



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 17, 2026 – 11:23 PM UTC

PDB ID : 6DK7 / pdb_00006dk7
Title : RetS histidine kinase region with cobalt
Authors : Mancl, J.M.; Schubot, F.D.
Deposited on : 2018-05-29
Resolution : 2.60 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
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

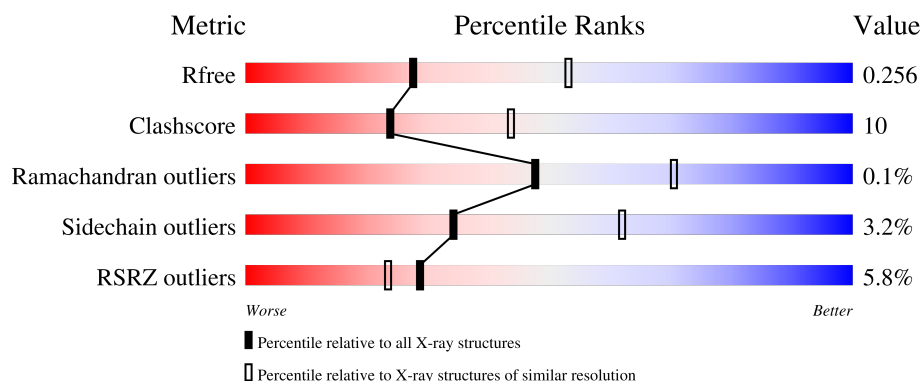
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.60 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	4008 (2.60-2.60)
Clashscore	190562	4347 (2.60-2.60)
Ramachandran outliers	187476	4277 (2.60-2.60)
Sidechain outliers	187428	4277 (2.60-2.60)
RSRZ outliers	180081	4008 (2.60-2.60)

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	227	7% 68% 30% .
1	B	227	5% 79% 18% ..
1	C	227	8% 78% 19% ..
1	D	227	6% 78% 19% ..
1	E	227	6% 79% 19% ..

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Mol	Chain	Length	Quality of chain
1	F	227	 5% 77% 20% ..
1	G	227	 3% 80% 17% ..
1	H	227	 7% 79% 19% ..

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 14138 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 RetS (Regulator of Exopolysaccharide and Type III Secretion).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	223	Total	C	N	O	S	0	0	0
			1724	1087	296	337	4			
1	C	225	Total	C	N	O	S	0	0	0
			1735	1093	298	340	4			
1	D	225	Total	C	N	O	S	0	0	0
			1735	1093	298	340	4			
1	B	224	Total	C	N	O	S	0	0	0
			1731	1091	297	339	4			
1	E	225	Total	C	N	O	S	0	0	0
			1736	1093	298	341	4			
1	F	223	Total	C	N	O	S	0	0	0
			1726	1087	297	338	4			
1	G	225	Total	C	N	O	S	0	0	0
			1739	1095	299	341	4			
1	H	225	Total	C	N	O	S	0	0	0
			1738	1095	299	340	4			

- Molecule 2 is COBALT (II) ION (CCD ID: CO) (formula: Co).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	2	Total	Co	0	0
			2	2		
2	C	4	Total	Co	0	0
			4	4		
2	D	3	Total	Co	0	0
			3	3		
2	B	4	Total	Co	0	0
			4	4		
2	E	4	Total	Co	0	0
			4	4		
2	F	2	Total	Co	0	0
			2	2		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	G	2	Total 2	O 2	0	0
2	H	3	Total 3	O 3	0	0

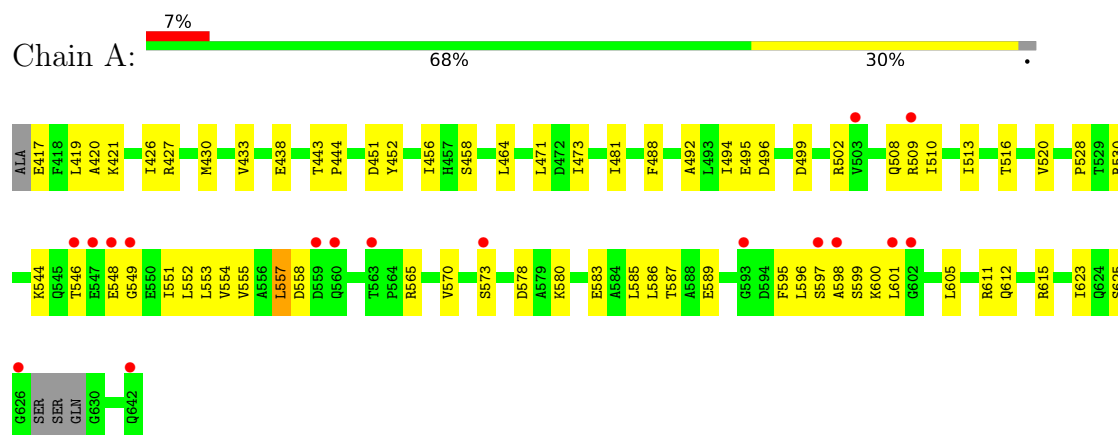
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	29	Total 29	O 29	0	0
3	C	23	Total 23	O 23	0	0
3	D	41	Total 41	O 41	0	0
3	B	33	Total 33	O 33	0	0
3	E	32	Total 32	O 32	0	0
3	F	38	Total 38	O 38	0	0
3	G	22	Total 22	O 22	0	0
3	H	32	Total 32	O 32	0	0

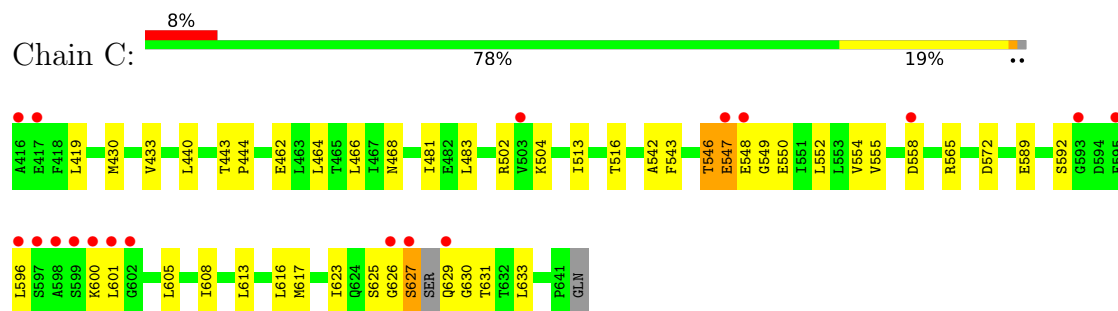
3 Residue-property plots [i](#)

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

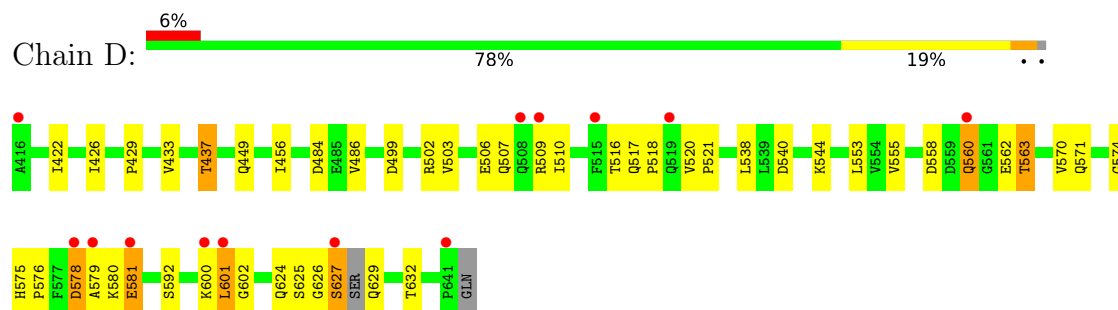
- Molecule 1: RetS (Regulator of Exopolysaccharide and Type III Secretion)



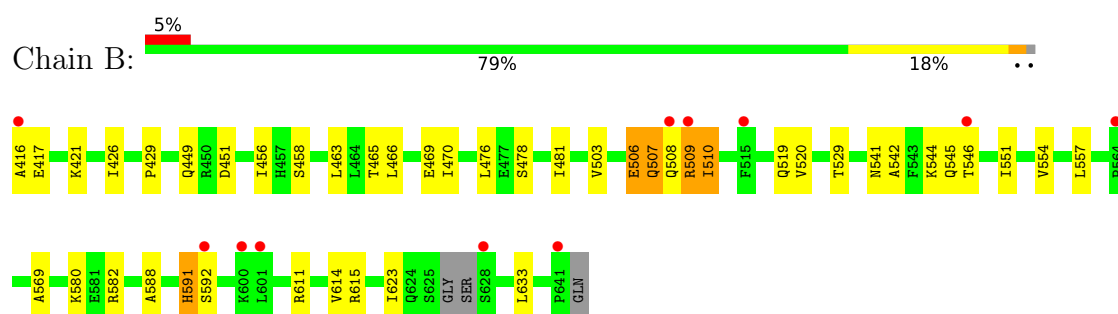
- Molecule 1: RetS (Regulator of Exopolysaccharide and Type III Secretion)



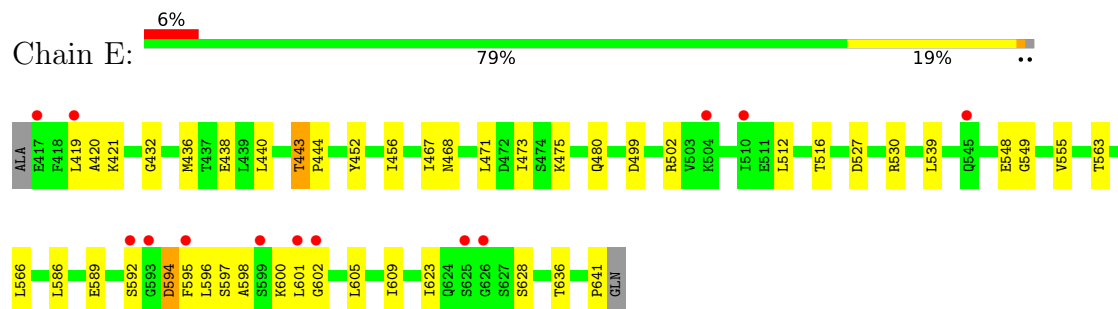
- Molecule 1: RetS (Regulator of Exopolysaccharide and Type III Secretion)



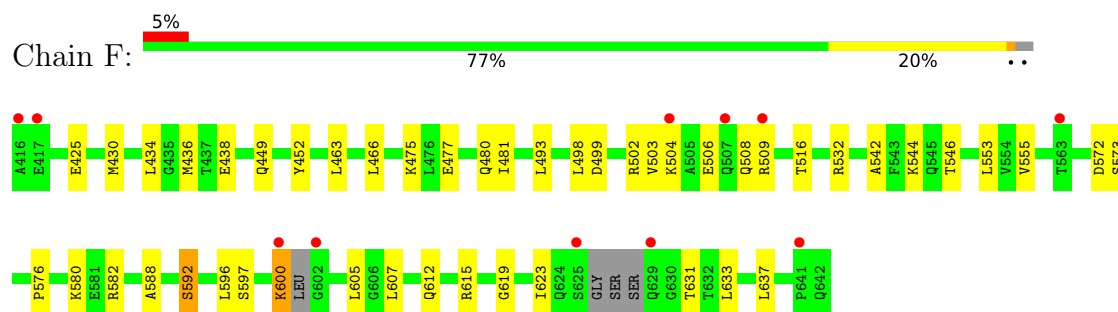
- Molecule 1: RetS (Regulator of Exopolysaccharide and Type III Secretion)



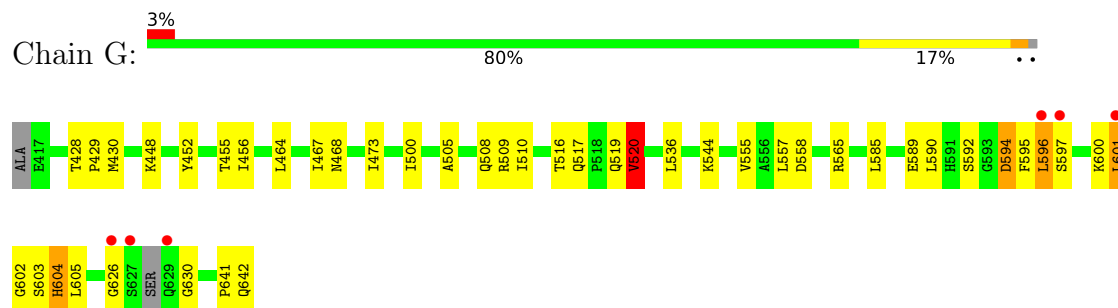
- Molecule 1: RetS (Regulator of Exopolysaccharide and Type III Secretion)



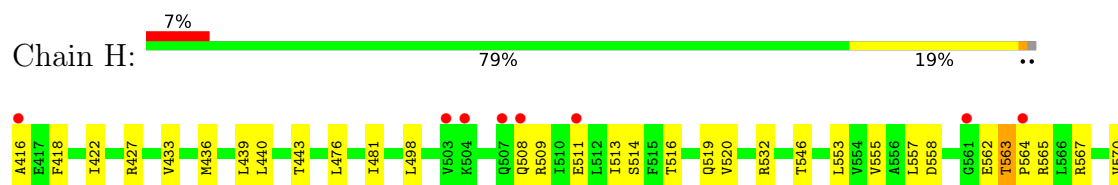
- Molecule 1: RetS (Regulator of Exopolysaccharide and Type III Secretion)

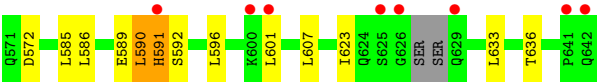


- Molecule 1: RetS (Regulator of Exopolysaccharide and Type III Secretion)



- Molecule 1: RetS (Regulator of Exopolysaccharide and Type III Secretion)





4 Data and refinement statistics

Property	Value	Source
Space group	P 41 21 2	Depositor
Cell constants a, b, c, α , β , γ	158.71Å 158.71Å 243.83Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	56.78 – 2.60 56.78 – 2.60	Depositor EDS
% Data completeness (in resolution range)	96.3 (56.78-2.60) 96.3 (56.78-2.60)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.42 (at 2.61Å)	Xtriage
Refinement program	PHENIX 1.10.1_2155	Depositor
R, R_{free}	0.211 , 0.261 0.211 , 0.256	Depositor DCC
R_{free} test set	4021 reflections (2.73%)	wwPDB-VP
Wilson B-factor (Å ²)	51.2	Xtriage
Anisotropy	0.226	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 47.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	14138	wwPDB-VP
Average B, all atoms (Å ²)	61.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 17.57% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section:
CO

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	0.58	0/1745	0.62	0/2360
1	B	0.37	0/1752	0.53	2/2370 (0.1%)
1	C	0.36	0/1756	0.52	2/2375 (0.1%)
1	D	0.60	3/1756 (0.2%)	0.68	5/2375 (0.2%)
1	E	0.26	0/1758	0.49	1/2379 (0.0%)
1	F	0.44	0/1746	0.57	2/2360 (0.1%)
1	G	0.58	2/1760 (0.1%)	0.68	7/2380 (0.3%)
1	H	0.46	1/1759 (0.1%)	0.63	4/2379 (0.2%)
All	All	0.47	6/14032 (0.0%)	0.59	23/18978 (0.1%)

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	H	591	HIS	CA-CB	6.89	1.62	1.53
1	D	563	THR	C-N	5.36	1.40	1.33
1	D	517	GLN	C-N	5.30	1.40	1.34
1	D	518	PRO	N-CD	5.17	1.54	1.47
1	G	520	VAL	C-N	5.09	1.40	1.33
1	G	517	GLN	C-N	5.05	1.40	1.34

All (23) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	H	563	THR	CA-C-N	-8.25	111.28	119.78
1	H	563	THR	C-N-CA	-8.25	111.28	119.78
1	C	549	GLY	N-CA-C	6.67	122.28	110.95
1	H	591	HIS	CA-CB-CG	6.65	120.45	113.80
1	D	560	GLN	N-CA-C	-6.39	101.66	110.35
1	D	563	THR	CA-C-N	-6.14	113.65	119.85
1	D	563	THR	C-N-CA	-6.14	113.65	119.85

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	592	SER	N-CA-C	-5.99	98.96	108.73
1	G	520	VAL	CA-C-N	-5.79	114.00	119.85
1	G	520	VAL	C-N-CA	-5.79	114.00	119.85
1	G	602	GLY	N-CA-C	-5.70	105.89	112.73
1	F	508	GLN	N-CA-C	5.67	117.37	109.31
1	C	550	GLU	N-CA-C	5.59	118.07	109.07
1	B	510	ILE	N-CA-C	5.56	115.89	108.11
1	G	592	SER	N-CA-C	-5.48	102.77	110.50
1	G	517	GLN	CA-C-N	-5.45	114.05	119.56
1	G	517	GLN	C-N-CA	-5.45	114.05	119.56
1	D	517	GLN	CA-C-N	-5.14	113.74	119.19
1	D	517	GLN	C-N-CA	-5.14	113.74	119.19
1	H	590	LEU	N-CA-C	5.12	117.32	109.07
1	G	604	HIS	N-CA-C	5.09	116.97	110.61
1	F	509	ARG	N-CA-C	-5.08	105.74	111.28
1	B	591	HIS	CA-CB-CG	5.05	118.85	113.80

There are no chirality outliers.

There are no planarity outliers.

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	1724	0	1758	48	0
1	B	1731	0	1765	28	0
1	C	1735	0	1768	32	0
1	D	1735	0	1768	35	0
1	E	1736	0	1769	45	0
1	F	1726	0	1756	43	0
1	G	1739	0	1771	52	0
1	H	1738	0	1771	37	0
2	A	2	0	0	0	0
2	B	4	0	0	0	0
2	C	4	0	0	0	0
2	D	3	0	0	0	0
2	E	4	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	F	2	0	0	0	0
2	G	2	0	0	0	0
2	H	3	0	0	0	0
3	A	29	0	0	6	0
3	B	33	0	0	5	0
3	C	23	0	0	2	0
3	D	41	0	0	3	0
3	E	32	0	0	2	0
3	F	38	0	0	2	0
3	G	22	0	0	1	0
3	H	32	0	0	5	0
All	All	14138	0	14126	284	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 10.

All (284) 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:627:SER:HB2	1:D:629:GLN:N	1.15	1.45
1:G:448:LYS:HE3	1:G:452:TYR:CZ	1.62	1.32
1:C:627:SER:HA	1:C:629:GLN:N	1.46	1.29
1:H:591:HIS:NE2	3:H:801:HOH:O	1.69	1.23
1:C:627:SER:CA	1:C:629:GLN:N	2.05	1.20
1:D:627:SER:CB	1:D:629:GLN:N	2.06	1.17
1:H:558:ASP:OD2	1:H:565:ARG:NH2	1.79	1.13
1:C:627:SER:C	1:C:629:GLN:N	2.06	1.13
1:D:581:GLU:OE1	1:D:601:LEU:O	1.66	1.11
1:G:448:LYS:CE	1:G:452:TYR:CZ	2.36	1.09
1:G:448:LYS:HE3	1:G:452:TYR:CE2	1.90	1.06
1:F:502:ARG:NH1	1:F:506:GLU:OE2	1.90	1.05
1:G:603:SER:HB2	1:G:604:HIS:CE1	1.96	1.00
1:H:519:GLN:OE1	3:H:802:HOH:O	1.80	0.99
1:A:419:LEU:HD13	1:A:481:ILE:HD13	1.51	0.92
1:C:543:PHE:O	3:C:801:HOH:O	1.87	0.91
1:G:603:SER:OG	1:G:604:HIS:CD2	2.26	0.89
1:E:421:LYS:NZ	1:F:600:LYS:NZ	2.21	0.89
1:H:427:ARG:NH1	3:H:803:HOH:O	2.07	0.88
1:C:542:ALA:O	1:C:546:THR:HG23	1.76	0.85
1:E:601:LEU:HD23	1:E:602:GLY:H	1.42	0.85
1:G:448:LYS:HE3	1:G:452:TYR:OH	1.75	0.85

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:484:ASP:O	3:D:801:HOH:O	1.95	0.84
1:D:581:GLU:OE1	1:D:601:LEU:C	2.22	0.82
1:A:444:PRO:HD3	1:F:544:LYS:HE3	1.62	0.82
1:C:625:SER:HB2	1:C:631:THR:HG23	1.61	0.81
1:B:591:HIS:CD2	3:B:805:HOH:O	2.33	0.81
1:E:499:ASP:HA	1:E:502:ARG:HG2	1.62	0.81
1:D:499:ASP:HA	1:D:502:ARG:HG3	1.63	0.81
1:B:507:GLN:OE1	1:B:509:ARG:NE	2.13	0.81
1:E:421:LYS:NZ	1:F:600:LYS:HZ2	1.77	0.81
1:E:421:LYS:HZ1	1:F:600:LYS:NZ	1.78	0.81
1:E:438:GLU:OE2	3:E:801:HOH:O	2.00	0.79
1:H:416:ALA:N	1:H:591:HIS:HE1	1.80	0.78
1:H:520:VAL:HG12	1:H:557:LEU:HG	1.64	0.78
1:E:452:TYR:HA	1:F:436:MET:HE3	1.64	0.78
1:C:513:ILE:HG13	1:C:552:LEU:HD23	1.66	0.77
1:C:626:GLY:O	1:C:629:GLN:HB3	1.84	0.76
1:G:448:LYS:NZ	1:G:452:TYR:CE1	2.54	0.76
1:G:448:LYS:NZ	1:G:452:TYR:CZ	2.54	0.75
1:G:590:LEU:HA	1:G:595:PHE:CD1	2.20	0.75
1:D:558:ASP:OD1	1:D:560:GLN:HB2	1.85	0.75
1:C:462:GLU:OE1	3:C:802:HOH:O	2.03	0.74
1:B:582:ARG:NH2	3:B:803:HOH:O	2.21	0.74
1:D:516:THR:HG23	1:D:555:VAL:HB	1.68	0.74
1:G:603:SER:HB2	1:G:604:HIS:NE2	2.03	0.73
1:B:520:VAL:HG12	1:B:557:LEU:HG	1.70	0.72
1:G:448:LYS:CE	1:G:452:TYR:OH	2.32	0.71
1:C:596:LEU:HD22	1:C:600:LYS:HB2	1.71	0.71
1:C:443:THR:HG21	1:D:449:GLN:HG2	1.73	0.71
1:A:612:GLN:OE1	3:A:802:HOH:O	2.09	0.70
1:A:438:GLU:OE2	3:A:801:HOH:O	2.08	0.70
1:A:598:ALA:HA	1:A:601:LEU:HD22	1.73	0.70
1:E:527:ASP:OD2	1:E:530:ARG:NH1	2.23	0.70
1:H:562:GLU:HG2	1:H:563:THR:HG23	1.73	0.69
1:H:567:ARG:NH2	3:H:806:HOH:O	2.25	0.69
1:E:480:GLN:NE2	3:E:802:HOH:O	2.25	0.67
1:E:471:LEU:HG	1:E:475:LYS:HZ2	1.60	0.67
1:G:596:LEU:HD12	1:G:601:LEU:HB2	1.75	0.66
1:H:567:ARG:HG3	1:H:636:THR:HG22	1.76	0.66
1:B:588:ALA:O	1:B:615:ARG:NH2	2.29	0.66
1:B:451:ASP:OD1	3:B:801:HOH:O	2.13	0.65
1:E:421:LYS:HZ3	1:F:600:LYS:NZ	1.92	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:507:GLN:HG3	1:D:509:ARG:HG2	1.78	0.65
1:H:509:ARG:O	3:H:804:HOH:O	2.14	0.65
1:A:549:GLY:HA3	1:A:573:SER:OG	1.97	0.65
1:F:588:ALA:O	1:F:615:ARG:NH2	2.30	0.65
1:G:452:TYR:CE2	1:H:439:LEU:HB3	2.32	0.64
1:F:546:THR:HG22	1:F:573:SER:H	1.62	0.63
1:C:516:THR:HG23	1:C:555:VAL:HB	1.80	0.63
1:E:421:LYS:NZ	1:F:600:LYS:HZ3	1.97	0.62
1:G:596:LEU:HD13	1:H:418:PHE:HE1	1.63	0.62
1:E:421:LYS:HZ1	1:F:600:LYS:HZ2	1.39	0.62
1:H:511:GLU:HG3	1:H:513:ILE:HD11	1.81	0.61
1:A:419:LEU:HD13	1:A:481:ILE:CD1	2.28	0.60
1:E:563:THR:HG21	1:E:641:PRO:HG3	1.81	0.60
1:H:476:LEU:HD23	1:H:481:ILE:HG13	1.82	0.60
1:H:498:LEU:HD21	1:H:553:LEU:HD23	1.82	0.60
1:G:473:ILE:HD12	1:G:605:LEU:HD22	1.83	0.60
1:C:589:GLU:HB2	1:C:592:SER:HB3	1.84	0.60
1:E:420:ALA:HB1	1:E:475:LYS:HZ3	1.66	0.60
1:E:443:THR:HG21	1:F:449:GLN:HG2	1.83	0.59
1:D:538:LEU:O	3:D:803:HOH:O	2.16	0.59
1:D:507:GLN:OE1	1:D:509:ARG:NE	2.34	0.58
1:G:596:LEU:HD23	1:G:596:LEU:C	2.29	0.58
1:G:596:LEU:CD1	1:H:418:PHE:HE1	2.16	0.58
1:H:416:ALA:N	1:H:591:HIS:CE1	2.68	0.58
1:D:626:GLY:O	1:D:629:GLN:N	2.35	0.57
1:A:451:ASP:OD2	3:A:803:HOH:O	2.16	0.57
1:H:601:LEU:HD12	1:H:601:LEU:H	1.69	0.57
1:A:430:MET:HG2	1:A:464:LEU:HD13	1.86	0.57
1:A:473:ILE:HD12	1:A:605:LEU:HD22	1.87	0.57
1:D:629:GLN:HG3	1:D:629:GLN:O	2.05	0.57
1:E:432:GLY:O	1:E:436:MET:HG2	2.05	0.57
1:E:601:LEU:HD21	1:F:425:GLU:HG2	1.86	0.56
1:A:585:LEU:O	1:A:611:ARG:NH1	2.32	0.56
1:B:465:THR:O	1:B:469:GLU:HG3	2.07	0.55
1:F:504:LYS:HD3	1:F:504:LYS:N	2.22	0.55
1:H:519:GLN:HB3	1:H:557:LEU:HD12	1.88	0.55
1:G:473:ILE:CD1	1:G:605:LEU:HD22	2.37	0.55
1:H:589:GLU:C	1:H:590:LEU:HD23	2.32	0.55
1:E:471:LEU:HG	1:E:475:LYS:NZ	2.21	0.55
1:G:600:LYS:O	1:G:603:SER:OG	2.16	0.55
1:D:601:LEU:O	1:D:601:LEU:HD23	2.06	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:542:ALA:O	1:B:546:THR:HG23	2.07	0.55
1:A:496:ASP:HA	1:A:499:ASP:HB2	1.88	0.54
1:C:466:LEU:HD11	1:C:601:LEU:HD21	1.89	0.54
1:F:546:THR:CG2	1:F:572:ASP:HB2	2.37	0.54
1:G:430:MET:HG2	1:G:464:LEU:HG	1.89	0.54
1:G:603:SER:CB	1:G:604:HIS:CD2	2.90	0.54
1:A:443:THR:HG21	1:B:449:GLN:CG	2.38	0.54
1:A:546:THR:HG21	1:A:551:ILE:HD11	1.89	0.54
1:D:433:VAL:O	1:D:437:THR:HG23	2.08	0.53
1:A:596:LEU:HD23	1:A:597:SER:O	2.09	0.53
1:D:581:GLU:HA	1:D:581:GLU:OE2	2.08	0.53
1:G:467:ILE:HG23	1:H:596:LEU:HD13	1.90	0.52
1:H:623:ILE:HG12	1:H:633:LEU:HD23	1.91	0.52
1:A:499:ASP:OD1	1:A:502:ARG:CZ	2.57	0.52
1:D:574:GLY:O	1:D:576:PRO:HD3	2.09	0.52
1:F:438:GLU:OE2	3:F:802:HOH:O	2.19	0.52
1:F:502:ARG:HG3	1:F:503:VAL:N	2.24	0.52
1:C:440:LEU:O	1:C:443:THR:HB	2.09	0.52
1:C:552:LEU:CD1	1:C:554:VAL:HG23	2.40	0.52
1:C:558:ASP:OD2	1:C:565:ARG:NH2	2.37	0.52
1:G:603:SER:OG	1:G:604:HIS:CG	2.63	0.51
1:D:509:ARG:NH2	3:D:802:HOH:O	2.04	0.51
1:B:591:HIS:HD2	3:B:805:HOH:O	1.83	0.51
1:A:513:ILE:HG13	1:A:552:LEU:CD2	2.41	0.51
1:E:598:ALA:HB1	1:F:425:GLU:CD	2.36	0.51
1:F:516:THR:HG23	1:F:555:VAL:HB	1.91	0.51
1:E:467:ILE:HG23	1:F:596:LEU:HD13	1.92	0.51
1:G:456:ILE:HG23	1:H:433:VAL:HG13	1.92	0.51
1:D:486:VAL:HG12	1:H:532:ARG:HH12	1.75	0.51
1:E:419:LEU:HD22	1:E:530:ARG:HE	1.75	0.51
1:E:440:LEU:O	1:E:443:THR:HB	2.11	0.51
1:E:471:LEU:HD11	1:F:597:SER:HB2	1.92	0.51
1:G:508:GLN:O	1:G:509:ARG:HB2	2.11	0.51
1:G:505:ALA:O	1:G:510:ILE:N	2.44	0.50
1:E:473:ILE:HG12	1:E:609:ILE:HG12	1.93	0.50
1:B:416:ALA:HB1	1:B:478:SER:HB3	1.92	0.50
1:C:552:LEU:HD11	1:C:554:VAL:HG23	1.93	0.50
1:A:419:LEU:CD2	1:A:530:ARG:HE	2.25	0.50
1:G:626:GLY:N	1:G:630:GLY:O	2.40	0.50
1:C:433:VAL:HG13	1:D:456:ILE:HG23	1.93	0.50
1:G:603:SER:CB	1:G:604:HIS:NE2	2.73	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:613:LEU:O	1:C:617:MET:HG3	2.11	0.49
1:B:611:ARG:O	1:B:614:VAL:HG22	2.12	0.49
1:D:601:LEU:C	1:D:601:LEU:CD2	2.85	0.49
1:F:480:GLN:HG2	1:F:481:ILE:HG23	1.94	0.49
1:B:541:ASN:O	1:B:545:GLN:HG2	2.13	0.49
1:A:488:PHE:CD1	1:A:528:PRO:HG3	2.48	0.49
1:F:466:LEU:HD21	1:F:605:LEU:HD12	1.94	0.49
1:B:503:VAL:O	1:B:506:GLU:HB2	2.12	0.49
1:E:421:LYS:HZ1	1:F:600:LYS:HZ3	1.54	0.49
1:F:493:LEU:HD11	1:F:532:ARG:HB2	1.94	0.49
1:A:583:GLU:O	1:A:587:THR:OG1	2.25	0.49
1:C:443:THR:CG2	1:D:449:GLN:HE21	2.26	0.49
1:G:520:VAL:HG12	1:G:557:LEU:HG	1.95	0.49
1:F:623:ILE:HG12	1:F:633:LEU:HD23	1.95	0.48
1:C:623:ILE:HG12	1:C:633:LEU:HD23	1.95	0.48
1:B:466:LEU:O	1:B:470:ILE:HG13	2.13	0.48
1:E:597:SER:OG	1:E:600:LYS:HG2	2.13	0.48
1:A:499:ASP:OD1	1:A:502:ARG:NH2	2.47	0.48
1:A:596:LEU:HD21	1:A:600:LYS:HB2	1.96	0.48
1:H:553:LEU:HD13	1:H:570:VAL:HG22	1.96	0.48
1:A:599:SER:OG	1:A:600:LYS:HE2	2.14	0.48
1:A:520:VAL:HG22	1:A:557:LEU:HD13	1.95	0.48
1:E:596:LEU:HD21	1:E:601:LEU:N	2.28	0.48
1:F:582:ARG:HG3	1:F:623:ILE:HB	1.96	0.48
1:E:566:LEU:O	1:E:636:THR:HA	2.15	0.47
1:G:589:GLU:O	1:G:595:PHE:HD1	1.97	0.47
1:E:594:ASP:O	1:E:595:PHE:C	2.57	0.47
1:G:595:PHE:HD2	1:G:596:LEU:HD13	1.79	0.47
1:B:519:GLN:HG3	1:B:557:LEU:HD12	1.95	0.47
1:B:623:ILE:HG12	1:B:633:LEU:HD23	1.95	0.47
1:E:443:THR:CG2	1:F:449:GLN:HE21	2.27	0.47
1:H:440:LEU:O	1:H:443:THR:OG1	2.31	0.47
1:A:494:ILE:HG13	1:A:555:VAL:HG21	1.96	0.47
1:C:430:MET:HG2	1:C:464:LEU:HG	1.96	0.47
1:A:558:ASP:OD1	1:A:565:ARG:NH2	2.37	0.47
1:C:601:LEU:HD13	1:D:422:ILE:HG21	1.97	0.47
1:E:548:GLU:OE2	1:E:549:GLY:N	2.47	0.47
1:H:516:THR:HG23	1:H:555:VAL:HB	1.97	0.47
1:H:586:LEU:HG	1:H:623:ILE:HD12	1.96	0.47
1:A:513:ILE:HG13	1:A:552:LEU:HD22	1.96	0.47
1:A:426:ILE:HG23	1:B:463:LEU:HD11	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:589:GLU:C	1:G:595:PHE:HD1	2.23	0.46
1:B:417:GLU:O	1:B:421:LYS:HG3	2.14	0.46
1:E:420:ALA:CB	1:E:475:LYS:HZ3	2.28	0.46
1:F:592:SER:OG	3:F:803:HOH:O	2.20	0.46
1:B:478:SER:OG	3:B:802:HOH:O	2.21	0.46
1:G:452:TYR:CZ	1:H:439:LEU:HD13	2.51	0.46
1:A:443:THR:HG21	1:B:449:GLN:HG3	1.97	0.46
1:A:544:LYS:NZ	3:A:810:HOH:O	2.49	0.46
1:F:499:ASP:O	1:F:502:ARG:HG2	2.16	0.46
1:F:542:ALA:O	1:F:546:THR:HG23	2.15	0.46
1:F:546:THR:CG2	1:F:573:SER:H	2.29	0.46
1:H:562:GLU:HG2	1:H:563:THR:CG2	2.44	0.46
1:C:483:LEU:HD11	1:C:616:LEU:HG	1.98	0.46
1:A:516:THR:HG23	1:A:555:VAL:HB	1.97	0.46
1:E:436:MET:HE2	1:F:452:TYR:HA	1.99	0.45
1:G:594:ASP:OD1	1:G:594:ASP:N	2.48	0.45
1:D:575:HIS:HA	1:D:576:PRO:HD2	1.83	0.45
1:H:563:THR:O	1:H:564:PRO:C	2.57	0.45
1:E:563:THR:CG2	1:E:641:PRO:HG3	2.46	0.45
1:A:586:LEU:HD21	1:A:623:ILE:HG22	1.99	0.45
1:D:553:LEU:HD13	1:D:570:VAL:HG22	1.99	0.45
1:B:544:LYS:HG2	1:E:444:PRO:HB3	1.98	0.45
1:G:601:LEU:HD13	1:H:422:ILE:HG21	1.99	0.45
1:H:585:LEU:HD22	1:H:607:LEU:HD21	1.99	0.45
1:F:498:LEU:HD21	1:F:553:LEU:HD23	1.98	0.45
1:G:452:TYR:OH	1:H:439:LEU:HD22	2.16	0.45
1:A:508:GLN:O	1:A:510:ILE:HG12	2.17	0.44
1:E:473:ILE:HD12	1:E:605:LEU:HD22	1.99	0.44
1:F:475:LYS:HD3	1:F:480:GLN:NE2	2.32	0.44
1:A:420:ALA:HB3	1:A:471:LEU:HD23	1.98	0.44
1:C:601:LEU:O	1:C:605:LEU:HG	2.18	0.44
1:A:420:ALA:CB	1:A:471:LEU:HD23	2.47	0.44
1:E:586:LEU:HD21	1:E:623:ILE:HG13	1.99	0.44
1:E:601:LEU:HD23	1:E:602:GLY:N	2.21	0.44
1:B:426:ILE:O	1:B:429:PRO:HD2	2.18	0.44
1:B:554:VAL:HG22	1:B:569:ALA:HB3	2.00	0.43
1:D:520:VAL:HA	1:D:521:PRO:HD3	1.87	0.43
1:F:580:LYS:H	1:F:580:LYS:HD2	1.83	0.43
1:D:540:ASP:O	1:D:544:LYS:HG3	2.19	0.43
1:D:571:GLN:HG3	1:D:632:THR:OG1	2.19	0.43
1:E:452:TYR:O	1:E:456:ILE:HG13	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:605:LEU:HA	1:G:605:LEU:HD23	1.76	0.43
1:G:516:THR:HG23	1:G:555:VAL:HB	2.01	0.43
1:A:452:TYR:O	1:A:456:ILE:HG13	2.19	0.43
1:C:629:GLN:HG2	1:C:630:GLY:N	2.32	0.43
1:G:428:THR:HB	1:G:429:PRO:HD3	2.01	0.43
1:A:589:GLU:C	1:A:595:PHE:HD1	2.27	0.43
1:G:641:PRO:O	1:G:642:GLN:HG2	2.19	0.42
1:C:419:LEU:HD13	1:C:481:ILE:CD1	2.48	0.42
1:D:624:GLN:OE1	1:D:624:GLN:HA	2.17	0.42
1:G:455:THR:HG21	1:H:436:MET:HE2	2.02	0.42
1:G:595:PHE:CD2	1:G:596:LEU:HB3	2.54	0.42
1:A:578:ASP:OD1	1:A:580:LYS:N	2.50	0.42
1:H:546:THR:CG2	1:H:572:ASP:HB2	2.48	0.42
1:A:509:ARG:O	1:A:548:GLU:OE2	2.37	0.42
1:C:546:THR:HG22	1:C:572:ASP:HB2	2.01	0.42
1:B:580:LYS:HA	1:B:580:LYS:HD3	1.82	0.42
1:E:421:LYS:HZ3	1:F:600:LYS:HZ2	1.56	0.42
1:G:603:SER:C	1:G:604:HIS:CG	2.97	0.42
1:A:615:ARG:NE	3:A:811:HOH:O	2.49	0.42
1:B:510:ILE:HG21	1:B:551:ILE:HD12	2.01	0.42
1:E:516:THR:HG23	1:E:555:VAL:HB	2.00	0.42
1:A:433:VAL:HG13	1:B:456:ILE:HG23	2.02	0.42
1:D:578:ASP:O	1:D:579:ALA:C	2.61	0.42
1:E:589:GLU:C	1:E:595:PHE:HD1	2.28	0.42
1:G:508:GLN:HE21	1:G:508:GLN:HB3	1.73	0.42
1:G:603:SER:C	1:G:604:HIS:ND1	2.77	0.42
1:H:585:LEU:CD2	1:H:607:LEU:HD21	2.50	0.42
1:A:552:LEU:HD12	1:A:554:VAL:HG23	2.02	0.42
1:F:576:PRO:HA	1:F:631:THR:OG1	2.20	0.42
1:D:426:ILE:O	1:D:429:PRO:HD2	2.20	0.42
1:G:558:ASP:OD1	1:G:565:ARG:NH2	2.49	0.42
1:A:578:ASP:OD1	1:A:580:LYS:HG2	2.19	0.42
1:G:596:LEU:N	1:G:596:LEU:CD2	2.83	0.41
1:F:607:LEU:HD12	1:F:607:LEU:HA	1.94	0.41
1:G:585:LEU:HD21	1:G:600:LYS:NZ	2.34	0.41
1:F:619:GLY:HA3	1:F:637:LEU:HD23	2.02	0.41
1:A:492:ALA:O	1:A:495:GLU:HG3	2.19	0.41
1:A:553:LEU:HD13	1:A:570:VAL:HG22	2.03	0.41
1:C:626:GLY:O	1:C:629:GLN:N	2.54	0.41
1:G:544:LYS:NZ	3:G:802:HOH:O	2.52	0.41
1:C:547:GLU:H	1:C:547:GLU:HG2	1.53	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:539:LEU:HD23	1:E:539:LEU:HA	1.89	0.41
1:A:516:THR:OG1	3:A:805:HOH:O	2.22	0.41
1:C:443:THR:HG23	1:C:444:PRO:HD2	2.02	0.41
1:D:509:ARG:HG3	1:D:510:ILE:HG12	2.03	0.41
1:G:585:LEU:HD21	1:G:600:LYS:HZ3	1.85	0.41
1:G:589:GLU:C	1:G:595:PHE:CD1	2.99	0.41
1:A:419:LEU:CD1	1:A:481:ILE:HD13	2.34	0.40
1:D:540:ASP:CG	1:D:544:LYS:HE3	2.47	0.40
1:E:596:LEU:HD21	1:E:601:LEU:HB3	2.01	0.40
1:F:430:MET:HE1	1:F:463:LEU:HD23	2.04	0.40
1:F:434:LEU:HA	1:F:434:LEU:HD23	1.87	0.40
1:A:419:LEU:HD22	1:A:530:ARG:HE	1.85	0.40
1:D:503:VAL:O	1:D:506:GLU:HB2	2.21	0.40
1:G:500:ILE:HD12	1:G:536:LEU:HD21	2.04	0.40
1:B:476:LEU:HD23	1:B:481:ILE:HG13	2.01	0.40
1:F:477:GLU:OE2	1:F:612:GLN:NE2	2.52	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	219/227 (96%)	213 (97%)	6 (3%)	0	100	100
1	B	220/227 (97%)	215 (98%)	5 (2%)	0	100	100
1	C	221/227 (97%)	221 (100%)	0	0	100	100
1	D	221/227 (97%)	218 (99%)	2 (1%)	1 (0%)	24	46
1	E	223/227 (98%)	219 (98%)	4 (2%)	0	100	100
1	F	217/227 (96%)	214 (99%)	3 (1%)	0	100	100
1	G	221/227 (97%)	219 (99%)	2 (1%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	H	221/227 (97%)	219 (99%)	2 (1%)	0	100	100
All	All	1763/1816 (97%)	1738 (99%)	24 (1%)	1 (0%)	48	70

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	602	GLY

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	192/195 (98%)	186 (97%)	6 (3%)	35	63
1	B	193/195 (99%)	186 (96%)	7 (4%)	31	58
1	C	193/195 (99%)	185 (96%)	8 (4%)	27	54
1	D	193/195 (99%)	182 (94%)	11 (6%)	18	40
1	E	194/195 (100%)	189 (97%)	5 (3%)	40	68
1	F	192/195 (98%)	190 (99%)	2 (1%)	68	86
1	G	194/195 (100%)	187 (96%)	7 (4%)	31	58
1	H	193/195 (99%)	190 (98%)	3 (2%)	55	79
All	All	1544/1560 (99%)	1495 (97%)	49 (3%)	34	62

All (49) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	417	GLU
1	A	421	LYS
1	A	427	ARG
1	A	458	SER
1	A	557	LEU
1	A	625	SER
1	C	468	ASN

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Mol	Chain	Res	Type
1	C	502	ARG
1	C	504	LYS
1	C	546	THR
1	C	547	GLU
1	C	548	GLU
1	C	608	ILE
1	C	627	SER
1	D	437	THR
1	D	562	GLU
1	D	563	THR
1	D	578	ASP
1	D	580	LYS
1	D	581	GLU
1	D	592	SER
1	D	600	LYS
1	D	601	LEU
1	D	625	SER
1	D	627	SER
1	B	458	SER
1	B	506	GLU
1	B	507	GLN
1	B	508	GLN
1	B	509	ARG
1	B	529	THR
1	B	592	SER
1	E	443	THR
1	E	468	ASN
1	E	512	LEU
1	E	594	ASP
1	E	628	SER
1	F	592	SER
1	F	600	LYS
1	G	468	ASN
1	G	519	GLN
1	G	520	VAL
1	G	594	ASP
1	G	596	LEU
1	G	597	SER
1	G	601	LEU
1	H	508	GLN
1	H	514	SER
1	H	592	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (18) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	457	HIS
1	A	541	ASN
1	A	560	GLN
1	A	591	HIS
1	B	454	GLN
1	E	487	GLN
1	E	541	ASN
1	E	545	GLN
1	E	560	GLN
1	E	571	GLN
1	F	480	GLN
1	F	487	GLN
1	F	571	GLN
1	G	508	GLN
1	G	517	GLN
1	G	571	GLN
1	G	604	HIS
1	H	519	GLN

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 ⓘ

Of 24 ligands modelled in this entry, 24 are monoatomic - leaving 0 for Mogul analysis.

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 ⓘ

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	223/227 (98%)	0.29	17 (7%)	20	16	35, 58, 95, 111	0
1	B	224/227 (98%)	0.27	11 (4%)	35	29	37, 58, 93, 112	0
1	C	225/227 (99%)	0.25	18 (8%)	18	14	32, 56, 103, 126	0
1	D	225/227 (99%)	0.20	13 (5%)	29	23	34, 53, 90, 117	0
1	E	225/227 (99%)	0.20	13 (5%)	29	23	34, 56, 102, 123	0
1	F	223/227 (98%)	0.22	11 (4%)	35	29	36, 57, 93, 109	0
1	G	225/227 (99%)	0.24	6 (2%)	56	50	35, 55, 100, 119	0
1	H	225/227 (99%)	0.34	16 (7%)	22	17	33, 61, 100, 117	0
All	All	1795/1816 (98%)	0.25	105 (5%)	29	23	32, 57, 99, 126	0

All (105) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	626	GLY	6.1
1	C	416	ALA	5.4
1	F	602	GLY	4.9
1	A	549	GLY	4.7
1	H	601	LEU	4.7
1	G	597	SER	4.6
1	C	597	SER	4.2
1	D	560	GLN	4.2
1	H	626	GLY	4.1
1	C	601	LEU	4.1
1	C	595	PHE	4.0
1	A	597	SER	3.9
1	C	602	GLY	3.9
1	G	596	LEU	3.9
1	C	596	LEU	3.8
1	C	627	SER	3.7

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Mol	Chain	Res	Type	RSRZ
1	F	625	SER	3.6
1	A	601	LEU	3.5
1	C	548	GLU	3.4
1	F	507	GLN	3.4
1	E	593	GLY	3.3
1	A	503	VAL	3.3
1	A	602	GLY	3.2
1	D	416	ALA	3.2
1	B	416	ALA	3.2
1	F	600	LYS	3.2
1	D	601	LEU	3.2
1	D	581	GLU	3.1
1	F	416	ALA	3.1
1	E	504	LYS	3.1
1	E	602	GLY	3.1
1	E	595	PHE	3.0
1	G	629	GLN	3.0
1	C	503	VAL	3.0
1	H	503	VAL	3.0
1	B	509	ARG	3.0
1	H	416	ALA	3.0
1	C	598	ALA	3.0
1	H	642	GLN	2.9
1	C	626	GLY	2.9
1	B	515	PHE	2.9
1	C	547	GLU	2.9
1	E	626	GLY	2.8
1	A	548	GLU	2.8
1	C	417	GLU	2.8
1	A	546	THR	2.8
1	H	508	GLN	2.8
1	F	504	LYS	2.8
1	D	641	PRO	2.8
1	G	601	LEU	2.8
1	F	509	ARG	2.8
1	D	519	GLN	2.7
1	C	599	SER	2.7
1	B	508	GLN	2.7
1	E	599	SER	2.7
1	A	547	GLU	2.7
1	E	545	GLN	2.6
1	B	601	LEU	2.6

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Mol	Chain	Res	Type	RSRZ
1	E	592	SER	2.6
1	F	629	GLN	2.6
1	D	579	ALA	2.6
1	H	641	PRO	2.6
1	G	626	GLY	2.5
1	A	560	GLN	2.5
1	B	592	SER	2.5
1	B	641	PRO	2.5
1	G	627	SER	2.5
1	H	625	SER	2.5
1	B	564	PRO	2.5
1	E	625	SER	2.5
1	D	578	ASP	2.4
1	A	642	GLN	2.4
1	F	641	PRO	2.4
1	D	600	LYS	2.4
1	A	598	ALA	2.4
1	A	573	SER	2.4
1	A	509	ARG	2.4
1	A	563	THR	2.4
1	C	600	LYS	2.4
1	D	508	GLN	2.4
1	E	419	LEU	2.3
1	E	601	LEU	2.3
1	E	417	GLU	2.3
1	H	564	PRO	2.3
1	H	591	HIS	2.3
1	C	593	GLY	2.3
1	F	417	GLU	2.2
1	H	507	GLN	2.2
1	H	504	LYS	2.2
1	B	546	THR	2.2
1	D	515	PHE	2.2
1	H	600	LYS	2.1
1	D	627	SER	2.1
1	E	510	ILE	2.1
1	D	509	ARG	2.1
1	H	511	GLU	2.1
1	H	629	GLN	2.1
1	A	559	ASP	2.1
1	A	593	GLY	2.1
1	B	600	LYS	2.0

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Mol	Chain	Res	Type	RSRZ
1	F	563	THR	2.0
1	C	558	ASP	2.0
1	B	628	SER	2.0
1	C	629	GLN	2.0
1	H	561	GLY	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(Å ²)	Q<0.9
2	CO	C	704	1/1	0.85	0.11	117,117,117,117	0
2	CO	A	701	1/1	0.86	0.14	132,132,132,132	0
2	CO	F	702	1/1	0.86	0.13	132,132,132,132	0
2	CO	H	702	1/1	0.88	0.10	123,123,123,123	0
2	CO	E	704	1/1	0.91	0.10	109,109,109,109	0
2	CO	D	703	1/1	0.91	0.14	124,124,124,124	0
2	CO	B	704	1/1	0.91	0.09	119,119,119,119	0
2	CO	H	703	1/1	0.92	0.09	57,57,57,57	0
2	CO	G	702	1/1	0.93	0.07	126,126,126,126	0
2	CO	H	701	1/1	0.94	0.06	106,106,106,106	0
2	CO	F	701	1/1	0.95	0.08	97,97,97,97	0
2	CO	B	701	1/1	0.95	0.07	56,56,56,56	0
2	CO	B	703	1/1	0.95	0.06	92,92,92,92	0
2	CO	A	702	1/1	0.96	0.14	89,89,89,89	0
2	CO	E	701	1/1	0.96	0.10	56,56,56,56	0
2	CO	C	702	1/1	0.96	0.11	56,56,56,56	0
2	CO	G	701	1/1	0.97	0.06	72,72,72,72	0
2	CO	E	702	1/1	0.98	0.10	59,59,59,59	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	CO	E	703	1/1	0.98	0.04	70,70,70,70	0
2	CO	C	701	1/1	0.98	0.07	64,64,64,64	0
2	CO	D	702	1/1	0.98	0.04	76,76,76,76	0
2	CO	B	702	1/1	0.98	0.11	56,56,56,56	0
2	CO	C	703	1/1	0.99	0.04	63,63,63,63	0
2	CO	D	701	1/1	1.00	0.02	34,34,34,34	0

6.5 Other polymers [i](#)

There are no such residues in this entry.