



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 06:54 PM GMT

PDB ID : 4MZO
Title : Mouse cathepsin s with covalent ligand (3S,4S)-N-[(2E)-2-IMINOETHYL]-4-(MORPHOLIN-4-YLCARBONYL)-1-(PHENYLSULFONYL)PYRROLIDINE-3-CARBOXAMIDE
Authors : Kuglstatter, A.; Stihle, M.
Deposited on : 2013-09-30
Resolution : 1.47 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
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix) : 1.9-1692
EDS : rb-20026688
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac : 5.8.0135
CCP4 : 6.5.0
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : trunk26865

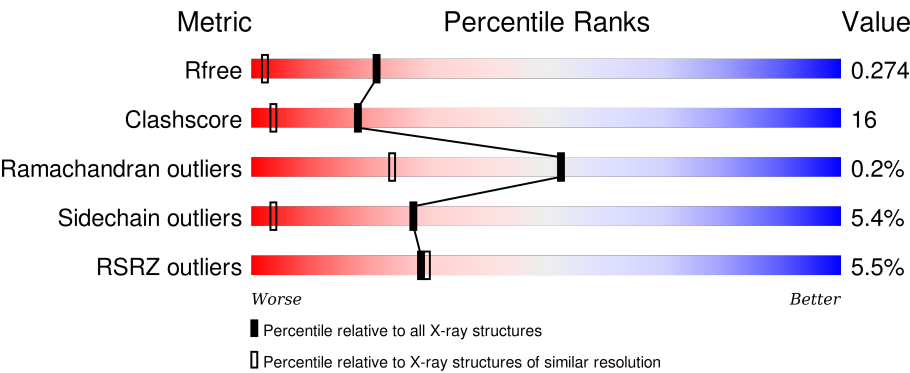
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.47 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}	91344	3129 (1.50-1.46)
Clashscore	102246	3380 (1.50-1.46)
Ramachandran outliers	100387	3310 (1.50-1.46)
Sidechain outliers	100360	3308 (1.50-1.46)
RSRZ outliers	91569	3133 (1.50-1.46)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=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	225	<div><div>2%</div><div>69%</div><div>23%</div><div>5%</div><div></div></div>
1	B	225	<div><div>9%</div><div>69%</div><div>24%</div><div></div><div></div></div>
1	C	225	<div><div>4%</div><div>69%</div><div>24%</div><div></div><div></div></div>
1	D	225	<div><div>5%</div><div>66%</div><div>28%</div><div></div><div></div></div>
1	E	225	<div><div>11%</div><div>57%</div><div>36%</div><div></div><div></div></div>

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Mol	Chain	Length	Quality of chain
1	F	225	<div><div><div></div><div></div><div></div></div><div><div>3%</div><div>65%</div><div>30%</div><div></div><div></div></div><div><div></div><div></div><div></div></div></div>
1	G	225	<div><div><div></div><div></div><div></div></div><div><div>3%</div><div>72%</div><div>19%</div><div>6%</div><div></div></div><div><div></div><div></div><div></div></div></div>
1	H	225	<div><div><div></div><div></div><div></div></div><div><div>5%</div><div>67%</div><div>28%</div><div></div><div></div></div><div><div></div><div></div><div></div></div></div>

2 Entry composition [i](#)

There are 3 unique types of molecules in this entry. The entry contains 14421 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.

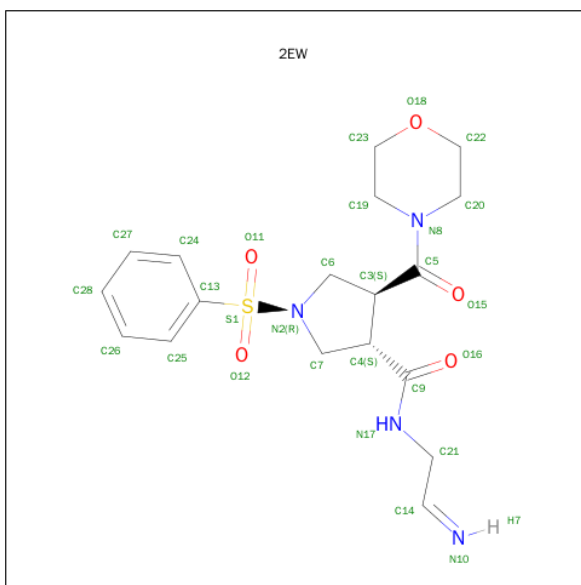
- Molecule 1 is a protein called Cathepsin S.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	218	Total	C	N	O	S	0	2	0
			1683	1059	281	330	13			
1	B	219	Total	C	N	O	S	0	1	0
			1682	1055	282	332	13			
1	C	218	Total	C	N	O	S	0	2	0
			1678	1054	280	331	13			
1	D	218	Total	C	N	O	S	0	2	0
			1683	1059	281	330	13			
1	E	218	Total	C	N	O	S	0	3	0
			1680	1058	280	328	14			
1	F	219	Total	C	N	O	S	0	1	0
			1679	1054	281	330	14			
1	G	218	Total	C	N	O	S	0	0	0
			1669	1048	280	328	13			
1	H	218	Total	C	N	O	S	0	0	0
			1669	1048	280	328	13			

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	218	MET	THR	VARIANT	UNP O70370
B	218	MET	THR	VARIANT	UNP O70370
C	218	MET	THR	VARIANT	UNP O70370
D	218	MET	THR	VARIANT	UNP O70370
E	218	MET	THR	VARIANT	UNP O70370
F	218	MET	THR	VARIANT	UNP O70370
G	218	MET	THR	VARIANT	UNP O70370
H	218	MET	THR	VARIANT	UNP O70370

- Molecule 2 is (3S,4S)-N-[(2E)-2-IMINOETHYL]-4-(MORPHOLIN-4-YLCARBONYL)-1-(PHENYLSULFONYL)PYRROLIDINE-3-CARBOXAMIDE (three-letter code: 2EW) (formula: C₁₈H₂₄N₄O₅S).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	S	0	0
			28	18	4	5	1		
2	B	1	Total	C	N	O	S	0	0
			28	18	4	5	1		
2	C	1	Total	C	N	O	S	0	0
			28	18	4	5	1		
2	D	1	Total	C	N	O	S	0	0
			28	18	4	5	1		
2	E	1	Total	C	N	O	S	0	0
			28	18	4	5	1		
2	F	1	Total	C	N	O	S	0	0
			28	18	4	5	1		
2	G	1	Total	C	N	O	S	0	0
			28	18	4	5	1		
2	H	1	Total	C	N	O	S	0	0
			28	18	4	5	1		

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	119	Total	O	0	0
			119	119		
3	B	101	Total	O	0	0
			101	101		
3	C	97	Total	O	0	0
			97	97		
3	D	86	Total	O	0	0
			86	86		

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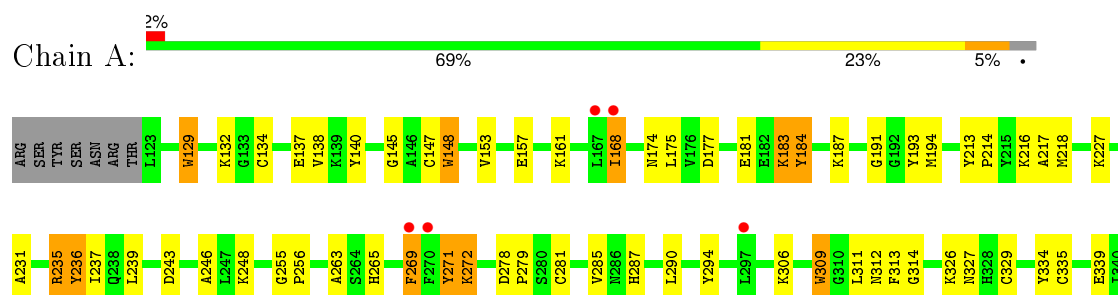
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	E	91	Total 91	O 91	0	0
3	F	97	Total 97	O 97	0	0
3	G	86	Total 86	O 86	0	0
3	H	97	Total 97	O 97	0	0

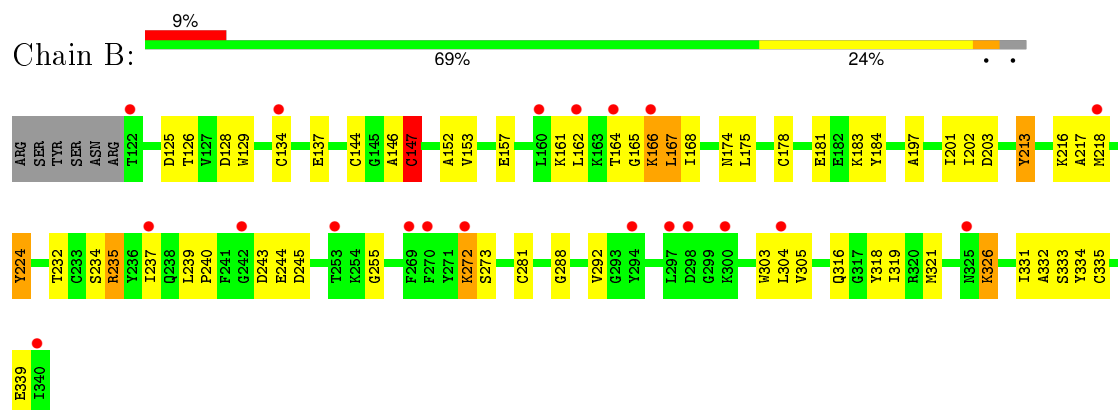
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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.

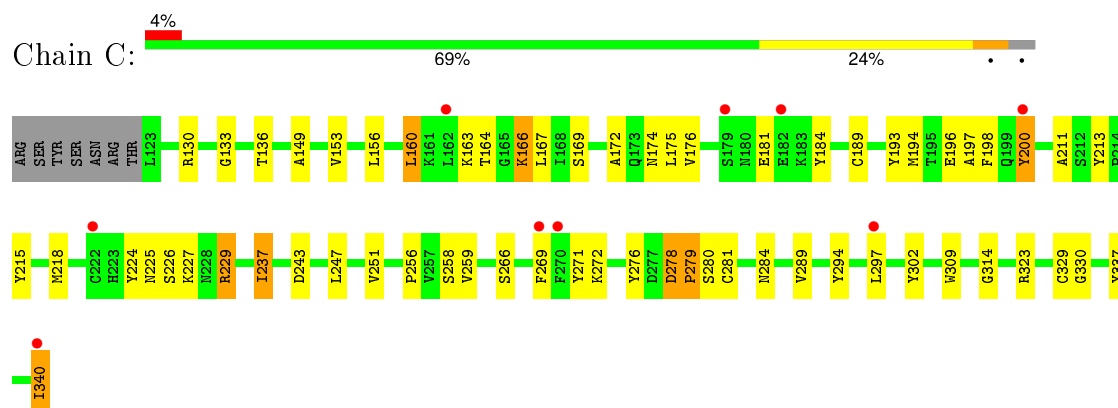
• Molecule 1: Cathepsin S



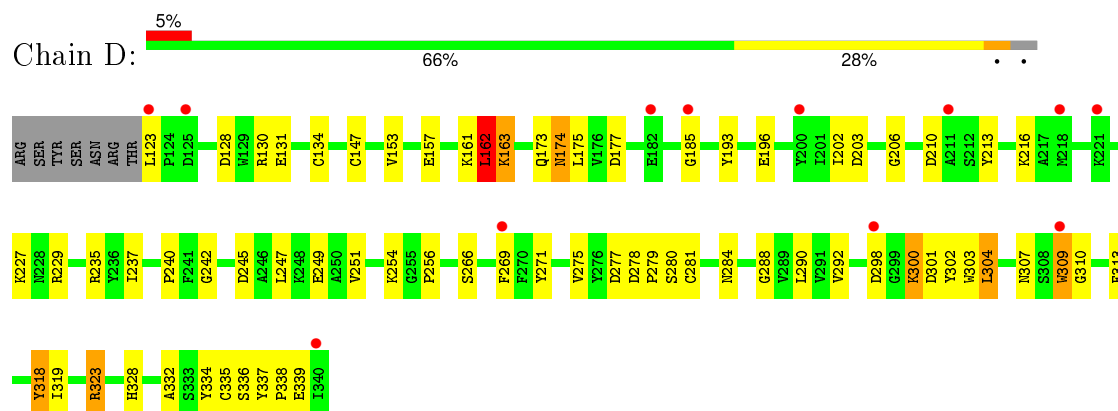
• Molecule 1: Cathepsin S



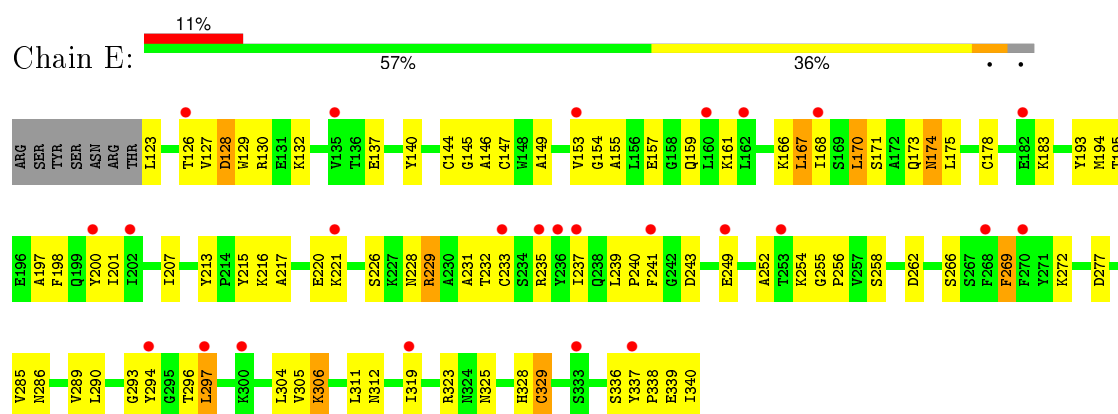
• Molecule 1: Cathepsin S



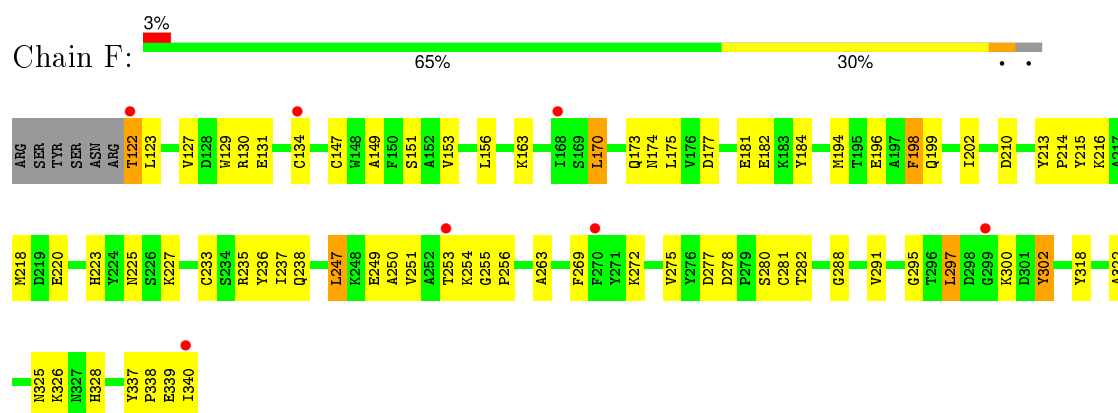
- Molecule 1: Cathepsin S



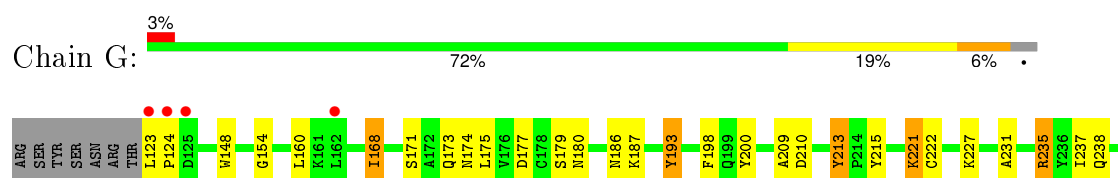
- Molecule 1: Cathepsin S

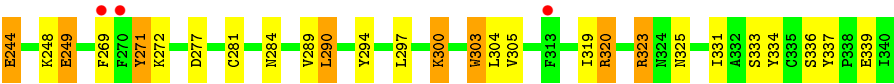


- Molecule 1: Cathepsin S

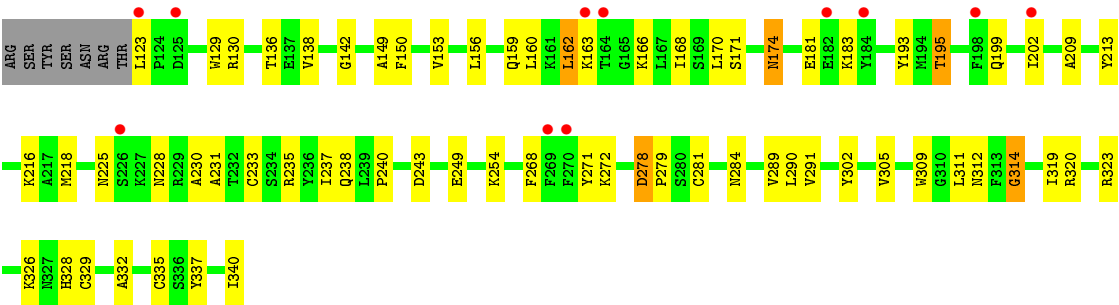


- Molecule 1: Cathepsin S





● Molecule 1: Cathepsin S



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	73.20Å 86.06Å 119.32Å 90.00° 90.46° 90.00°	Depositor
Resolution (Å)	49.03 – 1.47 49.03 – 1.47	Depositor EDS
% Data completeness (in resolution range)	92.5 (49.03-1.47) 92.5 (49.03-1.47)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.02 (at 1.47Å)	Xtriage
Refinement program	REFMAC 5.7.0029	Depositor
R, R_{free}	0.231 , 0.275 0.230 , 0.274	Depositor DCC
R_{free} test set	11771 reflections (5.29%)	DCC
Wilson B-factor (Å ²)	18.9	Xtriage
Anisotropy	0.153	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 19.0	EDS
Estimated twinning fraction	0.703 for H, K, L 0.297 for -H, -K, L 0.279 for h,-k,-l	Xtriage
Reported twinning fraction	0.703 for H, K, L 0.297 for -H, -K, L	Depositor
L-test for twinning ²	$\langle L \rangle = 0.39$, $\langle L^2 \rangle = 0.21$	Xtriage
Outliers	0 of 234146 reflections	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	14421	wwPDB-VP
Average B, all atoms (Å ²)	17.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 69.66 % of the origin peak, indicating pseudo translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo translational symmetry is equal to 3.5618e-06.*

¹ Intensities estimated from amplitudes.

² Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 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: 2EW

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	1.33	9/1726 (0.5%)	1.36	11/2331 (0.5%)
1	B	1.25	3/1721 (0.2%)	1.38	9/2325 (0.4%)
1	C	1.39	12/1723 (0.7%)	1.42	15/2327 (0.6%)
1	D	1.26	4/1726 (0.2%)	1.37	10/2331 (0.4%)
1	E	1.26	4/1728 (0.2%)	1.40	15/2335 (0.6%)
1	F	1.35	4/1721 (0.2%)	1.43	11/2325 (0.5%)
1	G	1.36	8/1708 (0.5%)	1.48	15/2307 (0.7%)
1	H	1.23	3/1708 (0.2%)	1.38	14/2307 (0.6%)
All	All	1.30	47/13761 (0.3%)	1.40	100/18588 (0.5%)

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	E	0	1
1	G	0	1
All	All	0	2

All (47) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	309	TRP	CB-CG	-9.34	1.33	1.50
1	C	276	TYR	CE1-CZ	8.60	1.49	1.38
1	E	144	CYS	CB-SG	-8.21	1.68	1.82
1	G	213	TYR	CZ-OH	-7.03	1.25	1.37
1	F	198	PHE	CG-CD2	6.91	1.49	1.38
1	A	148	TRP	CB-CG	-6.81	1.38	1.50
1	G	271	TYR	CE2-CZ	6.54	1.47	1.38
1	H	314	GLY	N-CA	-6.50	1.36	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	E	294	TYR	CE1-CZ	6.44	1.47	1.38
1	A	184	TYR	CE1-CZ	6.36	1.46	1.38
1	C	337	TYR	CG-CD1	6.34	1.47	1.39
1	F	318	TYR	CE1-CZ	6.33	1.46	1.38
1	C	215	TYR	CG-CD2	6.15	1.47	1.39
1	C	276	TYR	CD1-CE1	6.08	1.48	1.39
1	H	291	VAL	N-CA	-6.04	1.34	1.46
1	G	231	ALA	C-O	6.03	1.34	1.23
1	D	318	TYR	CE1-CZ	5.97	1.46	1.38
1	D	290	LEU	C-O	5.89	1.34	1.23
1	C	309	TRP	CB-CG	-5.76	1.39	1.50
1	A	129	TRP	CE3-CZ3	5.65	1.48	1.38
1	F	302	TYR	CD2-CE2	5.60	1.47	1.39
1	C	294	TYR	CE1-CZ	-5.55	1.31	1.38
1	A	184	TYR	CZ-OH	5.51	1.47	1.37
1	A	236	TYR	CE1-CZ	-5.49	1.31	1.38
1	C	279	PRO	N-CA	-5.42	1.38	1.47
1	G	333	SER	C-O	5.40	1.33	1.23
1	A	145	GLY	C-O	5.39	1.32	1.23
1	B	318	TYR	CG-CD1	5.34	1.46	1.39
1	C	198	PHE	CG-CD2	5.32	1.46	1.38
1	C	193	TYR	CG-CD2	5.31	1.46	1.39
1	E	329	CYS	C-O	5.30	1.33	1.23
1	G	303	TRP	CD1-NE1	5.30	1.47	1.38
1	B	224	TYR	CE1-CZ	5.29	1.45	1.38
1	G	271	TYR	CG-CD1	5.29	1.46	1.39
1	H	142	GLY	C-O	5.24	1.32	1.23
1	E	140	TYR	CG-CD2	5.23	1.46	1.39
1	D	334	TYR	CE2-CZ	-5.22	1.31	1.38
1	C	193	TYR	CE1-CZ	5.21	1.45	1.38
1	B	333	SER	CB-OG	5.14	1.49	1.42
1	F	220	GLU	CD-OE1	-5.13	1.20	1.25
1	G	148	TRP	CB-CG	-5.07	1.41	1.50
1	A	231	ALA	C-O	5.06	1.32	1.23
1	A	309	TRP	CB-CG	5.06	1.59	1.50
1	C	330	GLY	N-CA	5.06	1.53	1.46
1	A	271	TYR	C-O	-5.05	1.13	1.23
1	C	193	TYR	CG-CD1	5.05	1.45	1.39
1	G	148	TRP	CZ3-CH2	5.03	1.48	1.40

All (100) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	130	ARG	NE-CZ-NH1	10.36	125.48	120.30
1	C	276	TYR	CZ-CE2-CD2	9.69	128.52	119.80
1	G	175	LEU	CB-CG-CD1	9.51	127.16	111.00
1	H	130	ARG	NE-CZ-NH2	9.20	124.90	120.30
1	C	323	ARG	NE-CZ-NH1	-8.90	115.85	120.30
1	E	323	ARG	NE-CZ-NH2	-8.85	115.88	120.30
1	E	170	LEU	CB-CG-CD2	-8.64	96.31	111.00
1	A	243	ASP	CB-CG-OD2	8.25	125.73	118.30
1	C	297	LEU	CB-CG-CD2	-7.91	97.55	111.00
1	E	220	GLU	OE1-CD-OE2	-7.91	113.81	123.30
1	A	175	LEU	CB-CG-CD2	-7.74	97.85	111.00
1	H	278	ASP	CB-CG-OD1	7.71	125.24	118.30
1	H	243	ASP	CB-CG-OD2	7.67	125.20	118.30
1	A	177	ASP	CB-CG-OD1	-7.61	111.45	118.30
1	F	175	LEU	CB-CG-CD1	7.45	123.67	111.00
1	G	200	TYR	CB-CG-CD2	7.39	125.44	121.00
1	H	130	ARG	NE-CZ-NH1	-7.25	116.67	120.30
1	G	323	ARG	NE-CZ-NH2	-7.21	116.69	120.30
1	E	262	ASP	CB-CG-OD1	-7.02	111.98	118.30
1	F	210	ASP	CB-CG-OD1	-7.01	111.99	118.30
1	H	323	ARG	NE-CZ-NH1	-6.97	116.81	120.30
1	G	320	ARG	NE-CZ-NH2	-6.89	116.86	120.30
1	F	177	ASP	CB-CG-OD2	6.80	124.42	118.30
1	G	244	GLU	OE1-CD-OE2	-6.79	115.16	123.30
1	H	162	LEU	CB-CG-CD2	-6.76	99.51	111.00
1	C	276	TYR	CE1-CZ-CE2	-6.75	109.00	119.80
1	F	156	LEU	CB-CG-CD2	-6.68	99.64	111.00
1	G	334	TYR	CB-CG-CD2	6.59	124.96	121.00
1	C	302	TYR	CB-CG-CD2	6.55	124.93	121.00
1	F	275	VAL	CG1-CB-CG2	-6.53	100.45	110.90
1	C	289	VAL	CG1-CB-CG2	-6.53	100.45	110.90
1	D	210	ASP	CB-CG-OD1	-6.52	112.43	118.30
1	B	144	CYS	CA-CB-SG	6.51	125.72	114.00
1	G	235	ARG	NE-CZ-NH1	6.47	123.54	120.30
1	E	243	ASP	CB-CG-OD2	6.41	124.07	118.30
1	F	170	LEU	CB-CG-CD2	-6.29	100.30	111.00
1	D	210	ASP	CB-CG-OD2	6.27	123.94	118.30
1	E	306	LYS	CD-CE-NZ	6.25	126.08	111.70
1	D	162	LEU	CA-CB-CG	6.22	129.60	115.30
1	D	323	ARG	NE-CZ-NH1	-6.21	117.19	120.30
1	B	175	LEU	CB-CG-CD1	6.16	121.47	111.00
1	D	177	ASP	CB-CG-OD2	6.11	123.80	118.30
1	G	305	VAL	CA-CB-CG2	-6.11	101.73	110.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	259	VAL	CA-CB-CG2	-6.09	101.76	110.90
1	C	302	TYR	CB-CG-CD1	-6.07	117.36	121.00
1	D	175	LEU	CB-CG-CD1	-5.95	100.88	111.00
1	G	193	TYR	CB-CG-CD2	-5.93	117.44	121.00
1	F	247	LEU	CB-CG-CD1	-5.93	100.92	111.00
1	E	277	ASP	N-CA-C	-5.91	95.05	111.00
1	E	167	LEU	CB-CG-CD2	5.88	121.00	111.00
1	H	156	LEU	CB-CG-CD2	-5.87	101.02	111.00
1	A	193	TYR	CB-CG-CD1	-5.84	117.50	121.00
1	H	302	TYR	CB-CG-CD2	5.83	124.50	121.00
1	B	184	TYR	OH-CZ-CE2	-5.70	104.71	120.10
1	D	203	ASP	CB-CG-OD2	5.70	123.43	118.30
1	E	269	PHE	CB-CA-C	-5.67	99.05	110.40
1	C	278	ASP	CB-CG-OD2	5.66	123.39	118.30
1	B	128	ASP	CB-CG-OD2	5.64	123.38	118.30
1	G	198	PHE	CB-CG-CD1	5.62	124.73	120.80
1	H	290	LEU	CB-CG-CD2	-5.60	101.48	111.00
1	G	200	TYR	CB-CG-CD1	-5.59	117.65	121.00
1	E	285	VAL	CG1-CB-CG2	-5.55	102.02	110.90
1	G	289	VAL	CG1-CB-CG2	5.55	119.78	110.90
1	A	168	ILE	CB-CA-C	-5.54	100.52	111.60
1	A	311	LEU	CB-CG-CD2	-5.54	101.59	111.00
1	G	193	TYR	CB-CG-CD1	5.52	124.31	121.00
1	E	297	LEU	CA-CB-CG	5.50	127.95	115.30
1	D	302	TYR	CB-CG-CD2	5.49	124.29	121.00
1	E	175	LEU	CB-CG-CD2	-5.48	101.69	111.00
1	G	290	LEU	CA-CB-CG	5.45	127.83	115.30
1	C	130	ARG	NE-CZ-NH2	5.42	123.01	120.30
1	A	306	LYS	CD-CE-NZ	5.39	124.09	111.70
1	H	195	THR	CA-CB-CG2	-5.38	104.88	112.40
1	C	156	LEU	CB-CG-CD2	-5.37	101.87	111.00
1	E	128	ASP	CB-CG-OD2	5.37	123.13	118.30
1	H	302	TYR	N-CA-CB	5.35	120.22	110.60
1	A	329	CYS	CA-CB-SG	5.34	123.62	114.00
1	B	243	ASP	CB-CG-OD1	5.30	123.08	118.30
1	B	167	LEU	CB-CG-CD1	-5.29	102.01	111.00
1	A	168	ILE	CG1-CB-CG2	5.26	122.96	111.40
1	C	160	LEU	CB-CG-CD2	-5.24	102.09	111.00
1	B	147	CYS	CB-CA-C	-5.23	99.95	110.40
1	E	175	LEU	CB-CG-CD1	5.21	119.86	111.00
1	H	320	ARG	NE-CZ-NH1	5.21	122.91	120.30
1	C	243	ASP	CB-CG-OD2	5.20	122.98	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	177	ASP	CB-CG-OD1	-5.19	113.63	118.30
1	E	311	LEU	CB-CG-CD2	5.19	119.82	111.00
1	D	242	GLY	N-CA-C	5.15	125.97	113.10
1	B	125	ASP	CB-CG-OD2	5.14	122.93	118.30
1	C	237	ILE	CG1-CB-CG2	-5.14	100.08	111.40
1	F	131	GLU	OE1-CD-OE2	-5.13	117.15	123.30
1	H	136	THR	CA-CB-CG2	-5.12	105.23	112.40
1	A	313	PHE	CB-CG-CD2	-5.12	117.22	120.80
1	D	304	LEU	CB-CG-CD1	-5.11	102.32	111.00
1	H	326	LYS	CB-CA-C	5.11	120.61	110.40
1	F	127	VAL	CG1-CB-CG2	-5.07	102.79	110.90
1	C	237	ILE	CB-CA-C	-5.05	101.50	111.60
1	B	152	ALA	CB-CA-C	5.03	117.64	110.10
1	A	246	ALA	N-CA-CB	5.01	117.11	110.10
1	G	304	LEU	CB-CG-CD1	5.01	119.52	111.00

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	E	154	GLY	Mainchain
1	G	337	TYR	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	1683	0	1583	49	0
1	B	1682	0	1581	68	0
1	C	1678	0	1581	36	0
1	D	1683	0	1583	48	0
1	E	1680	0	1593	86	0
1	F	1679	0	1582	55	0
1	G	1669	0	1570	50	0
1	H	1669	0	1570	42	1
2	A	28	0	22	0	0
2	B	28	0	22	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	C	28	0	22	0	0
2	D	28	0	22	0	0
2	E	28	0	22	1	0
2	F	28	0	22	1	0
2	G	28	0	22	4	0
2	H	28	0	22	1	0
3	A	119	0	0	8	0
3	B	101	0	0	32	0
3	C	97	0	0	10	0
3	D	86	0	0	8	0
3	E	91	0	0	24	0
3	F	97	0	0	18	0
3	G	86	0	0	20	1
3	H	97	0	0	8	0
All	All	14421	0	12819	416	1

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 16.

All (416) 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:B:126:THR:HB	3:B:543:HOH:O	1.33	1.28
1:B:319:ILE:HG23	3:B:599:HOH:O	1.41	1.21
1:G:171:SER:HA	3:G:535:HOH:O	1.39	1.19
1:G:187:LYS:HE2	3:G:576:HOH:O	1.45	1.17
1:B:235:ARG:NH1	1:B:339:GLU:OE1	1.85	1.09
1:G:238:GLN:HB2	3:G:534:HOH:O	1.51	1.08
1:B:331:ILE:HG22	3:B:586:HOH:O	1.52	1.07
1:E:289[B]:VAL:CG2	1:E:306:LYS:O	2.02	1.07
1:G:272:LYS:HD2	1:H:240:PRO:HB3	1.36	1.04
3:E:532:HOH:O	2:H:401:2EW:H18	1.58	1.03
1:E:289[B]:VAL:HG22	1:E:290:LEU:H	1.18	1.02
1:B:218:MET:SD	3:B:526:HOH:O	2.20	1.00
1:E:153[B]:VAL:HG22	1:E:170:LEU:HB2	1.39	1.00
1:B:237:ILE:HD11	1:B:339:GLU:HG3	1.45	0.98
1:E:195:THR:HA	3:E:520:HOH:O	1.63	0.97
1:E:289[B]:VAL:HG23	1:E:306:LYS:O	1.66	0.96
1:E:297:LEU:HG	3:E:586:HOH:O	1.66	0.95
1:F:272:LYS:HE3	3:F:589:HOH:O	1.67	0.93
1:H:170:LEU:HD22	3:H:560:HOH:O	1.68	0.93

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:199:GLN:HA	1:H:202:ILE:HD12	1.47	0.92
1:D:338:PRO:HD2	3:D:568:HOH:O	1.68	0.92
1:B:134:CYS:SG	1:B:162:LEU:HD21	2.10	0.91
1:E:166:LYS:HA	3:E:516:HOH:O	1.69	0.91
1:H:193:TYR:CD1	3:H:531:HOH:O	2.25	0.90
1:B:181:GLU:HG3	3:B:598:HOH:O	1.71	0.89
1:B:153:VAL:O	1:B:157:GLU:HG3	1.73	0.88
1:F:326:LYS:HB3	3:F:573:HOH:O	1.71	0.88
1:E:272:LYS:HD3	3:E:554:HOH:O	1.75	0.87
1:B:164:THR:HG22	3:B:569:HOH:O	1.75	0.86
1:B:137:GLU:HG3	1:D:284:ASN:HD21	1.40	0.85
1:B:316:GLN:HG3	3:D:564:HOH:O	1.77	0.85
1:B:213:TYR:HE2	3:B:582:HOH:O	1.60	0.84
1:D:134:CYS:SG	1:D:162:LEU:CD1	2.66	0.83
1:B:164:THR:OG1	1:B:166:LYS:HG2	1.80	0.82
1:C:340:ILE:HA	3:C:559:HOH:O	1.79	0.81
1:G:215:TYR:HB2	3:G:580:HOH:O	1.81	0.81
1:D:216:LYS:HB2	3:D:562:HOH:O	1.81	0.81
1:C:269:PHE:HB2	3:C:580:HOH:O	1.78	0.80
1:B:316:GLN:CG	3:B:534:HOH:O	2.29	0.80
1:A:140:TYR:CE2	3:A:560:HOH:O	2.35	0.80
1:B:237:ILE:CD1	1:B:339:GLU:HG3	2.12	0.79
1:B:213:TYR:CE2	3:B:582:HOH:O	2.34	0.79
1:D:235:ARG:CG	1:D:339:GLU:HB2	2.13	0.79
1:E:289[B]:VAL:HG22	1:E:290:LEU:N	1.98	0.78
1:D:235:ARG:HG2	1:D:339:GLU:HB2	1.66	0.78
1:E:237:ILE:HD11	1:E:339:GLU:HG3	1.67	0.77
1:C:225:ASN:OD1	1:C:227:LYS:HG3	1.85	0.77
1:A:327:ASN:O	3:A:579:HOH:O	2.04	0.76
1:H:168:ILE:HD11	1:H:209:ALA:HB2	1.65	0.76
1:F:272:LYS:CE	3:F:589:HOH:O	2.27	0.76
1:E:198:PHE:HD1	3:E:520:HOH:O	1.69	0.76
1:F:198:PHE:HB3	3:F:530:HOH:O	1.86	0.76
1:E:237:ILE:HD13	1:E:337:TYR:CE2	2.21	0.75
1:E:153[B]:VAL:CG2	1:E:170:LEU:HB2	2.15	0.75
1:E:126:THR:HG22	3:E:507:HOH:O	1.86	0.75
1:C:266:SER:HB2	3:C:544:HOH:O	1.85	0.75
1:E:233[B]:CYS:SG	1:E:338:PRO:HB2	2.27	0.75
1:B:218:MET:HB2	3:B:526:HOH:O	1.86	0.74
1:B:232:THR:HB	3:B:575:HOH:O	1.86	0.74
1:B:134:CYS:SG	1:B:162:LEU:CD2	2.74	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:331:ILE:HG23	3:G:536:HOH:O	1.88	0.74
1:E:289[B]:VAL:HG22	1:E:306:LYS:O	1.86	0.73
1:A:237:ILE:N	1:A:237:ILE:HD12	2.04	0.73
1:B:232:THR:CB	3:B:575:HOH:O	2.35	0.73
1:F:325:ASN:HB3	3:F:516:HOH:O	1.89	0.73
1:D:134:CYS:SG	1:D:162:LEU:HD13	2.30	0.71
1:E:129:TRP:CE2	1:E:255:GLY:HA2	2.26	0.71
1:E:289[B]:VAL:HG21	1:E:305:VAL:CG1	2.19	0.71
1:D:173:GLN:NE2	3:D:562:HOH:O	2.24	0.71
1:A:134:CYS:SG	1:A:161:LYS:HG2	2.31	0.71
1:B:321:MET:SD	3:B:599:HOH:O	2.48	0.71
1:D:163:LYS:HD2	1:D:163:LYS:N	2.04	0.71
1:F:263:ALA:O	1:F:269:PHE:HE1	1.74	0.71
1:H:272:LYS:HD2	3:H:595:HOH:O	1.90	0.70
1:D:271:TYR:CD1	1:D:319:ILE:HG13	2.27	0.70
1:F:338:PRO:HB3	3:F:546:HOH:O	1.91	0.70
1:B:316:GLN:HG3	3:B:534:HOH:O	1.90	0.70
1:B:202:ILE:HD12	3:B:583:HOH:O	1.90	0.69
1:E:161:LYS:HD3	1:E:167:LEU:HB2	1.73	0.69
1:B:237:ILE:HD11	1:B:339:GLU:CG	2.22	0.69
1:F:297:LEU:HA	3:F:541:HOH:O	1.93	0.69
1:F:325:ASN:ND2	3:F:557:HOH:O	2.24	0.69
1:B:305:VAL:HB	3:B:599:HOH:O	1.93	0.68
1:B:235:ARG:HG3	1:B:339:GLU:HB2	1.74	0.68
1:G:272:LYS:HD2	1:H:240:PRO:CB	2.19	0.68
1:A:137:GLU:HG3	1:C:284:ASN:HD21	1.57	0.68
1:E:166:LYS:HD2	1:E:168:ILE:HD11	1.75	0.67
1:E:266:SER:HA	1:E:269:PHE:CD1	2.30	0.67
1:E:296:THR:HB	3:E:535:HOH:O	1.93	0.67
1:B:178:CYS:SG	3:B:582:HOH:O	2.53	0.66
1:A:263:ALA:O	1:A:269[A]:PHE:HE2	1.78	0.66
1:B:232:THR:HA	3:B:575:HOH:O	1.96	0.66
1:H:193:TYR:HD1	3:H:531:HOH:O	1.69	0.66
3:B:601:HOH:O	1:D:185:GLY:HA2	1.95	0.65
1:E:195:THR:HG22	3:E:520:HOH:O	1.95	0.65
1:G:221:LYS:HD2	1:G:221:LYS:H	1.62	0.65
1:C:340:ILE:CA	3:C:559:HOH:O	2.39	0.65
1:F:216:LYS:HD3	1:F:216:LYS:N	2.11	0.64
1:E:289[B]:VAL:HG21	1:E:305:VAL:HG12	1.80	0.64
1:E:198:PHE:CD1	3:E:520:HOH:O	2.45	0.64
1:B:321:MET:HG3	3:B:599:HOH:O	1.99	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:272:LYS:HE3	1:C:196:GLU:OE1	1.98	0.63
1:E:166:LYS:CD	1:E:168:ILE:HD11	2.29	0.63
1:B:244:GLU:HB3	1:B:303:TRP:HZ2	1.63	0.63
1:G:237:ILE:CD1	1:G:339:GLU:HG3	2.29	0.63
1:E:325:ASN:ND2	3:E:547:HOH:O	2.31	0.63
1:G:244:GLU:HG2	3:G:536:HOH:O	1.99	0.63
1:B:292:VAL:HG23	1:B:304:LEU:HD23	1.79	0.63
1:A:236:TYR:C	1:A:237:ILE:HD12	2.19	0.62
1:D:292:VAL:HG23	1:D:304:LEU:HD23	1.79	0.62
1:B:232:THR:CA	3:B:575:HOH:O	2.46	0.62
1:H:163:LYS:HB3	3:H:573:HOH:O	1.98	0.62
1:E:297:LEU:CG	3:E:586:HOH:O	2.32	0.61
1:E:129:TRP:CZ2	1:E:255:GLY:HA2	2.36	0.61
1:E:297:LEU:CB	3:E:586:HOH:O	2.48	0.61
1:C:227:LYS:HG2	1:F:182:GLU:O	2.01	0.61
1:G:215:TYR:CB	3:G:580:HOH:O	2.42	0.61
1:H:168:ILE:HD13	1:H:230:ALA:HB1	1.82	0.61
1:E:269:PHE:HB3	1:G:269:PHE:HZ	1.66	0.61
1:D:235:ARG:HG3	1:D:339:GLU:HB2	1.82	0.61
1:G:237:ILE:HD11	1:G:339:GLU:HG3	1.83	0.60
1:F:129:TRP:CE2	1:F:255:GLY:HA2	2.36	0.60
1:G:210:ASP:CB	3:G:535:HOH:O	2.50	0.60
1:A:161:LYS:NZ	1:B:334:TYR:OH	2.31	0.60
1:E:197:ALA:O	1:E:201:ILE:HG13	2.01	0.60
1:B:216:LYS:O	1:B:217:ALA:HB3	2.01	0.59
1:A:137:GLU:HG3	1:C:284:ASN:ND2	2.18	0.59
1:E:127:VAL:HG13	3:E:515:HOH:O	2.03	0.59
1:G:210:ASP:HB2	3:G:535:HOH:O	2.01	0.59
1:G:284:ASN:CB	3:G:538:HOH:O	2.50	0.59
1:G:284:ASN:HB3	3:G:538:HOH:O	2.01	0.59
1:D:247:LEU:O	1:D:251:VAL:HG23	2.03	0.59
1:F:338:PRO:HA	3:F:546:HOH:O	2.03	0.59
1:G:297:LEU:O	1:G:300:LYS:HG3	2.01	0.58
1:H:168:ILE:HD11	1:H:209:ALA:CB	2.33	0.58
1:A:235:ARG:HH11	1:A:235:ARG:CB	2.16	0.58
1:G:168:ILE:HD11	1:G:209:ALA:HB1	1.84	0.58
1:F:173:GLN:HG2	1:F:214:PRO:O	2.04	0.58
1:E:130:ARG:CZ	3:E:568:HOH:O	2.52	0.58
1:E:137:GLU:HG3	1:H:284:ASN:ND2	2.19	0.58
1:A:235:ARG:HG3	1:A:339:GLU:HG3	1.86	0.57
1:A:138:VAL:HG23	3:A:506:HOH:O	2.03	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:224:TYR:HB2	3:B:582:HOH:O	2.03	0.57
1:E:325:ASN:CG	3:E:552:HOH:O	2.43	0.57
1:G:210:ASP:CA	3:G:535:HOH:O	2.52	0.57
1:G:210:ASP:HA	3:G:535:HOH:O	2.04	0.57
1:C:149:ALA:O	1:C:153:VAL:HG22	2.05	0.57
1:D:277:ASP:HA	1:D:328:HIS:CE1	2.39	0.57
1:A:140:TYR:CD2	3:A:560:HOH:O	2.54	0.57
1:C:271:TYR:HE2	3:C:575:HOH:O	1.87	0.57
1:F:223:HIS:HE1	3:F:560:HOH:O	1.86	0.57
1:H:254:LYS:HG3	1:H:337:TYR:CZ	2.40	0.57
1:F:202:ILE:HD11	3:F:530:HOH:O	2.04	0.57
1:C:184:TYR:O	1:C:196:GLU:OE1	2.23	0.57
1:C:284:ASN:HB3	3:C:546:HOH:O	2.04	0.57
1:B:316:GLN:HG2	3:B:534:HOH:O	2.00	0.56
1:E:237:ILE:HD11	1:E:339:GLU:CG	2.34	0.56
1:D:256:PRO:HB3	1:D:292:VAL:HG12	1.87	0.56
1:G:248:LYS:HE3	1:G:294:TYR:CE2	2.39	0.56
1:E:137:GLU:HG3	1:H:284:ASN:HD21	1.69	0.56
1:F:295:GLY:HA3	1:F:302:TYR:CZ	2.40	0.56
1:B:129:TRP:CE2	1:B:255:GLY:HA2	2.40	0.56
1:E:256:PRO:HD2	3:E:529:HOH:O	2.06	0.56
1:B:272:LYS:HD2	3:B:548:HOH:O	2.06	0.55
1:F:338:PRO:CA	3:F:546:HOH:O	2.53	0.55
1:D:128:ASP:HB3	1:D:131:GLU:HG3	1.88	0.55
1:G:277:ASP:OD1	1:G:325:ASN:ND2	2.40	0.55
1:G:221:LYS:N	1:G:221:LYS:HD2	2.22	0.55
1:F:249:GLU:OE1	1:F:253:THR:CG2	2.53	0.55
1:B:126:THR:CB	3:B:543:HOH:O	2.15	0.55
1:C:163:LYS:NZ	1:F:238:GLN:O	2.39	0.55
1:A:187:LYS:HB3	3:A:564:HOH:O	2.06	0.55
1:E:289[B]:VAL:CG2	1:E:290:LEU:H	2.03	0.54
1:D:235:ARG:HG2	1:D:339:GLU:CB	2.37	0.54
1:D:275:VAL:HB	1:D:300:LYS:HD2	1.89	0.54
1:G:179:SER:C	3:G:568:HOH:O	2.46	0.54
1:H:271:TYR:O	1:H:272:LYS:HE3	2.08	0.54
1:C:164:THR:O	1:C:166:LYS:HD2	2.07	0.54
1:E:149:ALA:O	1:E:153[A]:VAL:HG22	2.07	0.54
1:A:187:LYS:HB2	1:A:191:GLY:O	2.08	0.54
1:F:236:TYR:HB3	3:F:546:HOH:O	2.06	0.54
1:A:271:TYR:O	1:A:314:GLY:HA2	2.08	0.54
1:H:268:PHE:CE2	1:H:319:ILE:HD13	2.42	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:269[A]:PHE:H	1:A:269[A]:PHE:HD2	1.55	0.54
1:F:215:TYR:C	1:F:216:LYS:HD3	2.29	0.54
1:F:235:ARG:HG2	1:F:339:GLU:HB2	1.89	0.54
1:G:215:TYR:HD2	3:G:580:HOH:O	1.91	0.53
1:F:236:TYR:C	1:F:237:ILE:HD12	2.28	0.53
1:B:167:LEU:O	1:B:168:ILE:HG13	2.08	0.53
1:G:271:TYR:CE1	1:G:319:ILE:HG13	2.44	0.53
1:F:233:CYS:SG	3:F:530:HOH:O	2.37	0.53
1:A:214:PRO:HD2	3:A:519:HOH:O	2.07	0.53
1:C:172:ALA:O	1:C:176:VAL:HG23	2.09	0.53
1:G:168:ILE:HD11	1:G:209:ALA:CB	2.38	0.53
1:D:271:TYR:CG	1:D:319:ILE:HG13	2.43	0.52
1:A:269[B]:PHE:CG	1:A:269[B]:PHE:O	2.62	0.52
1:H:225:ASN:HB3	1:H:228:ASN:HD22	1.75	0.52
1:D:173:GLN:CD	3:D:562:HOH:O	2.48	0.52
1:C:163:LYS:CE	1:F:238:GLN:O	2.57	0.52
1:G:193:TYR:CZ	2:G:401:2EW:H12	2.44	0.52
1:E:161:LYS:HA	1:E:166:LYS:O	2.10	0.52
1:A:269[B]:PHE:HD2	1:A:309:TRP:CZ3	2.27	0.52
1:B:319:ILE:CA	3:B:513:HOH:O	2.56	0.52
1:G:179:SER:CA	3:G:568:HOH:O	2.58	0.52
1:B:202:ILE:CD1	3:B:583:HOH:O	2.54	0.52
1:H:160:LEU:HD13	1:H:231:ALA:CB	2.40	0.52
1:F:338:PRO:CB	3:F:546:HOH:O	2.53	0.51
1:D:245:ASP:HB3	3:D:543:HOH:O	2.10	0.51
1:D:301:ASP:HB2	1:D:323:ARG:O	2.10	0.51
1:C:256:PRO:HD2	3:C:519:HOH:O	2.09	0.51
1:C:133:GLY:O	1:C:167:LEU:HD13	2.09	0.51
1:A:269[B]:PHE:CD2	1:A:309:TRP:CZ3	2.98	0.51
1:F:147:CYS:HB2	1:F:288:GLY:O	2.10	0.51
1:B:147:CYS:HB2	1:B:288:GLY:O	2.11	0.51
1:D:134:CYS:SG	1:D:162:LEU:HD11	2.48	0.51
1:B:237:ILE:N	1:B:237:ILE:HD12	2.26	0.51
1:C:340:ILE:C	3:C:559:HOH:O	2.49	0.51
1:A:263:ALA:O	1:A:269[A]:PHE:CE2	2.61	0.51
1:D:227:LYS:HD2	1:E:183:LYS:O	2.11	0.51
1:B:235:ARG:NH2	3:B:541:HOH:O	2.44	0.50
1:B:235:ARG:HB2	3:B:528:HOH:O	2.10	0.50
1:F:256:PRO:HA	1:F:291:VAL:O	2.12	0.50
1:D:237:ILE:O	1:D:336[B]:SER:HA	2.12	0.50
1:A:269[A]:PHE:N	1:A:269[A]:PHE:CD2	2.79	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:304:LEU:HD21	3:E:568:HOH:O	2.11	0.50
1:G:173:GLN:HB2	3:G:580:HOH:O	2.12	0.50
1:E:221:LYS:HE3	3:E:584:HOH:O	2.12	0.50
1:F:249:GLU:OE1	1:F:253:THR:HG23	2.11	0.49
1:F:184:TYR:HE2	1:F:199:GLN:HG2	1.77	0.49
1:H:166:LYS:HG3	1:H:166:LYS:O	2.11	0.49
1:G:160:LEU:HD23	1:G:168:ILE:HG22	1.94	0.49
1:D:123:LEU:HD13	1:D:249:GLU:HA	1.94	0.49
1:A:237:ILE:N	1:A:237:ILE:CD1	2.69	0.49
1:A:239:LEU:HD12	1:A:335:CYS:HB3	1.94	0.49
1:A:269[B]:PHE:HD2	1:A:309:TRP:HZ3	1.60	0.49
1:H:163:LYS:HD2	1:H:340:ILE:HB	1.94	0.49
1:H:159:GLN:HB3	3:H:589:HOH:O	2.12	0.49
1:G:179:SER:O	1:G:186:ASN:HB2	2.12	0.49
1:B:326:LYS:HE2	1:B:326:LYS:O	2.13	0.49
1:E:123:LEU:HD11	1:E:249:GLU:OE1	2.13	0.49
1:A:129:TRP:CE2	1:A:255:GLY:HA2	2.48	0.49
1:G:179:SER:HA	3:G:568:HOH:O	2.13	0.48
1:A:214:PRO:HG2	1:A:216:LYS:HE2	1.93	0.48
1:B:183:LYS:HE2	1:B:203:ASP:OD1	2.13	0.48
1:G:123:LEU:HD21	1:G:249:GLU:OE1	2.12	0.48
1:C:224:TYR:HE1	1:C:226[B]:SER:HG	1.60	0.48
1:F:254:LYS:HG3	1:F:337:TYR:CZ	2.49	0.48
1:H:254:LYS:HG3	1:H:337:TYR:CE2	2.49	0.48
1:F:250:ALA:O	1:F:254:LYS:HB2	2.14	0.48
1:A:269[A]:PHE:N	1:A:269[A]:PHE:HD2	2.10	0.48
1:D:206:GLY:HA3	1:D:229:ARG:HG3	1.94	0.48
1:H:237:ILE:HD13	1:H:337:TYR:CE2	2.49	0.47
1:E:226:SER:C	1:E:228:ASN:H	2.18	0.47
1:D:153:VAL:O	1:D:157:GLU:HG3	2.13	0.47
1:B:316:GLN:NE2	1:D:193:TYR:OH	2.47	0.47
1:E:237:ILE:CD1	1:E:339:GLU:CG	2.92	0.47
1:E:312:ASN:HB2	3:E:510:HOH:O	2.14	0.47
1:E:146:ALA:O	1:E:147:CYS:C	2.51	0.47
1:H:235:ARG:NH1	3:H:550:HOH:O	2.45	0.47
1:B:235:ARG:CZ	1:B:339:GLU:OE1	2.58	0.47
1:A:153:VAL:O	1:A:157:GLU:HG3	2.14	0.47
2:G:401:2EW:H1	2:G:401:2EW:H13	1.61	0.47
1:A:239:LEU:HB2	1:A:335:CYS:HB2	1.96	0.47
1:H:160:LEU:HD13	1:H:231:ALA:HB2	1.96	0.47
1:E:128:ASP:OD2	1:E:130:ARG:HB2	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:331:ILE:CG2	3:G:536:HOH:O	2.55	0.47
1:A:237:ILE:HD11	1:A:339:GLU:HG3	1.96	0.47
1:C:200:TYR:C	1:C:200:TYR:CD1	2.88	0.47
1:A:216:LYS:O	1:A:217:ALA:HB3	2.14	0.46
1:E:207:ILE:HG22	1:E:231:ALA:HB3	1.97	0.46
1:F:237:ILE:N	1:F:237:ILE:HD12	2.29	0.46
1:G:154:GLY:HA3	1:G:290:LEU:HD22	1.97	0.46
1:B:234:SER:C	1:B:235:ARG:HG2	2.33	0.46
1:C:175:LEU:HD13	1:C:197:ALA:HB1	1.96	0.46
1:E:328:HIS:O	1:E:329:CYS:HB2	2.16	0.46
1:F:278:ASP:OD2	1:F:280:SER:HB2	2.14	0.46
1:C:340:ILE:OXT	3:C:559:HOH:O	2.20	0.46
1:G:271:TYR:CD1	1:G:319:ILE:HG13	2.49	0.46
1:A:285:VAL:HG21	1:A:334:TYR:HD1	1.80	0.46
2:F:401:2EW:H13	2:F:401:2EW:H1	1.66	0.46
1:E:289[B]:VAL:CG2	1:E:305:VAL:CG1	2.90	0.46
1:G:272:LYS:HB2	1:G:272:LYS:HE2	1.57	0.46
1:E:127:VAL:O	1:E:293:GLY:HA3	2.16	0.46
1:F:196:GLU:O	1:F:199:GLN:HB3	2.16	0.46
1:D:147:CYS:HB2	1:D:288:GLY:O	2.15	0.46
1:E:239:LEU:HB3	1:E:240:PRO:HD2	1.97	0.46
1:G:303:TRP:CE2	1:G:323:ARG:HG3	2.50	0.46
1:F:173:GLN:HB2	1:F:215:TYR:HA	1.96	0.46
1:F:216:LYS:O	1:F:218:MET:HG3	2.17	0.46
1:H:319:ILE:HD13	1:H:319:ILE:HG21	1.74	0.46
1:C:237:ILE:HD12	1:C:237:ILE:N	2.31	0.46
1:D:278:ASP:HA	1:D:279:PRO:HD2	1.87	0.46
1:H:309:TRP:O	3:H:546:HOH:O	2.21	0.46
1:B:319:ILE:N	3:B:513:HOH:O	2.49	0.45
1:G:297:LEU:O	1:G:300:LYS:HE3	2.16	0.45
1:C:160:LEU:HD23	3:C:504:HOH:O	2.16	0.45
1:H:328:HIS:CE1	1:H:329:CYS:SG	3.09	0.45
1:H:202:ILE:HA	1:H:233:CYS:O	2.17	0.45
1:D:237:ILE:O	1:D:336[A]:SER:HA	2.16	0.45
1:A:248:LYS:HE3	1:A:294:TYR:CE2	2.52	0.45
1:D:254:LYS:HD3	1:D:254:LYS:HA	1.84	0.45
1:C:211:ALA:HB1	1:E:340:ILE:HG21	1.99	0.45
1:E:155:ALA:HB1	1:E:338:PRO:HD3	1.97	0.45
1:A:235:ARG:NH1	1:A:235:ARG:HB2	2.32	0.45
1:A:265:HIS:O	1:A:269[A]:PHE:CD2	2.70	0.45
1:F:282:THR:CG2	3:F:579:HOH:O	2.64	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:237:ILE:HD13	1:E:337:TYR:HE2	1.79	0.45
1:A:290:LEU:HD22	3:A:618:HOH:O	2.16	0.45
1:D:196:GLU:OE2	1:D:196:GLU:HA	2.16	0.45
1:F:322:ALA:HB1	1:F:325:ASN:HD22	1.81	0.45
1:D:237:ILE:HD13	1:D:337:TYR:CE2	2.52	0.45
1:C:278:ASP:HA	1:C:279:PRO:HD2	1.56	0.45
1:B:237:ILE:CD1	1:B:339:GLU:CG	2.86	0.44
1:F:249:GLU:OE1	1:F:253:THR:HG21	2.17	0.44
1:E:170:LEU:HA	1:E:170:LEU:HD23	1.81	0.44
1:A:285:VAL:HG21	1:A:334:TYR:CD1	2.52	0.44
1:C:136:THR:HG21	1:C:169:SER:HA	1.99	0.44
1:E:289[B]:VAL:HG11	1:E:305:VAL:HG11	1.99	0.44
1:G:193:TYR:OH	2:G:401:2EW:H12	2.17	0.44
1:C:229:ARG:NH2	1:F:199:GLN:OE1	2.50	0.44
1:F:170:LEU:HD23	1:F:170:LEU:HA	1.60	0.44
1:H:332:ALA:HA	1:H:335:CYS:SG	2.57	0.44
1:B:235:ARG:NH1	1:B:235:ARG:HG3	2.33	0.44
1:C:272:LYS:CD	1:D:240:PRO:HB3	2.47	0.44
1:B:319:ILE:C	3:B:513:HOH:O	2.55	0.44
1:E:167:LEU:N	3:E:516:HOH:O	2.45	0.44
1:D:266:SER:HA	1:D:269[A]:PHE:CD1	2.52	0.44
1:E:171:SER:OG	1:E:174:ASN:HB2	2.17	0.44
1:G:235:ARG:HB2	3:G:533:HOH:O	2.18	0.44
1:F:297:LEU:HD13	3:F:541:HOH:O	2.17	0.44
1:F:122:THR:HB	1:F:123:LEU:H	1.43	0.44
1:E:241:PHE:CD1	1:E:241:PHE:C	2.90	0.44
1:E:195:THR:CG2	3:E:520:HOH:O	2.62	0.44
1:E:159:GLN:HG3	1:E:338:PRO:O	2.18	0.43
1:A:235:ARG:HD3	1:A:339:GLU:OE1	2.17	0.43
1:A:148:TRP:O	1:A:194:MET:HG3	2.18	0.43
1:G:123:LEU:HA	1:G:124:PRO:HD2	1.76	0.43
1:H:289:VAL:HG21	1:H:305:VAL:HG11	2.00	0.43
1:H:195:THR:HG21	1:H:238:GLN:OE1	2.18	0.43
1:D:332:ALA:HA	1:D:335:CYS:SG	2.59	0.43
1:F:202:ILE:CD1	3:F:530:HOH:O	2.66	0.43
1:A:235:ARG:CB	1:A:235:ARG:NH1	2.81	0.43
1:C:271:TYR:O	1:C:314:GLY:HA2	2.17	0.43
1:E:289[B]:VAL:CG2	1:E:290:LEU:N	2.71	0.43
1:H:278:ASP:HA	1:H:279:PRO:HD2	1.71	0.43
1:F:129:TRP:O	1:F:134[B]:CYS:HB2	2.18	0.43
1:G:320:ARG:HH11	1:G:320:ARG:HG3	1.83	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:147:CYS:HB3	1:A:287:HIS:CE1	2.54	0.43
1:B:239:LEU:HB2	1:B:335:CYS:HB2	2.01	0.43
1:H:216:LYS:HD2	1:H:216:LYS:HA	1.63	0.43
1:E:305:VAL:HB	1:E:319:ILE:HG23	2.01	0.43
1:H:129:TRP:CZ3	1:H:162:LEU:HD21	2.54	0.43
1:D:174:ASN:HD22	1:D:174:ASN:C	2.19	0.43
1:B:161:LYS:NZ	1:B:165:GLY:O	2.50	0.42
1:D:309:TRP:HE3	1:D:313:PHE:CD2	2.37	0.42
1:E:127:VAL:HG21	1:E:252:ALA:HA	2.01	0.42
1:E:178:CYS:HB3	1:E:200:TYR:OH	2.19	0.42
1:A:278:ASP:HA	1:A:279:PRO:HD3	1.81	0.42
1:A:183:LYS:HG2	1:A:184:TYR:CE1	2.54	0.42
1:F:269:PHE:N	1:F:269:PHE:CD1	2.88	0.42
1:E:127:VAL:HG12	1:E:128:ASP:N	2.33	0.42
1:E:312:ASN:ND2	3:E:565:HOH:O	2.35	0.42
1:A:235:ARG:HH11	1:A:235:ARG:HB3	1.85	0.42
1:H:195:THR:CG2	1:H:238:GLN:OE1	2.67	0.42
1:B:332:ALA:HA	1:B:335:CYS:SG	2.60	0.42
1:H:271:TYR:O	1:H:314:GLY:HA2	2.20	0.42
1:E:269:PHE:CD1	1:G:269:PHE:HE2	2.37	0.42
1:G:193:TYR:CE2	2:G:401:2EW:H4	2.55	0.42
1:E:229:ARG:HD2	1:E:232:THR:HG23	2.02	0.42
1:B:321:MET:CG	3:B:599:HOH:O	2.58	0.42
1:E:216:LYS:O	1:E:217:ALA:HB3	2.20	0.42
1:F:151:SER:HB3	1:F:194:MET:HG2	2.02	0.42
1:F:149:ALA:O	1:F:153:VAL:HG22	2.20	0.42
1:A:265:HIS:HD2	3:A:527:HOH:O	2.02	0.42
1:F:184:TYR:CE2	1:F:199:GLN:HG2	2.55	0.41
1:A:239:LEU:HD12	1:A:335:CYS:CB	2.50	0.41
1:F:247:LEU:O	1:F:251:VAL:HG23	2.20	0.41
1:E:237:ILE:O	1:E:336:SER:HA	2.19	0.41
1:B:146:ALA:O	1:B:147:CYS:C	2.57	0.41
1:E:153[B]:VAL:CG2	1:E:170:LEU:CB	2.93	0.41
1:B:134:CYS:SG	1:B:162:LEU:HD23	2.58	0.41
1:C:189:CYS:SG	1:C:218:MET:HA	2.61	0.41
1:H:150:PHE:HA	1:H:153:VAL:HG22	2.02	0.41
1:H:168:ILE:O	1:H:168:ILE:HG23	2.21	0.41
1:C:247:LEU:O	1:C:251:VAL:HG23	2.20	0.41
1:D:130:ARG:HD3	1:D:318:TYR:CZ	2.56	0.41
1:B:197:ALA:O	1:B:201:ILE:HG13	2.20	0.41
1:F:129:TRP:CZ2	1:F:255:GLY:HA2	2.55	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:277:ASP:HA	1:F:328:HIS:CE1	2.54	0.41
1:E:173:GLN:HB2	1:E:215:TYR:HA	2.03	0.41
1:C:194:MET:HG2	1:C:258:SER:HB3	2.02	0.41
1:D:202:ILE:HG22	3:D:533:HOH:O	2.21	0.41
1:B:316:GLN:CD	1:D:193:TYR:OH	2.59	0.41
1:D:307:ASN:ND2	1:D:309:TRP:CE3	2.89	0.41
1:E:193:TYR:CZ	2:E:401:2EW:H12	2.56	0.41
1:F:272:LYS:HA	1:F:272:LYS:HD2	1.93	0.41
1:B:239:LEU:O	1:B:240:PRO:C	2.58	0.41
1:H:171:SER:OG	1:H:174:ASN:HB2	2.21	0.41
1:B:134:CYS:HA	1:B:161:LYS:HG2	2.02	0.41
1:C:184:TYR:O	1:C:196:GLU:HG3	2.21	0.41
1:G:168:ILE:O	1:G:168:ILE:HG23	2.19	0.41
1:B:137:GLU:HG3	1:D:284:ASN:ND2	2.19	0.40
1:G:237:ILE:O	1:G:336:SER:HA	2.22	0.40
1:E:201:ILE:O	1:E:201:ILE:HG22	2.21	0.40
1:D:247:LEU:HD23	1:D:303:TRP:CZ2	2.56	0.40
1:E:237:ILE:CD1	1:E:339:GLU:HG2	2.51	0.40
1:E:130:ARG:NH2	3:E:568:HOH:O	2.53	0.40
1:E:194:MET:HG2	1:E:258:SER:HB3	2.02	0.40
1:H:149:ALA:O	1:H:153:VAL:HG22	2.21	0.40
1:H:138:VAL:HB	1:H:311:LEU:HD23	2.04	0.40
1:E:290:LEU:HA	1:E:290:LEU:HD12	2.00	0.40
1:B:129:TRP:CZ2	1:B:255:GLY:HA2	2.55	0.40
1:D:310:GLY:HA2	3:D:571:HOH:O	2.21	0.40
1:G:177:ASP:HB3	1:G:222:CYS:HA	2.02	0.40

All (1) 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:H:312:ASN:OD1	3:G:534:HOH:O[1_655]	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	218/225 (97%)	207 (95%)	11 (5%)	0	100	100
1	B	218/225 (97%)	207 (95%)	11 (5%)	0	100	100
1	C	218/225 (97%)	203 (93%)	13 (6%)	2 (1%)	21	4
1	D	218/225 (97%)	206 (94%)	12 (6%)	0	100	100
1	E	219/225 (97%)	207 (94%)	10 (5%)	2 (1%)	21	4
1	F	218/225 (97%)	206 (94%)	12 (6%)	0	100	100
1	G	216/225 (96%)	207 (96%)	9 (4%)	0	100	100
1	H	216/225 (96%)	204 (94%)	12 (6%)	0	100	100
All	All	1741/1800 (97%)	1647 (95%)	90 (5%)	4 (0%)	52	24

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	181	GLU
1	E	286	ASN
1	C	329	CYS
1	E	145	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	177/182 (97%)	161 (91%)	16 (9%)	12	1
1	B	177/182 (97%)	167 (94%)	10 (6%)	26	3
1	C	177/182 (97%)	169 (96%)	8 (4%)	34	5
1	D	177/182 (97%)	168 (95%)	9 (5%)	29	4
1	E	178/182 (98%)	172 (97%)	6 (3%)	44	11
1	F	177/182 (97%)	166 (94%)	11 (6%)	23	2
1	G	175/182 (96%)	166 (95%)	9 (5%)	29	4

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	H	175/182 (96%)	167 (95%)	8 (5%)	33 5
All	All	1413/1456 (97%)	1336 (95%)	77 (5%)	27 4

All (77) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	132	LYS
1	A	168	ILE
1	A	174	ASN
1	A	181	GLU
1	A	183	LYS
1	A	213	TYR
1	A	218	MET
1	A	227	LYS
1	A	235	ARG
1	A	256	PRO
1	A	269[A]	PHE
1	A	269[B]	PHE
1	A	272	LYS
1	A	281	CYS
1	A	312	ASN
1	A	326	LYS
1	B	147	CYS
1	B	166	LYS
1	B	174	ASN
1	B	213	TYR
1	B	235	ARG
1	B	245	ASP
1	B	272	LYS
1	B	273	SER
1	B	281	CYS
1	B	326	LYS
1	C	166	LYS
1	C	174	ASN
1	C	200	TYR
1	C	213	TYR
1	C	229	ARG
1	C	280	SER
1	C	281	CYS
1	C	340	ILE
1	D	161	LYS
1	D	162	LEU

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Mol	Chain	Res	Type
1	D	163	LYS
1	D	174	ASN
1	D	213	TYR
1	D	280	SER
1	D	281	CYS
1	D	298	ASP
1	D	300	LYS
1	E	132	LYS
1	E	174	ASN
1	E	213	TYR
1	E	229	ARG
1	E	235	ARG
1	E	254	LYS
1	F	122	THR
1	F	163	LYS
1	F	174	ASN
1	F	181	GLU
1	F	213	TYR
1	F	225	ASN
1	F	227	LYS
1	F	281	CYS
1	F	297	LEU
1	F	300	LYS
1	F	340	ILE
1	G	168	ILE
1	G	174	ASN
1	G	180	ASN
1	G	213	TYR
1	G	221	LYS
1	G	227	LYS
1	G	249	GLU
1	G	281	CYS
1	G	300	LYS
1	H	123	LEU
1	H	174	ASN
1	H	181	GLU
1	H	183	LYS
1	H	213	TYR
1	H	218	MET
1	H	249	GLU
1	H	281	CYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (19) such

sidechains are listed below:

Mol	Chain	Res	Type
1	A	284	ASN
1	B	312	ASN
1	B	316	GLN
1	C	284	ASN
1	D	284	ASN
1	E	159	GLN
1	E	284	ASN
1	E	325	ASN
1	F	223	HIS
1	F	225	ASN
1	F	312	ASN
1	F	325	ASN
1	G	180	ASN
1	G	223	HIS
1	G	228	ASN
1	H	223	HIS
1	H	228	ASN
1	H	284	ASN
1	H	316	GLN

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 carbohydrates in this entry.

5.6 Ligand geometry [i](#)

8 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
2	2EW	A	401	1	29,30,30	1.26	2 (6%)	37,42,42	2.26	15 (40%)
2	2EW	B	401	1	29,30,30	1.77	7 (24%)	37,42,42	2.66	16 (43%)
2	2EW	C	401	1	29,30,30	1.58	6 (20%)	37,42,42	3.41	15 (40%)
2	2EW	D	401	1	29,30,30	1.68	8 (27%)	37,42,42	2.57	18 (48%)
2	2EW	E	401	1	29,30,30	1.58	4 (13%)	37,42,42	2.63	17 (45%)
2	2EW	F	401	1	29,30,30	1.31	3 (10%)	37,42,42	3.35	12 (32%)
2	2EW	G	401	1	29,30,30	1.91	6 (20%)	37,42,42	1.98	13 (35%)
2	2EW	H	401	1	29,30,30	1.51	3 (10%)	37,42,42	3.17	14 (37%)

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
2	2EW	A	401	1	-	0/27/48/48	0/3/3/3
2	2EW	B	401	1	-	0/27/48/48	0/3/3/3
2	2EW	C	401	1	-	0/27/48/48	0/3/3/3
2	2EW	D	401	1	-	0/27/48/48	0/3/3/3
2	2EW	E	401	1	-	0/27/48/48	0/3/3/3
2	2EW	F	401	1	-	0/27/48/48	0/3/3/3
2	2EW	G	401	1	-	0/27/48/48	0/3/3/3
2	2EW	H	401	1	-	0/27/48/48	0/3/3/3

All (39) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	G	401	2EW	O11-S1	-6.76	1.35	1.43
2	H	401	2EW	O11-S1	-5.21	1.37	1.43
2	G	401	2EW	O12-S1	-4.11	1.38	1.43
2	E	401	2EW	O12-S1	-3.95	1.38	1.43
2	G	401	2EW	C7-N2	-2.96	1.45	1.48
2	F	401	2EW	O12-S1	-2.56	1.40	1.43
2	D	401	2EW	C6-N2	-2.08	1.46	1.48
2	C	401	2EW	O12-S1	-2.02	1.41	1.43
2	B	401	2EW	C20-N8	2.09	1.50	1.47
2	D	401	2EW	O12-S1	2.10	1.46	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	G	401	2EW	C5-N8	2.12	1.38	1.34
2	B	401	2EW	C6-N2	2.16	1.50	1.48
2	D	401	2EW	O11-S1	2.17	1.46	1.43
2	D	401	2EW	C7-N2	2.22	1.50	1.48
2	E	401	2EW	C9-N17	2.23	1.38	1.33
2	B	401	2EW	C19-N8	2.24	1.50	1.47
2	D	401	2EW	O16-C9	2.27	1.27	1.23
2	C	401	2EW	S1-N2	2.33	1.66	1.63
2	F	401	2EW	C13-S1	2.38	1.80	1.76
2	F	401	2EW	C9-N17	2.41	1.38	1.33
2	A	401	2EW	C20-N8	2.41	1.51	1.47
2	H	401	2EW	S1-N2	2.47	1.67	1.63
2	D	401	2EW	S1-N2	2.59	1.67	1.63
2	B	401	2EW	C6-C3	2.62	1.56	1.53
2	G	401	2EW	C13-S1	2.68	1.80	1.76
2	G	401	2EW	C19-N8	2.70	1.51	1.47
2	C	401	2EW	C6-C3	2.71	1.57	1.53
2	E	401	2EW	O11-S1	2.81	1.47	1.43
2	C	401	2EW	C6-N2	3.13	1.51	1.48
2	B	401	2EW	S1-N2	3.26	1.68	1.63
2	B	401	2EW	O11-S1	3.30	1.47	1.43
2	H	401	2EW	C5-N8	3.38	1.39	1.34
2	C	401	2EW	C25-C13	3.61	1.44	1.38
2	D	401	2EW	C6-C3	3.72	1.58	1.53
2	C	401	2EW	C9-N17	3.73	1.41	1.33
2	D	401	2EW	C9-N17	4.14	1.42	1.33
2	A	401	2EW	C19-N8	4.16	1.54	1.47
2	E	401	2EW	S1-N2	4.88	1.70	1.63
2	B	401	2EW	O12-S1	5.04	1.50	1.43

All (120) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	F	401	2EW	C13-S1-N2	-11.25	93.45	107.32
2	C	401	2EW	O12-S1-N2	-9.94	96.87	106.69
2	C	401	2EW	O12-S1-C13	-9.34	95.87	108.00
2	H	401	2EW	O11-S1-C13	-8.63	96.80	108.00
2	H	401	2EW	O12-S1-N2	-8.46	98.33	106.69
2	B	401	2EW	O11-S1-N2	-6.69	100.08	106.69
2	D	401	2EW	O12-S1-N2	-6.53	100.24	106.69
2	A	401	2EW	O12-S1-N2	-6.49	100.28	106.69
2	E	401	2EW	C13-S1-N2	-6.24	99.63	107.32

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	401	2EW	C13-S1-N2	-5.96	99.97	107.32
2	E	401	2EW	O12-S1-N2	-5.95	100.81	106.69
2	F	401	2EW	C25-C13-S1	-5.31	113.93	119.79
2	D	401	2EW	C28-C27-C24	-5.08	112.75	120.19
2	B	401	2EW	C7-N2-S1	-5.06	112.57	119.62
2	F	401	2EW	O12-S1-C13	-4.96	101.56	108.00
2	C	401	2EW	O18-C22-C20	-4.93	100.54	111.84
2	C	401	2EW	C13-S1-N2	-4.72	101.50	107.32
2	C	401	2EW	O15-C5-N8	-4.58	115.94	121.66
2	G	401	2EW	O11-S1-C13	-4.32	102.40	108.00
2	E	401	2EW	C7-N2-S1	-4.30	113.64	119.62
2	F	401	2EW	C7-N2-S1	-4.17	113.81	119.62
2	B	401	2EW	O16-C9-C4	-4.10	116.86	121.56
2	H	401	2EW	C13-S1-N2	-4.04	102.33	107.32
2	D	401	2EW	C7-N2-S1	-3.89	114.21	119.62
2	D	401	2EW	C26-C25-C13	-3.68	114.96	118.95
2	D	401	2EW	C13-S1-N2	-3.59	102.89	107.32
2	H	401	2EW	O15-C5-N8	-3.43	117.38	121.66
2	A	401	2EW	C24-C13-S1	-3.42	116.01	119.79
2	A	401	2EW	O15-C5-C3	-3.33	115.77	121.92
2	G	401	2EW	C6-N2-S1	-3.30	115.03	119.62
2	E	401	2EW	C23-C19-N8	-3.27	102.88	109.90
2	B	401	2EW	C23-C19-N8	-3.19	103.05	109.90
2	B	401	2EW	C6-N2-S1	-3.04	115.39	119.62
2	G	401	2EW	O15-C5-N8	-3.03	117.88	121.66
2	G	401	2EW	O12-S1-C13	-3.00	104.11	108.00
2	B	401	2EW	C7-C4-C3	-2.96	98.72	103.43
2	H	401	2EW	O18-C22-C20	-2.89	105.21	111.84
2	E	401	2EW	O16-C9-C4	-2.86	118.27	121.56
2	D	401	2EW	C7-C4-C3	-2.81	98.96	103.43
2	H	401	2EW	C28-C27-C24	-2.68	116.26	120.19
2	D	401	2EW	O15-C5-C3	-2.68	116.97	121.92
2	A	401	2EW	C23-C19-N8	-2.62	104.30	109.90
2	A	401	2EW	C13-S1-N2	-2.60	104.11	107.32
2	C	401	2EW	O18-C23-C19	-2.54	106.01	111.84
2	D	401	2EW	C25-C13-S1	-2.52	117.01	119.79
2	G	401	2EW	C13-S1-N2	-2.48	104.26	107.32
2	F	401	2EW	O18-C22-C20	-2.48	106.16	111.84
2	E	401	2EW	C26-C25-C13	-2.39	116.36	118.95
2	B	401	2EW	C27-C28-C26	-2.38	115.75	119.93
2	G	401	2EW	C21-N17-C9	-2.32	115.91	123.00
2	A	401	2EW	O11-S1-N2	-2.27	104.45	106.69

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	401	2EW	C25-C13-S1	-2.26	117.30	119.79
2	G	401	2EW	C7-N2-S1	-2.25	116.50	119.62
2	C	401	2EW	C4-C7-N2	-2.22	99.49	102.98
2	F	401	2EW	C22-C20-N8	-2.19	105.21	109.90
2	B	401	2EW	C20-N8-C5	-2.19	115.17	123.19
2	C	401	2EW	C28-C26-C25	-2.14	117.05	120.19
2	A	401	2EW	C7-C4-C3	-2.14	100.03	103.43
2	A	401	2EW	C6-N2-S1	-2.12	116.68	119.62
2	G	401	2EW	C4-C3-C5	-2.07	106.67	111.37
2	G	401	2EW	C28-C27-C24	-2.07	117.16	120.19
2	D	401	2EW	O16-C9-C4	-2.06	119.19	121.56
2	B	401	2EW	O15-C5-C3	-2.05	118.14	121.92
2	E	401	2EW	O18-C22-C20	-2.01	107.24	111.84
2	D	401	2EW	O11-S1-N2	2.02	108.69	106.69
2	E	401	2EW	C22-O18-C23	2.14	117.10	109.89
2	H	401	2EW	C27-C24-C13	2.17	121.31	118.95
2	D	401	2EW	C24-C13-C25	2.20	123.36	120.42
2	C	401	2EW	C22-O18-C23	2.30	117.62	109.89
2	F	401	2EW	C4-C3-C5	2.31	116.64	111.37
2	C	401	2EW	O11-S1-C13	2.36	111.07	108.00
2	F	401	2EW	O11-S1-O12	2.36	123.54	119.47
2	B	401	2EW	O15-C5-N8	2.37	124.62	121.66
2	E	401	2EW	C27-C24-C13	2.38	121.53	118.95
2	B	401	2EW	C27-C24-C13	2.44	121.59	118.95
2	H	401	2EW	O12-S1-C13	2.47	111.21	108.00
2	A	401	2EW	C24-C13-C25	2.50	123.77	120.42
2	A	401	2EW	C27-C28-C26	2.52	124.35	119.93
2	A	401	2EW	O12-S1-C13	2.54	111.30	108.00
2	E	401	2EW	C22-C20-N8	2.60	115.48	109.90
2	C	401	2EW	C24-C13-C25	2.61	123.90	120.42
2	A	401	2EW	C22-O18-C23	2.62	118.72	109.89
2	H	401	2EW	O18-C23-C19	2.71	118.04	111.84
2	D	401	2EW	C20-N8-C19	2.76	117.67	112.56
2	C	401	2EW	C27-C28-C26	2.78	124.81	119.93
2	B	401	2EW	O12-S1-C13	2.78	111.62	108.00
2	E	401	2EW	C28-C26-C25	2.83	124.33	120.19
2	B	401	2EW	C4-C7-N2	2.84	107.45	102.98
2	D	401	2EW	C27-C28-C26	2.84	124.91	119.93
2	G	401	2EW	C27-C24-C13	2.85	122.03	118.95
2	D	401	2EW	C22-O18-C23	2.86	119.52	109.89
2	H	401	2EW	O11-S1-N2	2.86	109.52	106.69
2	E	401	2EW	O16-C9-N17	3.04	129.18	123.08

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	F	401	2EW	C3-C6-N2	3.05	107.78	102.98
2	D	401	2EW	C4-C7-N2	3.09	107.85	102.98
2	A	401	2EW	C3-C6-N2	3.21	108.03	102.98
2	G	401	2EW	O11-S1-O12	3.35	125.24	119.47
2	G	401	2EW	O12-S1-N2	3.35	110.00	106.69
2	E	401	2EW	C21-N17-C9	3.36	133.26	123.00
2	H	401	2EW	C20-N8-C19	3.41	118.88	112.56
2	E	401	2EW	C20-N8-C19	3.42	118.90	112.56
2	D	401	2EW	C3-C6-N2	3.44	108.40	102.98
2	C	401	2EW	O11-S1-N2	3.49	110.14	106.69
2	E	401	2EW	C3-C6-N2	3.64	108.70	102.98
2	G	401	2EW	C20-N8-C19	3.69	119.41	112.56
2	H	401	2EW	C4-C3-C5	3.73	119.87	111.37
2	A	401	2EW	C20-N8-C19	3.81	119.63	112.56
2	E	401	2EW	O12-S1-C13	3.90	113.07	108.00
2	D	401	2EW	C27-C24-C13	3.92	123.19	118.95
2	E	401	2EW	O11-S1-N2	4.23	110.87	106.69
2	F	401	2EW	C20-N8-C19	4.36	120.65	112.56
2	H	401	2EW	C22-O18-C23	4.43	124.79	109.89
2	A	401	2EW	O11-S1-O12	4.53	127.29	119.47
2	B	401	2EW	O12-S1-N2	4.68	111.31	106.69
2	D	401	2EW	O11-S1-O12	4.83	127.80	119.47
2	B	401	2EW	C20-N8-C19	4.88	121.61	112.56
2	F	401	2EW	C24-C13-S1	6.99	127.50	119.79
2	H	401	2EW	O11-S1-O12	9.02	135.02	119.47
2	F	401	2EW	O11-S1-N2	9.58	116.16	106.69
2	C	401	2EW	O11-S1-O12	9.65	136.11	119.47

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

4 monomers are involved in 7 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	E	401	2EW	1	0
2	F	401	2EW	1	0
2	G	401	2EW	4	0
2	H	401	2EW	1	0

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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	218/225 (96%)	0.61	5 (2%) 64 67	9, 15, 22, 31	15 (6%)
1	B	219/225 (97%)	0.85	20 (9%) 11 11	9, 16, 25, 38	16 (7%)
1	C	218/225 (96%)	0.61	9 (4%) 41 43	8, 15, 23, 35	15 (6%)
1	D	218/225 (96%)	0.69	12 (5%) 29 30	9, 17, 27, 38	15 (6%)
1	E	218/225 (96%)	1.00	25 (11%) 6 6	9, 18, 27, 32	15 (6%)
1	F	219/225 (97%)	0.63	7 (3%) 51 53	9, 15, 22, 30	16 (7%)
1	G	218/225 (96%)	0.50	7 (3%) 51 53	8, 15, 21, 30	15 (6%)
1	H	218/225 (96%)	0.73	11 (5%) 32 34	10, 17, 27, 33	15 (6%)
All	All	1746/1800 (97%)	0.70	96 (5%) 29 30	8, 16, 25, 38	122 (6%)

All (96) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	269[A]	PHE	5.1
1	D	123	LEU	5.0
1	B	162	LEU	4.8
1	F	122	THR	4.7
1	B	297	LEU	4.7
1	E	337	TYR	4.6
1	F	340	ILE	4.6
1	E	237	ILE	4.5
1	G	123	LEU	4.5
1	G	269	PHE	4.1
1	D	309	TRP	4.0
1	B	242	GLY	3.9
1	E	202	ILE	3.7
1	B	269	PHE	3.7
1	C	182	GLU	3.6
1	E	233[A]	CYS	3.4

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Mol	Chain	Res	Type	RSRZ
1	E	135	VAL	3.3
1	E	241	PHE	3.3
1	H	123	LEU	3.3
1	A	270	PHE	3.3
1	B	122	THR	3.3
1	E	162	LEU	3.2
1	H	269	PHE	3.1
1	H	163	LYS	3.1
1	E	168	ILE	3.1
1	B	270	PHE	3.1
1	B	160	LEU	3.0
1	C	162	LEU	3.0
1	D	269[A]	PHE	2.9
1	E	294	TYR	2.9
1	G	124	PRO	2.9
1	H	182	GLU	2.9
1	H	202	ILE	2.9
1	G	125	ASP	2.8
1	C	297	LEU	2.8
1	B	294	TYR	2.8
1	D	298	ASP	2.7
1	E	126	THR	2.7
1	E	200	TYR	2.7
1	F	168	ILE	2.7
1	G	270	PHE	2.7
1	B	300	LYS	2.7
1	E	160	LEU	2.7
1	H	270	PHE	2.7
1	B	325	ASN	2.6
1	F	270	PHE	2.6
1	E	236	TYR	2.6
1	D	211	ALA	2.6
1	E	319	ILE	2.5
1	E	333	SER	2.5
1	D	182	GLU	2.5
1	B	166	LYS	2.5
1	E	297	LEU	2.5
1	D	218	MET	2.5
1	C	270	PHE	2.5
1	B	304	LEU	2.5
1	E	253	THR	2.5
1	E	235	ARG	2.5

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Mol	Chain	Res	Type	RSRZ
1	F	134[A]	CYS	2.5
1	C	200	TYR	2.4
1	H	198	PHE	2.4
1	C	269	PHE	2.4
1	C	222	CYS	2.4
1	B	237	ILE	2.4
1	D	185	GLY	2.3
1	E	221	LYS	2.3
1	A	297	LEU	2.3
1	B	340	ILE	2.3
1	H	164	THR	2.3
1	B	218	MET	2.2
1	B	134	CYS	2.2
1	A	168	ILE	2.2
1	C	340	ILE	2.2
1	C	179	SER	2.2
1	E	270	PHE	2.2
1	G	162	LEU	2.2
1	E	249	GLU	2.1
1	E	268	PHE	2.1
1	D	200	TYR	2.1
1	B	298	ASP	2.1
1	D	125	ASP	2.1
1	E	300	LYS	2.1
1	F	299	GLY	2.1
1	H	125	ASP	2.1
1	G	313	PHE	2.1
1	H	184	TYR	2.1
1	E	182	GLU	2.1
1	D	221	LYS	2.1
1	F	253	THR	2.1
1	H	226	SER	2.1
1	A	167	LEU	2.1
1	E	153[A]	VAL	2.0
1	B	164	THR	2.0
1	B	253	THR	2.0
1	D	340	ILE	2.0
1	B	272	LYS	2.0

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

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

6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 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	LLDF	B-factors(\AA^2)	Q<0.9
2	2EW	A	401	28/28	0.89	0.12	1.17	12,18,21,22	0
2	2EW	F	401	28/28	0.90	0.12	0.60	13,20,24,26	0
2	2EW	G	401	28/28	0.91	0.11	0.36	11,17,23,24	0
2	2EW	B	401	28/28	0.90	0.12	0.35	12,17,23,26	0
2	2EW	E	401	28/28	0.91	0.12	0.27	12,21,26,27	0
2	2EW	H	401	28/28	0.90	0.12	0.24	15,19,23,25	0
2	2EW	D	401	28/28	0.90	0.11	-0.28	9,17,24,26	0
2	2EW	C	401	28/28	0.94	0.10	-0.51	11,15,20,23	0

6.5 Other polymers [i](#)

There are no such residues in this entry.