG2	2.18	0.43
1:I:778:VAL:HG12	1:I:823:ALA:O	2.18	0.43
1:C:732:TYR:O	1:C:733:HIS:ND1	2.52	0.43
1:C:721:ARG:O	1:C:748:ASN:N	2.46	0.43
1:D:733:HIS:HB2	1:D:746:VAL:N	2.33	0.43
1:F:666:ALA:HB2	1:F:771:GLY:HA2	2.01	0.43
1:G:663:SER:CB	1:H:711:ALA:HB1	2.49	0.43
1:G:668:TYR:CE2	1:G:710:ALA:HB1	2.53	0.43
1:I:674:ARG:HE	1:I:674:ARG:HB3	1.65	0.42
1:I:813:ALA:O	1:I:815:ASP:N	2.52	0.42
1:D:732:TYR:O	1:D:746:VAL:HG13	2.19	0.42
1:D:744:GLN:HB3	1:H:674:ARG:HE	1.82	0.42
1:D:789:ARG:NH2	1:D:806:ILE:HG12	2.34	0.42
1:F:760:ARG:HD2	1:F:767:TRP:CE2	2.53	0.42
1:A:700:ILE:HG13	1:A:701:GLY:N	2.34	0.42
1:A:756:PRO:C	1:A:758:VAL:N	2.77	0.42
1:G:679:LEU:O	1:G:779:ARG:NE	2.39	0.42
1:E:708:ILE:HG13	1:F:711:ALA:CB	2.49	0.42
1:H:726:GLU:HG3	1:H:727:PHE:CD2	2.54	0.42
1:I:691:ARG:HH12	1:I:694:SER:HB3	1.85	0.42
1:C:677:ILE:CD1	1:C:690:VAL:HG23	2.49	0.42
1:H:674:ARG:NE	1:H:765:GLU:OE2	2.53	0.42
1:D:782:SER:HB3	1:D:814:TYR:HD2	1.83	0.42
1:B:722:TYR:HB3	1:B:730:LEU:HD11	2.01	0.42
1:G:670:GLU:OE1	1:G:767:TRP:NE1	2.53	0.42
1:I:698:ASP:OD1	1:I:698:ASP:N	2.52	0.42
1:A:811:LYS:HB3	1:A:811:LYS:HE3	1.84	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:737:VAL:O	1:D:739:GLY:N	2.53	0.42
1:D:775:GLN:OE1	1:D:808:MET:HE1	2.20	0.42
1:D:828:LYS:NZ	1:E:699:ILE:O	2.49	0.42
1:I:676:VAL:HG23	1:I:764:PRO:HB2	2.02	0.42
1:A:683:VAL:HG21	1:A:770:ILE:HD12	2.01	0.42
1:G:733:HIS:NE2	1:G:735:VAL:HG23	2.35	0.42
1:H:670:GLU:OE2	1:H:688:ARG:NH2	2.42	0.42
1:A:666:ALA:O	1:A:710:ALA:HA	2.19	0.41
1:C:779:ARG:HG3	1:C:820:TYR:CG	2.55	0.41
1:D:733:HIS:HD2	1:D:734:ASP:H	1.68	0.41
1:C:778:VAL:N	1:C:823:ALA:O	2.36	0.41
1:F:664:ASP:OD2	1:F:706:THR:HB	2.20	0.41
1:F:721:ARG:HB2	1:F:751:TYR:CG	2.54	0.41
1:C:789:ARG:HD3	1:C:803:ASN:HA	2.02	0.41
1:D:733:HIS:CD2	1:D:734:ASP:N	2.89	0.41
1:H:676:VAL:CG2	1:H:765:GLU:HG3	2.50	0.41
1:G:676:VAL:HG22	1:G:764:PRO:HB2	2.01	0.41
1:H:679:LEU:HD23	1:H:703:VAL:HG12	2.02	0.41
1:I:699:ILE:HD13	1:I:805:MET:HE2	2.01	0.41
1:I:734:ASP:HA	1:I:743:ARG:HA	2.03	0.41
1:A:815:ASP:HB3	1:A:818:LYS:HB2	2.01	0.41
1:D:733:HIS:ND1	1:D:746:VAL:HA	2.35	0.41
1:F:701:GLY:HA3	1:F:771:GLY:O	2.21	0.41
1:I:780:VAL:HB	1:I:784:VAL:HB	2.02	0.41
1:A:729:GLU:H	1:A:729:GLU:HG2	1.64	0.41
1:G:722:TYR:CD1	1:G:745:PRO:HG2	2.55	0.41
1:F:777:HIS:HA	1:F:823:ALA:O	2.20	0.41
1:F:812:GLN:H	1:F:822:VAL:HB	1.86	0.41
1:H:693:ALA:HB1	1:H:792:ALA:HB1	2.03	0.41
1:B:775:GLN:HG2	1:B:808:MET:HE1	2.02	0.41
1:F:742:GLU:HG2	1:F:743:ARG:N	2.35	0.41
1:A:733:HIS:ND1	1:A:744:GLN:O	2.39	0.41
1:C:789:ARG:NH1	1:C:804:GLY:H	2.13	0.41
1:H:708:ILE:HG13	1:I:711:ALA:CB	2.50	0.41
1:C:732:TYR:HB2	1:C:744:GLN:O	2.21	0.41
1:E:665:TYR:HE1	1:E:709:LEU:HD23	1.86	0.41
1:F:685:LEU:HD23	1:F:685:LEU:HA	1.91	0.41
1:F:727:PHE:C	1:F:729:GLU:H	2.29	0.41
1:H:815:ASP:HB3	1:H:818:LYS:HB2	2.04	0.41
1:A:733:HIS:HB3	1:A:746:VAL:HG22	2.03	0.40
1:D:668:TYR:CZ	1:D:769:CYS:HB2	2.55	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:714:SER:CB	1:E:719:GLY:HA2	2.40	0.40
1:I:751:TYR:CG	1:I:752:ASP:N	2.89	0.40
1:B:692:PRO:HG2	1:I:753:PRO:HB3	2.04	0.40
1:B:780:VAL:HG11	1:B:823:ALA:HB3	2.03	0.40
1:D:670:GLU:OE2	1:D:671:ASN:O	2.39	0.40
1:E:805:MET:HB3	1:E:806:ILE:H	1.59	0.40
1:G:695:ALA:HB2	1:G:794:ASP:N	2.36	0.40
1:H:685:LEU:HD22	1:H:687:GLY:O	2.21	0.40
1:A:791:ALA:N	1:A:799:VAL:O	2.42	0.40
1:B:812:GLN:HB3	1:B:822:VAL:H	1.86	0.40
1:C:726:GLU:H	1:C:726:GLU:HG3	1.60	0.40
1:E:730:LEU:HD23	1:E:730:LEU:HA	1.97	0.40
1:A:808:MET:HG2	1:A:824:LEU:O	2.22	0.40
1:B:666:ALA:O	1:B:710:ALA:HA	2.21	0.40
1:D:726:GLU:OE2	1:F:820:TYR:OH	2.39	0.40
1:F:665:TYR:HB3	1:F:773:VAL:HG12	2.03	0.40
1:F:782:SER:O	1:F:784:VAL:HG23	2.22	0.40
1:B:725:GLY:HA3	1:B:731:LEU:HD21	2.02	0.40
1:B:726:GLU:H	1:B:726:GLU:HG3	1.59	0.40
1:D:666:ALA:O	1:D:710:ALA:HA	2.22	0.40
1:D:687:GLY:C	1:D:689:LYS:H	2.30	0.40
1:D:743:ARG:HH21	1:D:743:ARG:HG2	1.86	0.40
1:E:704:SER:HB2	1:E:776:LEU:HD21	2.02	0.40
1:H:676:VAL:HG23	1:H:765:GLU:HG3	2.04	0.40

All (5) 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:754:SER:N	1:G:738:ASP:O[4_455]	1.93	0.27
1:A:814:TYR:OH	1:I:794:ASP:OD2[1_545]	2.10	0.10
1:D:750:GLU:OE2	1:G:694:SER:OG[1_445]	2.11	0.09
1:B:708:ILE:O	1:C:814:TYR:OH[4_455]	2.14	0.06
1:D:816:SER:OG	1:H:670:GLU:OE1[1_455]	2.15	0.05

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	165/173 (95%)	142 (86%)	19 (12%)	4 (2%)	4	24
1	B	160/173 (92%)	137 (86%)	19 (12%)	4 (2%)	4	23
1	C	159/173 (92%)	130 (82%)	20 (13%)	9 (6%)	1	9
1	D	160/173 (92%)	131 (82%)	21 (13%)	8 (5%)	1	11
1	E	160/173 (92%)	134 (84%)	24 (15%)	2 (1%)	9	35
1	F	159/173 (92%)	134 (84%)	17 (11%)	8 (5%)	1	11
1	G	160/173 (92%)	122 (76%)	34 (21%)	4 (2%)	4	23
1	H	159/173 (92%)	131 (82%)	22 (14%)	6 (4%)	2	16
1	I	159/173 (92%)	139 (87%)	15 (9%)	5 (3%)	3	20
All	All	1441/1557 (92%)	1200 (83%)	191 (13%)	50 (4%)	3	18

All (50) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	720	GLY
1	D	738	ASP
1	F	750	GLU
1	G	738	ASP
1	H	751	TYR
1	H	797	ILE
1	I	697	ASP
1	I	746	VAL
1	A	739	GLY
1	A	743	ARG
1	B	814	TYR
1	B	815	ASP
1	D	692	PRO
1	D	728	GLY
1	D	794	ASP
1	I	814	TYR

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Mol	Chain	Res	Type
1	B	733	HIS
1	C	695	ALA
1	C	742	GLU
1	D	726	GLU
1	E	816	SER
1	F	741	ILE
1	G	736	ASP
1	H	730	LEU
1	H	734	ASP
1	I	800	PRO
1	A	757	ASN
1	C	729	GLU
1	C	743	ARG
1	D	672	SER
1	D	673	ALA
1	E	695	ALA
1	G	805	MET
1	H	721	ARG
1	F	719	GLY
1	F	745	PRO
1	F	759	PRO
1	F	813	ALA
1	H	756	PRO
1	C	745	PRO
1	D	813	ALA
1	F	751	TYR
1	B	753	PRO
1	C	763	ARG
1	G	739	GLY
1	I	737	VAL
1	C	746	VAL
1	C	784	VAL
1	A	676	VAL
1	F	737	VAL

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	128/134 (96%)	128 (100%)	0	100	100
1	B	124/134 (92%)	124 (100%)	0	100	100
1	C	123/134 (92%)	123 (100%)	0	100	100
1	D	123/134 (92%)	123 (100%)	0	100	100
1	E	124/134 (92%)	124 (100%)	0	100	100
1	F	123/134 (92%)	123 (100%)	0	100	100
1	G	123/134 (92%)	123 (100%)	0	100	100
1	H	123/134 (92%)	123 (100%)	0	100	100
1	I	123/134 (92%)	123 (100%)	0	100	100
All	All	1114/1206 (92%)	1114 (100%)	0	100	100

There are no protein residues with a non-rotameric sidechain to report.

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (7) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	762	GLN
1	E	757	ASN
1	F	744	GLN
1	F	775	GLN
1	H	744	GLN
1	H	803	ASN
1	I	733	HIS

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry

1 ligand is modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
2	ACT	A	201	-	3,3,3	1.23	0	3,3,3	1.37	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.

No monomer is involved in short contacts.

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 [i](#)

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

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	167/173 (96%)	-0.14	0 100 100	24, 49, 88, 106	0
1	B	164/173 (94%)	-0.01	1 (0%) 85 73	27, 68, 111, 118	0
1	C	163/173 (94%)	-0.10	0 100 100	21, 43, 97, 121	0
1	D	164/173 (94%)	0.07	2 (1%) 76 58	39, 72, 113, 136	0
1	E	164/173 (94%)	-0.07	1 (0%) 85 73	25, 48, 118, 144	0
1	F	163/173 (94%)	-0.05	2 (1%) 76 58	34, 78, 109, 149	0
1	G	164/173 (94%)	0.06	0 100 100	46, 69, 115, 130	0
1	H	163/173 (94%)	0.09	1 (0%) 85 73	44, 63, 113, 128	0
1	I	163/173 (94%)	0.05	3 (1%) 67 49	36, 61, 104, 120	0
All	All	1475/1557 (94%)	-0.01	10 (0%) 84 70	21, 63, 111, 149	0

All (10) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	662	GLY	2.7
1	H	825	CYS	2.4
1	I	798	GLY	2.2
1	D	799	VAL	2.2
1	E	796	GLY	2.2
1	D	696	GLY	2.1
1	F	816	SER	2.1
1	I	791	ALA	2.1
1	I	790	VAL	2.1
1	F	734	ASP	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(\AA^2)	Q<0.9
2	ACT	A	201	4/4	0.98	0.08	26,26,26,26	0

6.5 Other polymers [i](#)

There are no such residues in this entry.