



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 12:09 PM UTC

PDB ID : 3GLS / pdb_00003gls
Title : Crystal Structure of Human SIRT3
Authors : Jin, L.; Wei, W.; Jiang, Y.; Peng, H.; Cai, J.; Mao, C.; Dai, H.; Bemis, J.E.;
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Deposited on : 2009-03-12
Resolution : 2.70 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

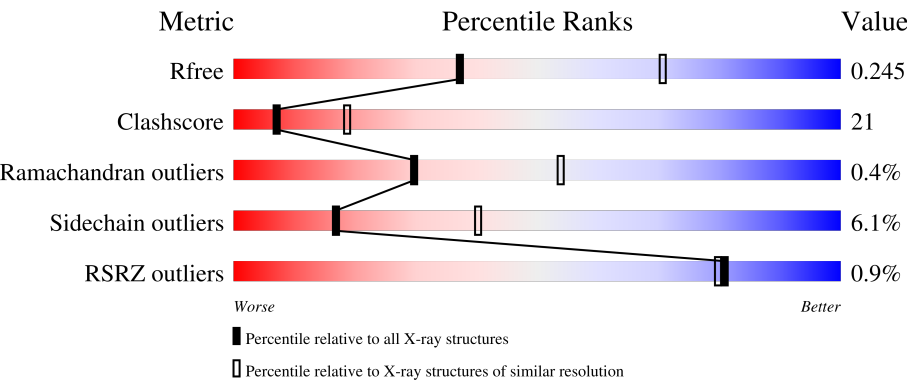
MolProbity : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry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

1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.70 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	3538 (2.70-2.70)
Clashscore	190562	3843 (2.70-2.70)
Ramachandran outliers	187476	3778 (2.70-2.70)
Sidechain outliers	187428	3778 (2.70-2.70)
RSRZ outliers	180081	3538 (2.70-2.70)

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	285	% 63%30% . .
1	B	285	% 59%32% . . 5%
1	C	285	% 58%34% . .
1	D	285	% 52%39% 5% .
1	E	285	59%35% . .

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Mol	Chain	Length	Quality of chain
1	F	285	% 62% 29% • 5%

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 12998 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 NAD-dependent deacetylase sirtuin-3, mitochondrial.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	273	Total	C	N	O	S	4	0	0
			2144	1382	369	384	9			
1	B	272	Total	C	N	O	S	3	0	0
			2135	1376	367	383	9			
1	C	273	Total	C	N	O	S	4	0	0
			2144	1382	369	384	9			
1	D	274	Total	C	N	O	S	4	0	0
			2148	1384	370	385	9			
1	E	274	Total	C	N	O	S	5	0	0
			2148	1384	370	385	9			
1	F	272	Total	C	N	O	S	3	0	0
			2135	1376	367	383	9			

There are 18 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	115	SER	-	expression tag	UNP Q9NTG7
A	116	ASN	-	expression tag	UNP Q9NTG7
A	117	ALA	-	expression tag	UNP Q9NTG7
B	115	SER	-	expression tag	UNP Q9NTG7
B	116	ASN	-	expression tag	UNP Q9NTG7
B	117	ALA	-	expression tag	UNP Q9NTG7
C	115	SER	-	expression tag	UNP Q9NTG7
C	116	ASN	-	expression tag	UNP Q9NTG7
C	117	ALA	-	expression tag	UNP Q9NTG7
D	115	SER	-	expression tag	UNP Q9NTG7
D	116	ASN	-	expression tag	UNP Q9NTG7
D	117	ALA	-	expression tag	UNP Q9NTG7
E	115	SER	-	expression tag	UNP Q9NTG7
E	116	ASN	-	expression tag	UNP Q9NTG7
E	117	ALA	-	expression tag	UNP Q9NTG7
F	115	SER	-	expression tag	UNP Q9NTG7
F	116	ASN	-	expression tag	UNP Q9NTG7

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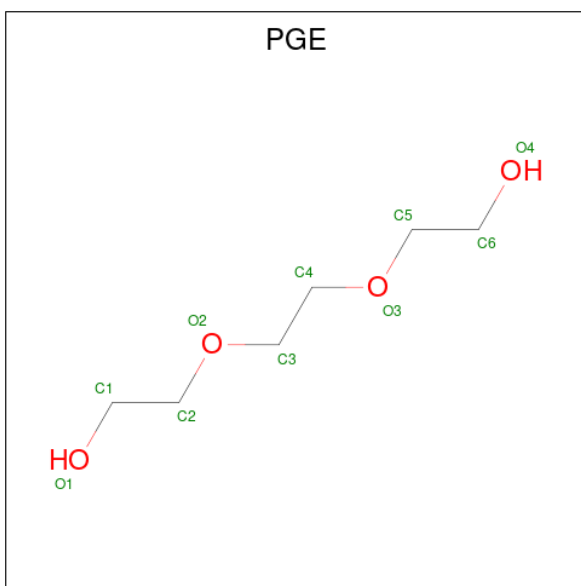
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Chain	Residue	Modelled	Actual	Comment	Reference
F	117	ALA	-	expression tag	UNP Q9NTG7

- Molecule 2 is ZINC ION (CCD ID: ZN) (formula: Zn).

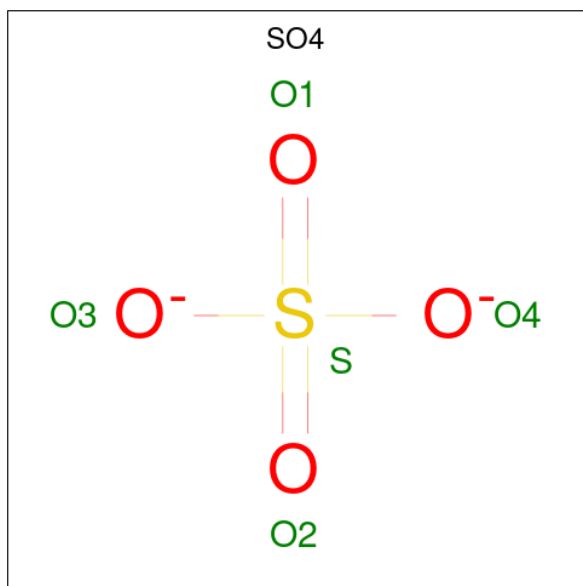
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	1	Total	Zn	0	0
			1	1		
2	B	1	Total	Zn	0	0
			1	1		
2	C	1	Total	Zn	0	0
			1	1		
2	D	1	Total	Zn	0	0
			1	1		
2	E	1	Total	Zn	0	0
			1	1		
2	F	1	Total	Zn	0	0
			1	1		

- Molecule 3 is TRIETHYLENE GLYCOL (CCD ID: PGE) (formula: C₆H₁₄O₄).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			7	4	3		
3	F	1	Total	C	O	0	0
			7	4	3		

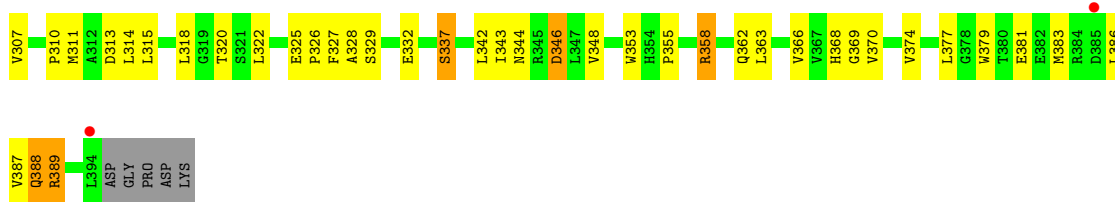
- Molecule 4 is SULFATE ION (CCD ID: SO4) (formula: O₄S).



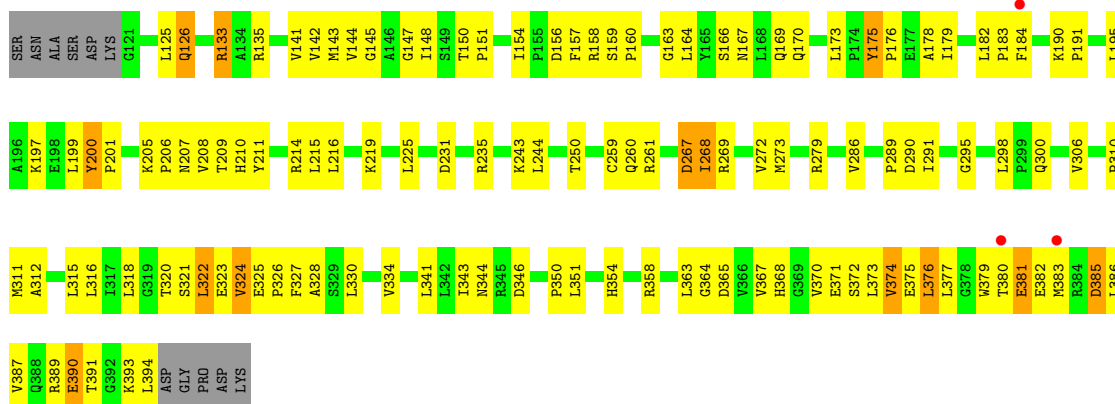
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	E	1	Total	O	S	0	0
			5	4	1		

- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	16	Total	O	0	0
			16	16		
5	B	17	Total	O	0	0
			17	17		
5	C	22	Total	O	0	0
			22	22		
5	D	19	Total	O	0	0
			19	19		
5	E	19	Total	O	0	0
			19	19		
5	F	26	Total	O	0	0
			26	26		



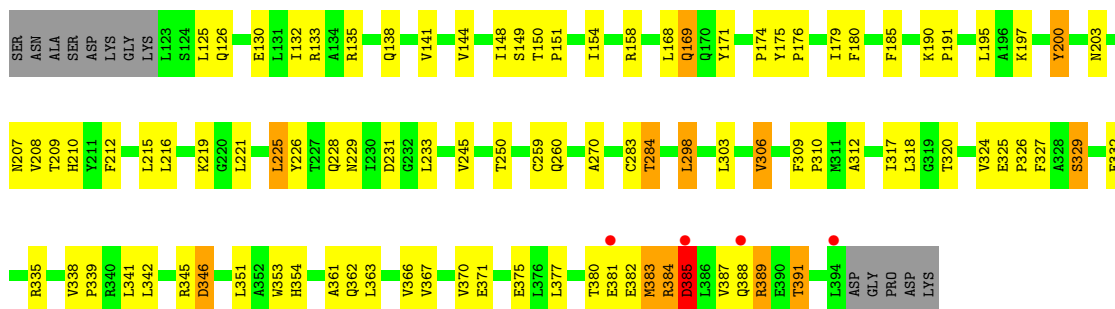
- Molecule 1: NAD-dependent deacetylase sirtuin-3, mitochondrial



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4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	85.37Å 143.94Å 91.66Å 90.00° 117.10° 90.00°	Depositor
Resolution (Å)	65.00 – 2.70 65.00 – 2.70	Depositor EDS
% Data completeness (in resolution range)	84.7 (65.00-2.70) 84.7 (65.00-2.70)	Depositor EDS
R_{merge}	0.12	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.69 (at 2.69Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.182 , 0.244 0.183 , 0.245	Depositor DCC
R_{free} test set	2313 reflections (5.05%)	wwPDB-VP
Wilson B-factor (Å ²)	32.1	Xtriage
Anisotropy	0.242	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 41.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	0.026 for h,-k,-h-l	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	12998	wwPDB-VP
Average B, all atoms (Å ²)	27.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.68% 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: ZN, SO4, PGE

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	1.01	1/2199 (0.0%)	1.06	10/2996 (0.3%)
1	B	1.01	2/2190 (0.1%)	1.05	5/2985 (0.2%)
1	C	1.03	3/2199 (0.1%)	1.01	3/2996 (0.1%)
1	D	0.93	3/2203 (0.1%)	1.01	3/3001 (0.1%)
1	E	0.99	2/2203 (0.1%)	1.04	6/3001 (0.2%)
1	F	1.01	2/2190 (0.1%)	1.10	7/2985 (0.2%)
All	All	1.00	13/13184 (0.1%)	1.05	34/17964 (0.2%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	C	0	2
1	D	0	1
All	All	0	3

All (13) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	F	385	ASP	CG-OD1	14.67	1.53	1.25
1	C	235	ARG	CZ-NH2	-11.60	1.18	1.33
1	B	126	GLN	CD-NE2	10.02	1.54	1.33
1	B	126	GLN	CD-OE1	-9.48	1.05	1.23
1	E	332	GLU	CD-OE2	9.11	1.42	1.25
1	C	332	GLU	CD-OE2	9.05	1.42	1.25
1	C	332	GLU	CG-CD	-7.45	1.33	1.52
1	D	126	GLN	CD-NE2	7.39	1.48	1.33
1	D	385	ASP	CB-CG	7.20	1.70	1.52
1	E	235	ARG	CZ-NH2	-6.32	1.25	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	235	ARG	CD-NE	-5.74	1.38	1.46
1	F	361	ALA	CA-CB	-5.71	1.45	1.53
1	D	385	ASP	CG-OD1	-5.58	1.14	1.25

All (34) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	385	ASP	CA-CB-CG	-12.21	100.39	112.60
1	F	126	GLN	OE1-CD-NE2	9.37	131.97	122.60
1	F	200	TYR	CA-C-N	8.91	128.99	119.90
1	F	200	TYR	C-N-CA	8.91	128.99	119.90
1	C	235	ARG	NE-CZ-NH2	8.71	127.04	119.20
1	A	239	ILE	CA-C-N	8.42	128.18	119.76
1	A	239	ILE	C-N-CA	8.42	128.18	119.76
1	C	332	GLU	CB-CG-CD	7.43	125.23	112.60
1	A	235	ARG	CD-NE-CZ	7.27	134.57	124.40
1	E	296	GLU	CA-C-N	-7.25	112.45	120.14
1	E	296	GLU	C-N-CA	-7.25	112.45	120.14
1	A	349	GLY	CA-C-N	6.59	126.83	119.32
1	A	349	GLY	C-N-CA	6.59	126.83	119.32
1	F	324	VAL	N-CA-C	6.50	118.14	109.37
1	E	194	THR	N-CA-C	-6.40	104.22	111.07
1	A	268	ILE	N-CA-C	-6.37	106.53	112.83
1	E	391	THR	N-CA-C	-5.97	104.90	111.82
1	B	288	LYS	CA-C-N	5.83	127.13	119.84
1	B	288	LYS	C-N-CA	5.83	127.13	119.84
1	F	346	ASP	N-CA-C	5.70	116.80	108.14
1	A	374	VAL	CB-CA-C	-5.69	104.46	112.14
1	B	306	VAL	CB-CA-C	-5.66	104.63	112.04
1	A	235	ARG	NE-CZ-NH2	-5.63	114.13	119.20
1	F	298	LEU	CA-C-N	-5.35	114.25	119.76
1	F	298	LEU	C-N-CA	-5.35	114.25	119.76
1	E	235	ARG	NE-CZ-NH2	5.28	123.95	119.20
1	D	268	ILE	N-CA-C	-5.25	107.86	112.90
1	A	306	VAL	CB-CA-C	-5.18	104.48	112.05
1	E	244	LEU	N-CA-C	5.12	118.41	110.17
1	B	172	ASP	N-CA-CB	-5.11	103.08	110.70
1	A	295	GLY	N-CA-C	-5.10	108.94	115.42
1	D	163	GLY	N-CA-C	-5.10	106.61	112.73
1	B	332	GLU	CB-CG-CD	5.06	121.21	112.60
1	C	126	GLN	OE1-CD-NE2	-5.03	117.57	122.60

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	C	126	GLN	Sidechain
1	C	389	ARG	Peptide
1	D	380	THR	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	2144	0	2160	81	0
1	B	2135	0	2147	85	0
1	C	2144	0	2160	97	0
1	D	2148	0	2163	113	0
1	E	2148	0	2163	89	0
1	F	2135	0	2147	88	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
2	C	1	0	0	0	0
2	D	1	0	0	0	0
2	E	1	0	0	0	0
2	F	1	0	0	0	0
3	A	7	0	9	0	0
3	F	7	0	9	1	0
4	E	5	0	0	1	0
5	A	16	0	0	5	0
5	B	17	0	0	2	0
5	C	22	0	0	3	0
5	D	19	0	0	4	0
5	E	19	0	0	4	0
5	F	26	0	0	6	0
All	All	12998	0	12958	538	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 21.

All (538) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:135:ARG:NH2	4:E:400:SO4:O2	1.75	1.19
1:B:384:ARG:O	1:B:388:GLN:HG2	1.46	1.16
1:C:358:ARG:HG3	1:C:358:ARG:HH11	1.15	1.11
1:F:385:ASP:O	1:F:389:ARG:HG3	1.51	1.09
1:B:125:LEU:HD21	1:B:362:GLN:HG2	1.28	1.08
1:A:389:ARG:CG	1:A:389:ARG:HH11	1.66	1.08
1:F:389:ARG:HG2	1:F:389:ARG:HH11	0.93	1.07
1:B:212:PHE:HA	1:B:383:MET:HE1	1.35	1.04
1:F:389:ARG:HH11	1:F:389:ARG:CG	1.71	1.02
1:D:133:ARG:HG2	1:D:133:ARG:HH11	1.21	1.01
1:F:383:MET:O	1:F:387:VAL:HG23	1.62	1.00
1:D:164:LEU:HD21	1:D:195:LEU:HD12	1.47	0.97
1:A:389:ARG:HH11	1:A:389:ARG:HG2	1.25	0.97
1:B:125:LEU:CD2	1:B:362:GLN:HG2	1.95	0.96
1:A:207:ASN:H	1:A:210:HIS:HD2	1.00	0.95
1:C:346:ASP:HA	1:C:363:LEU:CD2	1.97	0.94
1:A:207:ASN:H	1:A:210:HIS:CD2	1.87	0.93
1:C:346:ASP:HA	1:C:363:LEU:HD22	1.50	0.92
1:C:303:LEU:O	1:C:306:VAL:HG23	1.71	0.91
1:E:325:GLU:OE1	1:E:326:PRO:HA	1.71	0.90
1:F:148:ILE:HB	1:F:209:THR:HG21	1.53	0.90
1:F:389:ARG:HG2	1:F:389:ARG:NH1	1.64	0.90
1:F:384:ARG:O	1:F:388:GLN:HG3	1.70	0.90
1:F:154:ILE:HD13	1:F:231:ASP:CB	2.04	0.87
1:B:212:PHE:CA	1:B:383:MET:HE1	2.02	0.87
1:C:358:ARG:HG3	1:C:358:ARG:NH1	1.87	0.86
1:D:259:CYS:SG	1:D:261:ARG:HD2	2.16	0.85
1:E:207:ASN:H	1:E:210:HIS:HD2	1.23	0.85
1:B:317:ILE:C	1:B:318:LEU:HD23	2.01	0.84
1:E:374:VAL:HG21	1:E:383:MET:HE2	1.59	0.83
1:C:175:TYR:HB2	1:C:176:PRO:HD2	1.59	0.83
1:F:283:CYS:C	1:F:284:THR:HG23	2.03	0.83
1:E:259:CYS:SG	1:E:261:ARG:HG3	2.18	0.83
1:D:133:ARG:HG2	1:D:133:ARG:NH1	1.93	0.82
1:A:228:GLN:NE2	1:A:327:PHE:CD2	2.48	0.81
1:B:279:ARG:NH1	1:C:311:MET:HE1	1.97	0.80
1:A:158:ARG:HD3	1:A:177:GLU:OE2	1.81	0.80
1:F:154:ILE:CD1	1:F:231:ASP:HB2	2.12	0.80
1:D:173:LEU:CD2	1:D:184:PHE:CZ	2.64	0.80
1:D:173:LEU:HD23	1:D:184:PHE:CZ	2.18	0.79
1:F:207:ASN:H	1:F:210:HIS:HD2	1.31	0.79
1:F:154:ILE:HD13	1:F:231:ASP:HB3	1.64	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:256:CYS:SG	1:A:280:CYS:HB2	2.24	0.78
1:D:173:LEU:HD22	1:D:178:ALA:HB3	1.66	0.77
1:E:172:ASP:HB3	5:E:57:HOH:O	1.84	0.77
1:A:167:ASN:O	1:A:170:GLN:HG2	1.84	0.77
1:E:123:LEU:HD22	1:E:127:ASP:HB2	1.64	0.77
1:F:353:TRP:CD1	1:F:354:HIS:CD2	2.73	0.77
1:D:391:THR:HA	1:D:394:LEU:HD12	1.67	0.76
1:A:389:ARG:CG	1:A:389:ARG:NH1	2.38	0.76
1:B:317:ILE:HD13	1:B:351:LEU:HD11	1.66	0.76
1:B:167:ASN:O	1:B:170:GLN:HG3	1.84	0.75
1:E:173:LEU:HD23	1:E:184:PHE:CZ	2.21	0.75
1:A:389:ARG:HH11	1:A:389:ARG:HG3	1.51	0.75
1:F:371:GLU:O	1:F:375:GLU:HG3	1.85	0.75
1:C:283:CYS:C	1:C:284:THR:HG23	2.11	0.75
1:C:346:ASP:CA	1:C:363:LEU:CD2	2.65	0.75
1:D:164:LEU:HD21	1:D:195:LEU:CD1	2.15	0.75
1:B:354:HIS:CD2	5:B:402:HOH:O	2.40	0.74
1:A:280:CYS:SG	1:A:281:PRO:HD2	2.27	0.74
1:A:205:LYS:HG3	1:A:394:LEU:HD13	1.70	0.74
1:A:389:ARG:HG2	1:A:389:ARG:NH1	2.00	0.74
1:D:214:ARG:HG2	1:D:214:ARG:HH21	1.52	0.74
1:A:228:GLN:NE2	1:A:327:PHE:CG	2.56	0.74
1:D:321:SER:O	1:D:322:LEU:HB2	1.87	0.73
1:D:346:ASP:C	1:D:363:LEU:HD22	2.12	0.73
1:E:212:PHE:HB2	1:E:383:MET:HE1	1.70	0.73
1:B:125:LEU:HD23	1:B:362:GLN:OE1	1.88	0.73
1:C:161:GLY:O	1:E:127:ASP:CB	2.37	0.72
1:D:390:GLU:OE2	1:D:393:LYS:HE3	1.89	0.72
1:B:279:ARG:HH11	1:C:311:MET:HE1	1.53	0.72
1:E:318:LEU:HD23	1:E:343:ILE:HB	1.71	0.72
1:F:154:ILE:CD1	1:F:231:ASP:CB	2.66	0.72
1:A:149:SER:HB2	5:A:402:HOH:O	1.90	0.72
1:D:346:ASP:CA	1:D:363:LEU:HD22	2.19	0.72
1:D:386:LEU:O	1:D:390:GLU:HB2	1.90	0.71
1:F:259:CYS:O	1:F:260:GLN:HB2	1.90	0.71
1:E:123:LEU:HD22	1:E:127:ASP:CB	2.20	0.71
1:C:161:GLY:O	1:E:127:ASP:HB3	1.89	0.71
1:F:325:GLU:OE1	1:F:325:GLU:HA	1.91	0.71
1:B:389:ARG:O	1:B:393:LYS:HG3	1.91	0.70
1:B:207:ASN:H	1:B:210:HIS:HD2	1.36	0.70
1:C:342:LEU:HD11	1:C:344:ASN:CB	2.21	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:161:GLY:O	1:E:127:ASP:HA	1.91	0.70
1:B:165:TYR:O	1:B:169:GLN:HG3	1.91	0.69
1:D:215:LEU:HD22	1:D:383:MET:CE	2.22	0.69
1:D:365:ASP:HB3	1:D:368:HIS:HB3	1.74	0.69
1:A:149:SER:CB	5:A:402:HOH:O	2.40	0.69
1:E:283:CYS:C	1:E:284:THR:HG23	2.17	0.69
1:D:173:LEU:HD23	1:D:184:PHE:CE1	2.28	0.69
1:F:144:VAL:HG12	1:F:318:LEU:HB2	1.75	0.69
1:B:144:VAL:HB	1:B:148:ILE:HD13	1.75	0.68
1:C:346:ASP:CA	1:C:363:LEU:HD22	2.21	0.68
1:C:153:GLY:HA2	1:E:358:ARG:HD3	1.76	0.68
1:D:173:LEU:HD21	1:D:184:PHE:CZ	2.29	0.68
1:F:381:GLU:HA	1:F:384:ARG:HB2	1.76	0.67
1:F:219:LYS:NZ	5:F:5:HOH:O	2.27	0.67
1:E:207:ASN:H	1:E:210:HIS:CD2	2.09	0.66
1:B:342:LEU:HD11	1:B:344:ASN:HB2	1.76	0.66
1:F:381:GLU:O	1:F:384:ARG:CB	2.43	0.66
1:C:346:ASP:HA	1:C:363:LEU:HD21	1.75	0.66
1:A:261:ARG:HB3	1:A:263:PHE:CE2	2.30	0.66
1:B:126:GLN:O	1:B:130:GLU:HB2	1.96	0.66
1:D:382:GLU:O	1:D:386:LEU:N	2.26	0.65
1:B:186:PHE:CZ	1:C:303:LEU:HD13	2.30	0.65
1:D:390:GLU:OE2	1:D:390:GLU:HA	1.95	0.65
1:E:156:ASP:OD1	1:E:158:ARG:HG2	1.96	0.65
1:C:346:ASP:CA	1:C:363:LEU:HD21	2.27	0.65
1:E:190:LYS:N	1:E:191:PRO:CD	2.60	0.64
1:F:383:MET:O	1:F:383:MET:HG3	1.97	0.64
1:A:325:GLU:HB3	1:A:326:PRO:HA	1.80	0.64
1:D:207:ASN:H	1:D:210:HIS:HD2	1.46	0.64
1:D:382:GLU:HA	1:D:385:ASP:HB2	1.78	0.64
1:F:353:TRP:CD1	1:F:354:HIS:NE2	2.65	0.64
1:C:358:ARG:NH1	1:C:358:ARG:CG	2.60	0.64
1:E:150:THR:N	1:E:151:PRO:CD	2.59	0.64
1:B:210:HIS:HE1	5:B:25:HOH:O	1.80	0.64
1:C:342:LEU:HD11	1:C:344:ASN:HB2	1.80	0.63
1:D:144:VAL:HG12	1:D:318:LEU:HB2	1.80	0.63
1:F:212:PHE:HA	1:F:383:MET:HE1	1.80	0.63
1:E:224:ARG:NH1	1:E:242:SER:O	2.31	0.63
1:D:142:VAL:HB	1:D:225:LEU:HD13	1.79	0.63
1:D:389:ARG:O	1:D:393:LYS:HE3	1.99	0.63
1:A:266:GLU:CD	1:A:266:GLU:H	2.07	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:158:ARG:NH2	1:C:177:GLU:OE2	2.28	0.62
1:C:175:TYR:HB2	1:C:176:PRO:CD	2.27	0.62
1:B:208:VAL:HG11	1:B:367:VAL:HG13	1.80	0.62
1:D:372:SER:O	1:D:375:GLU:HB3	1.99	0.62
1:C:366:VAL:O	1:C:370:VAL:HG23	1.98	0.62
1:A:280:CYS:O	1:A:284:THR:HA	1.98	0.62
1:C:261:ARG:NH2	1:C:282:VAL:HG11	2.14	0.62
1:A:390:GLU:OE1	1:A:390:GLU:HA	1.98	0.61
1:B:325:GLU:HB3	1:B:326:PRO:HA	1.81	0.61
1:C:161:GLY:O	1:E:127:ASP:CA	2.47	0.61
1:E:318:LEU:CD2	1:E:343:ILE:HB	2.30	0.61
1:B:212:PHE:HA	1:B:383:MET:CE	2.22	0.61
1:C:176:PRO:O	1:C:179:ILE:HG12	2.00	0.61
1:A:345:ARG:HH12	1:A:365:ASP:HA	1.65	0.61
1:D:346:ASP:HA	1:D:363:LEU:HD22	1.82	0.61
1:A:259:CYS:O	1:A:260:GLN:HB2	2.00	0.61
1:D:346:ASP:C	1:D:363:LEU:CD2	2.74	0.61
1:E:173:LEU:HD22	1:E:178:ALA:HB3	1.81	0.61
1:E:382:GLU:HG3	5:E:16:HOH:O	2.00	0.61
1:C:138:GLN:N	1:C:313:ASP:OD2	2.33	0.61
1:E:266:GLU:CD	1:E:266:GLU:H	2.09	0.61
1:F:225:LEU:C	1:F:225:LEU:HD12	2.25	0.61
1:F:141:VAL:HG21	1:F:312:ALA:HB2	1.81	0.61
1:B:182:LEU:HB2	1:B:183:PRO:HD3	1.83	0.60
1:B:150:THR:N	1:B:151:PRO:CD	2.63	0.60
1:B:212:PHE:N	1:B:383:MET:HE1	2.17	0.60
1:C:346:ASP:C	1:C:363:LEU:HD21	2.26	0.60
1:C:268:ILE:O	1:C:272:VAL:HG23	2.01	0.60
1:E:212:PHE:CA	1:E:383:MET:HE1	2.32	0.60
1:D:125:LEU:HD11	1:D:373:LEU:HD13	1.83	0.60
1:E:123:LEU:CD2	1:E:127:ASP:CB	2.80	0.60
1:B:303:LEU:O	1:B:306:VAL:HG23	2.02	0.60
1:E:212:PHE:CB	1:E:383:MET:HE1	2.32	0.60
1:B:166:SER:HA	1:B:169:GLN:HE21	1.66	0.60
1:B:381:GLU:OE2	1:B:381:GLU:HA	2.01	0.60
1:A:315:LEU:HD21	1:A:317:ILE:HD11	1.84	0.59
1:A:345:ARG:HB2	5:A:95:HOH:O	2.01	0.59
1:D:268:ILE:O	1:D:272:VAL:HG23	2.02	0.59
1:D:383:MET:O	1:D:387:VAL:HG23	2.02	0.59
1:D:267:ASP:N	1:D:267:ASP:OD1	2.35	0.59
1:D:318:LEU:CD2	1:D:343:ILE:HB	2.31	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:141:VAL:CG2	1:D:312:ALA:HB2	2.32	0.59
1:C:342:LEU:HD11	1:C:344:ASN:HB3	1.84	0.59
1:F:141:VAL:CG2	1:F:312:ALA:HB2	2.33	0.59
1:A:158:ARG:CD	1:A:177:GLU:OE2	2.51	0.58
1:D:379:TRP:C	1:D:381:GLU:HB2	2.28	0.58
1:F:154:ILE:HD11	1:F:231:ASP:HB2	1.84	0.58
1:F:283:CYS:C	1:F:284:THR:CG2	2.76	0.58
1:F:381:GLU:O	1:F:384:ARG:HB3	2.04	0.58
1:B:186:PHE:HD1	1:C:306:VAL:HG21	1.67	0.57
1:C:342:LEU:HD12	1:C:343:ILE:N	2.18	0.57
1:A:219:LYS:HE3	1:A:379:TRP:CE2	2.39	0.57
1:C:249:GLY:HA2	5:C:404:HOH:O	2.04	0.57
1:D:148:ILE:HB	1:D:209:THR:HG21	1.86	0.57
1:D:365:ASP:HB3	1:D:368:HIS:CB	2.34	0.57
1:A:126:GLN:O	1:A:130:GLU:HG2	2.03	0.57
1:E:175:TYR:HB2	1:E:176:PRO:HD2	1.86	0.57
1:B:317:ILE:O	1:B:318:LEU:HD23	2.04	0.57
1:E:382:GLU:CG	5:E:16:HOH:O	2.52	0.57
1:F:174:PRO:HB2	1:F:175:TYR:CD1	2.40	0.57
1:A:261:ARG:CZ	1:A:282:VAL:HG21	2.35	0.57
1:A:293:PHE:O	1:A:296:GLU:HB2	2.05	0.57
1:C:274:ALA:O	1:C:275:ASP:HB2	2.05	0.57
1:E:164:LEU:HD21	1:E:195:LEU:HD12	1.86	0.57
1:E:212:PHE:HA	1:E:383:MET:HE1	1.86	0.57
1:F:387:VAL:O	1:F:391:THR:OG1	2.22	0.57
1:C:133:ARG:HD3	1:C:377:LEU:O	2.05	0.56
1:F:384:ARG:O	1:F:388:GLN:CG	2.49	0.56
1:E:175:TYR:HB2	1:E:176:PRO:CD	2.36	0.56
1:C:207:ASN:H	1:C:210:HIS:HD2	1.54	0.56
1:F:380:THR:O	1:F:384:ARG:NE	2.38	0.56
1:A:207:ASN:N	1:A:210:HIS:HD2	1.86	0.56
1:A:190:LYS:N	1:A:191:PRO:CD	2.69	0.56
1:E:182:LEU:HB2	1:E:183:PRO:HD3	1.88	0.56
1:C:322:LEU:HD12	1:C:348:VAL:HG23	1.87	0.55
1:E:279:ARG:HH21	1:E:284:THR:CB	2.20	0.55
1:E:342:LEU:HD22	1:E:351:LEU:HD12	1.88	0.55
1:C:388:GLN:HA	1:C:388:GLN:OE1	2.06	0.55
1:E:340:ARG:NH2	1:E:356:ARG:HG3	2.21	0.55
1:B:346:ASP:OD1	1:B:346:ASP:N	2.40	0.55
1:C:283:CYS:O	1:C:284:THR:HG23	2.06	0.55
1:D:298:LEU:HD11	1:D:326:PRO:HD2	1.89	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:252:ALA:O	1:C:265:GLY:N	2.36	0.55
1:B:208:VAL:CG1	1:B:367:VAL:HG13	2.37	0.55
1:B:274:ALA:O	1:B:275:ASP:HB2	2.07	0.55
1:C:337:SER:O	1:C:358:ARG:NH1	2.39	0.55
1:F:283:CYS:O	1:F:284:THR:HG23	2.06	0.55
1:D:219:LYS:HE3	1:D:379:TRP:CE2	2.42	0.54
1:C:235:ARG:HG3	1:C:244:LEU:CD1	2.37	0.54
1:F:154:ILE:HD13	1:F:231:ASP:HB2	1.74	0.54
1:E:374:VAL:CG2	1:E:383:MET:HE2	2.32	0.54
1:F:383:MET:O	1:F:387:VAL:CG2	2.48	0.54
1:B:207:ASN:H	1:B:210:HIS:CD2	2.23	0.54
1:D:215:LEU:HD22	1:D:383:MET:HE1	1.89	0.54
1:C:158:ARG:HD3	1:C:177:GLU:OE2	2.07	0.54
1:A:211:TYR:O	1:A:214:ARG:HB3	2.08	0.54
1:A:389:ARG:NH1	1:A:389:ARG:HG3	2.17	0.54
1:B:139:ARG:N	1:B:313:ASP:OD1	2.42	0.53
1:C:353:TRP:C	1:C:355:PRO:HD3	2.34	0.53
1:C:387:VAL:HG12	1:C:387:VAL:O	2.08	0.53
1:D:156:ASP:OD1	1:D:158:ARG:HG2	2.08	0.53
1:B:342:LEU:HD12	1:B:343:ILE:N	2.23	0.53
1:D:389:ARG:HD2	5:D:18:HOH:O	2.08	0.53
1:E:160:PRO:HA	1:E:165:TYR:CD2	2.43	0.53
1:F:215:LEU:HD22	1:F:383:MET:HE2	1.90	0.53
1:F:380:THR:O	1:F:384:ARG:NH2	2.40	0.53
1:B:190:LYS:N	1:B:191:PRO:CD	2.72	0.53
1:C:219:LYS:HE3	1:C:379:TRP:CE2	2.44	0.53
1:D:141:VAL:HG23	1:D:312:ALA:HB2	1.90	0.53
1:E:279:ARG:HH21	1:E:284:THR:HB	1.74	0.53
1:D:259:CYS:C	1:D:260:GLN:HG2	2.33	0.53
1:A:176:PRO:HD3	1:B:353:TRP:CD2	2.43	0.53
1:A:182:LEU:HB2	1:A:183:PRO:HD3	1.92	0.53
1:C:381:GLU:HB3	5:C:86:HOH:O	2.09	0.53
1:D:358:ARG:NH1	1:D:358:ARG:HG3	2.23	0.53
1:C:325:GLU:OE1	1:C:329:SER:HB3	2.08	0.52
1:D:173:LEU:HD21	1:D:184:PHE:CE2	2.44	0.52
1:B:134:ALA:O	1:B:135:ARG:HB3	2.08	0.52
1:D:371:GLU:O	1:D:372:SER:C	2.52	0.52
1:D:375:GLU:OE2	1:D:375:GLU:HA	2.08	0.52
1:A:276:ARG:O	1:A:278:PRO:HD3	2.09	0.52
1:B:219:LYS:HE3	1:B:379:TRP:CE2	2.44	0.52
1:D:358:ARG:HG3	1:D:358:ARG:HH11	1.75	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:190:LYS:N	1:C:191:PRO:HD2	2.25	0.52
1:C:374:VAL:HG21	1:C:383:MET:HE2	1.91	0.52
1:D:381:GLU:OE2	1:D:381:GLU:HA	2.08	0.52
1:F:215:LEU:CD2	1:F:383:MET:HE2	2.40	0.52
1:D:306:VAL:O	1:D:310:PRO:HG2	2.09	0.52
1:F:179:ILE:CD1	1:F:195:LEU:HD22	2.40	0.51
1:C:327:PHE:O	1:C:328:ALA:C	2.54	0.51
1:F:158:ARG:NH2	5:F:72:HOH:O	2.31	0.51
1:E:190:LYS:N	1:E:191:PRO:HD2	2.24	0.51
1:A:266:GLU:CD	1:A:266:GLU:N	2.68	0.51
1:A:345:ARG:HH12	1:A:365:ASP:CA	2.23	0.51
1:D:325:GLU:HB3	1:D:326:PRO:HA	1.92	0.51
1:E:182:LEU:N	1:E:183:PRO:CD	2.73	0.51
1:F:385:ASP:O	1:F:389:ARG:CG	2.42	0.51
1:C:280:CYS:O	1:C:284:THR:HA	2.10	0.51
1:D:133:ARG:NH1	1:D:133:ARG:CG	2.68	0.51
1:D:214:ARG:HG2	1:D:214:ARG:NH2	2.23	0.51
1:E:139:ARG:HB3	1:E:223:LEU:HD22	1.91	0.51
1:E:283:CYS:O	1:E:284:THR:HG23	2.10	0.51
1:E:342:LEU:HB2	1:E:351:LEU:CD1	2.41	0.51
1:A:182:LEU:O	1:A:183:PRO:C	2.52	0.50
1:F:341:LEU:HD12	1:F:342:LEU:N	2.26	0.50
1:A:387:VAL:O	1:A:387:VAL:CG1	2.59	0.50
1:B:135:ARG:O	1:B:135:ARG:HG3	2.12	0.50
1:D:323:GLU:O	1:D:324:VAL:C	2.55	0.50
1:D:383:MET:HA	1:D:383:MET:HE2	1.94	0.50
1:F:306:VAL:O	1:F:310:PRO:HG2	2.11	0.50
1:A:356:ARG:HD2	5:A:28:HOH:O	2.11	0.50
1:B:216:LEU:O	1:B:221:LEU:HB2	2.12	0.50
1:E:374:VAL:HG21	1:E:383:MET:CE	2.35	0.50
1:A:142:VAL:HB	1:A:225:LEU:HD13	1.93	0.50
1:B:215:LEU:HD22	1:B:383:MET:SD	2.52	0.49
1:D:289:PRO:C	1:D:291:ILE:H	2.19	0.49
1:C:207:ASN:H	1:C:210:HIS:CD2	2.30	0.49
1:C:219:LYS:CD	1:C:379:TRP:CZ2	2.96	0.49
1:C:320:THR:HG23	1:C:320:THR:O	2.12	0.49
1:D:219:LYS:HE3	1:D:379:TRP:CZ2	2.47	0.49
1:C:190:LYS:N	1:C:191:PRO:CD	2.75	0.49
1:D:190:LYS:N	1:D:191:PRO:CD	2.75	0.49
1:F:362:GLN:O	1:F:362:GLN:HG3	2.11	0.49
1:B:292:VAL:HG21	1:B:299:PRO:HD3	1.93	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:212:PHE:CA	1:B:383:MET:CE	2.83	0.49
1:D:207:ASN:H	1:D:210:HIS:CD2	2.28	0.49
1:F:245:VAL:HA	5:F:52:HOH:O	2.13	0.49
1:C:208:VAL:HG12	5:C:38:HOH:O	2.12	0.49
1:E:231:ASP:OD1	1:E:233:LEU:HG	2.12	0.49
1:A:345:ARG:HA	1:A:345:ARG:HD3	1.55	0.49
1:E:141:VAL:HG23	1:E:312:ALA:HB2	1.95	0.49
1:F:270:ALA:HB3	5:F:79:HOH:O	2.13	0.49
1:B:264:PRO:HB2	1:B:266:GLU:OE1	2.13	0.49
1:E:313:ASP:OD1	1:E:313:ASP:C	2.54	0.49
1:F:175:TYR:HB2	1:F:176:PRO:HD2	1.95	0.49
1:F:366:VAL:O	1:F:370:VAL:HG23	2.12	0.49
1:D:195:LEU:HG	1:D:199:LEU:HD12	1.94	0.48
1:F:133:ARG:NH1	1:F:377:LEU:O	2.46	0.48
1:C:163:GLY:HA2	1:C:166:SER:OG	2.13	0.48
1:F:132:ILE:O	1:F:135:ARG:N	2.40	0.48
1:D:390:GLU:OE2	1:D:393:LYS:CE	2.61	0.48
1:B:342:LEU:HD12	1:B:343:ILE:H	1.78	0.48
1:C:307:VAL:O	1:C:310:PRO:HD2	2.14	0.48
1:A:162:SER:OG	1:A:163:GLY:N	2.45	0.48
1:C:182:LEU:N	1:C:183:PRO:CD	2.76	0.48
1:D:315:LEU:HB2	1:D:334:VAL:HG11	1.95	0.48
1:B:129:ALA:O	1:B:133:ARG:HG3	2.14	0.48
1:C:283:CYS:C	1:C:284:THR:CG2	2.81	0.48
1:E:150:THR:N	1:E:151:PRO:HD2	2.27	0.48
1:D:197:LYS:HB2	1:D:272:VAL:HG12	1.96	0.48
1:E:123:LEU:CD2	1:E:127:ASP:HB3	2.43	0.48
1:E:173:LEU:CD2	1:E:184:PHE:CE2	2.97	0.48
1:E:222:LEU:O	1:E:243:LYS:HE3	2.14	0.48
1:F:179:ILE:HD12	1:F:195:LEU:HD22	1.95	0.48
1:D:318:LEU:HD23	1:D:343:ILE:HB	1.95	0.47
1:F:169:GLN:C	1:F:171:TYR:H	2.22	0.47
1:F:389:ARG:CG	1:F:389:ARG:NH1	2.42	0.47
1:C:212:PHE:HB2	1:C:383:MET:HE1	1.96	0.47
1:C:191:PRO:O	1:C:194:THR:HB	2.14	0.47
1:B:177:GLU:N	1:B:177:GLU:OE1	2.47	0.47
1:D:157:PHE:HB3	1:D:195:LEU:HD11	1.97	0.47
1:D:225:LEU:HB3	1:D:244:LEU:HD23	1.97	0.47
1:D:295:GLY:C	5:D:82:HOH:O	2.58	0.47
1:E:148:ILE:HB	1:E:209:THR:HG21	1.97	0.47
3:F:400:PGE:H5	5:F:401:HOH:O	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:228:GLN:HG3	1:E:327:PHE:CZ	2.50	0.47
1:E:344:ASN:O	1:E:363:LEU:HA	2.14	0.47
1:A:148:ILE:HB	1:A:209:THR:HG21	1.95	0.47
1:B:198:GLU:O	1:B:198:GLU:HG3	2.15	0.47
1:C:211:TYR:HB3	1:C:386:LEU:HD23	1.97	0.47
1:C:269:ARG:O	1:C:270:ALA:C	2.57	0.47
1:B:149:SER:C	1:B:151:PRO:HD2	2.39	0.47
1:D:133:ARG:C	1:D:135:ARG:H	2.23	0.47
1:E:166:SER:HA	1:E:169:GLN:HE21	1.80	0.47
1:F:346:ASP:HA	1:F:363:LEU:HD22	1.97	0.47
1:A:311:MET:HE3	1:A:311:MET:HB2	1.61	0.47
1:B:212:PHE:N	1:B:383:MET:CE	2.78	0.47
1:D:133:ARG:HD2	1:D:377:LEU:HA	1.97	0.47
1:A:215:LEU:HG	1:A:219:LYS:HE2	1.97	0.46
1:D:141:VAL:HG21	1:D:312:ALA:HB2	1.97	0.46
1:F:381:GLU:O	1:F:384:ARG:N	2.41	0.46
1:D:173:LEU:HD22	1:D:178:ALA:CB	2.42	0.46
1:E:207:ASN:N	1:E:210:HIS:HD2	2.02	0.46
1:F:125:LEU:HD12	1:F:125:LEU:HA	1.71	0.46
1:C:150:THR:N	1:C:151:PRO:CD	2.77	0.46
1:D:269:ARG:NH1	1:D:273:MET:HE2	2.31	0.46
1:A:387:VAL:O	1:A:387:VAL:HG12	2.15	0.46
1:C:173:LEU:O	1:D:354:HIS:CE1	2.68	0.46
1:C:139:ARG:NH2	1:C:311:MET:O	2.49	0.46
1:D:383:MET:HE2	1:D:383:MET:CA	2.45	0.46
1:C:346:ASP:N	1:C:363:LEU:HD22	2.30	0.46
1:E:219:LYS:HE3	1:E:379:TRP:CE2	2.51	0.46
1:A:144:VAL:HG12	1:A:318:LEU:HB2	1.97	0.46
1:A:271:ASP:OD1	1:A:276:ARG:NH2	2.49	0.46
1:C:314:LEU:HG	1:C:315:LEU:N	2.31	0.46
1:D:182:LEU:O	1:D:183:PRO:C	2.58	0.46
1:A:190:LYS:N	1:A:191:PRO:HD2	2.30	0.46
1:F:225:LEU:HD12	1:F:226:TYR:N	2.31	0.46
1:F:303:LEU:O	1:F:306:VAL:HG23	2.16	0.46
1:A:150:THR:O	1:A:151:PRO:C	2.58	0.45
1:C:141:VAL:O	1:C:315:LEU:HD12	2.15	0.45
1:E:180:PHE:HB2	1:E:294:PHE:CE2	2.51	0.45
1:F:329:SER:O	1:F:332:GLU:HB2	2.15	0.45
1:A:259:CYS:SG	1:A:261:ARG:HB2	2.56	0.45
1:A:318:LEU:HD22	1:A:343:ILE:HB	1.98	0.45
1:B:345:ARG:HA	1:B:345:ARG:HD3	1.68	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:313:ASP:OD1	1:C:313:ASP:C	2.60	0.45
1:D:389:ARG:O	1:D:393:LYS:CE	2.64	0.45
1:E:246:GLU:O	1:E:247:ALA:C	2.58	0.45
1:A:311:MET:HE1	1:D:279:ARG:NH1	2.31	0.45
1:C:368:HIS:O	1:C:369:GLY:C	2.58	0.45
1:B:367:VAL:O	1:B:368:HIS:C	2.59	0.45
1:D:295:GLY:HA3	5:D:82:HOH:O	2.15	0.45
1:E:174:PRO:HB2	1:E:175:TYR:CD2	2.52	0.45
1:A:303:LEU:O	1:A:306:VAL:HG23	2.16	0.45
1:B:322:LEU:HD22	1:B:328:ALA:HA	1.99	0.45
1:E:372:SER:O	1:E:375:GLU:HB3	2.17	0.45
1:A:125:LEU:HD11	1:A:373:LEU:HD13	1.98	0.45
1:F:380:THR:O	1:F:384:ARG:CZ	2.64	0.45
1:A:142:VAL:HG22	1:A:316:LEU:HB3	1.98	0.45
1:D:370:VAL:O	1:D:374:VAL:HG23	2.17	0.45
1:E:259:CYS:O	1:E:260:GLN:HB2	2.17	0.45
1:A:345:ARG:NH1	1:A:365:ASP:N	2.65	0.44
1:C:259:CYS:O	1:C:260:GLN:HB2	2.16	0.44
1:F:135:ARG:HA	1:F:135:ARG:HD3	1.82	0.44
1:E:160:PRO:HA	1:E:165:TYR:CE2	2.53	0.44
1:E:283:CYS:C	1:E:284:THR:CG2	2.86	0.44
1:B:150:THR:HB	1:B:151:PRO:HD3	2.00	0.44
1:F:325:GLU:CD	1:F:329:SER:OG	2.60	0.44
1:A:194:THR:HA	5:A:62:HOH:O	2.17	0.44
1:A:307:VAL:HG13	1:D:286:VAL:HG23	2.00	0.44
1:B:318:LEU:HD23	1:B:318:LEU:N	2.31	0.44
1:D:323:GLU:O	1:D:325:GLU:N	2.51	0.44
1:E:144:VAL:HG12	1:E:318:LEU:HB2	2.00	0.44
1:F:174:PRO:HB2	1:F:175:TYR:CE1	2.53	0.44
1:E:173:LEU:HD21	1:E:184:PHE:CE2	2.53	0.44
1:F:197:LYS:O	1:F:203:ASN:ND2	2.51	0.44
1:B:124:SER:O	1:B:128:VAL:HG23	2.18	0.44
1:D:372:SER:O	1:D:375:GLU:CB	2.65	0.44
1:E:129:ALA:HB1	1:E:377:LEU:HD23	2.00	0.44
1:F:382:GLU:C	1:F:384:ARG:H	2.24	0.44
1:D:143:MET:HE2	1:D:327:PHE:CE2	2.53	0.43
1:D:182:LEU:HB2	1:D:183:PRO:HD3	2.00	0.43
1:D:330:LEU:HD23	1:D:330:LEU:HA	1.86	0.43
1:F:317:ILE:HD13	1:F:351:LEU:HD11	2.00	0.43
1:B:152:SER:OG	1:B:205:LYS:O	2.31	0.43
1:D:145:GLY:HA3	1:D:320:THR:HB	1.99	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:130:GLU:OE2	1:F:130:GLU:HA	2.17	0.43
1:A:325:GLU:HA	1:A:325:GLU:OE1	2.18	0.43
1:B:182:LEU:HB2	1:B:183:PRO:CD	2.49	0.43
1:B:379:TRP:O	1:B:380:THR:C	2.58	0.43
1:D:157:PHE:HB3	1:D:195:LEU:CD1	2.48	0.43
1:D:344:ASN:O	1:D:363:LEU:HA	2.18	0.43
1:D:376:LEU:H	1:D:376:LEU:HG	1.69	0.43
1:C:156:ASP:C	1:C:158:ARG:H	2.27	0.43
1:C:344:ASN:O	1:C:363:LEU:HD23	2.18	0.43
1:D:206:PRO:HG2	1:D:211:TYR:OH	2.18	0.43
1:E:130:GLU:OE1	1:E:130:GLU:HA	2.19	0.43
1:E:141:VAL:CG2	1:E:312:ALA:HB2	2.48	0.43
1:E:279:ARG:HE	1:E:279:ARG:HB3	1.39	0.43
1:F:169:GLN:C	1:F:171:TYR:N	2.76	0.43
1:A:131:LEU:HB3	1:A:137:CYS:SG	2.59	0.43
1:C:219:LYS:HD3	1:C:379:TRP:CZ2	2.54	0.43
1:E:146:ALA:O	1:E:147:GLY:C	2.62	0.43
1:E:289:PRO:O	1:E:291:ILE:N	2.46	0.43
1:F:176:PRO:O	1:F:179:ILE:HG12	2.18	0.43
1:A:150:THR:HB	1:A:151:PRO:HD3	2.00	0.43
1:D:150:THR:HB	1:D:151:PRO:HD3	1.99	0.43
1:E:156:ASP:HB3	1:E:159:SER:HB2	2.01	0.43
1:F:185:PHE:HB2	5:F:404:HOH:O	2.18	0.43
1:B:224:ARG:HG3	1:B:225:LEU:N	2.33	0.43
1:C:182:LEU:HB2	1:C:183:PRO:HD3	2.01	0.43
1:C:225:LEU:C	1:C:225:LEU:HD12	2.44	0.43
1:E:214:ARG:HD3	1:E:237:SER:O	2.19	0.43
1:C:148:ILE:HB	1:C:209:THR:HG21	2.01	0.43
1:C:292:VAL:HG21	1:C:299:PRO:HD3	2.01	0.43
1:F:179:ILE:HG13	1:F:180:PHE:CD2	2.54	0.43
1:F:231:ASP:OD1	1:F:233:LEU:HB2	2.18	0.43
1:D:205:LYS:CE	5:D:56:HOH:O	2.66	0.43
1:C:235:ARG:HE	1:C:246:GLU:CD	2.26	0.43
1:D:214:ARG:HH21	1:D:214:ARG:CG	2.29	0.43
1:D:364:GLY:O	1:D:365:ASP:C	2.62	0.43
1:E:225:LEU:C	1:E:225:LEU:HD12	2.44	0.43
1:C:155:PRO:HB3	1:C:162:SER:HB3	2.01	0.42
1:A:256:CYS:SG	1:A:280:CYS:CB	2.95	0.42
1:B:339:PRO:HA	1:B:358:ARG:O	2.19	0.42
1:E:138:GLN:O	1:E:221:LEU:HA	2.19	0.42
1:A:159:SER:HA	1:A:160:PRO:HD3	1.84	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:134:ALA:O	1:B:135:ARG:CB	2.67	0.42
1:D:167:ASN:O	1:D:170:GLN:HB2	2.19	0.42
1:D:374:VAL:HG11	1:D:383:MET:HB2	2.01	0.42
1:B:280:CYS:O	1:B:284:THR:HA	2.20	0.42
1:C:318:LEU:HD23	1:C:343:ILE:HB	2.00	0.42
1:C:325:GLU:OE1	1:C:326:PRO:HA	2.19	0.42
1:D:175:TYR:HB2	1:D:176:PRO:HD2	2.00	0.42
1:D:215:LEU:HD22	1:D:383:MET:HE2	2.00	0.42
1:D:322:LEU:HD13	1:D:350:PRO:HD2	2.02	0.42
1:E:269:ARG:O	1:E:270:ALA:C	2.62	0.42
1:F:168:LEU:O	1:F:171:TYR:HB2	2.19	0.42
1:F:335:ARG:HE	1:F:335:ARG:HB2	1.73	0.42
1:A:122:LYS:HA	1:A:122:LYS:HD3	1.42	0.42
1:E:154:ILE:HD12	1:E:154:ILE:HA	1.77	0.42
1:E:212:PHE:HB2	1:E:383:MET:CE	2.46	0.42
1:E:353:TRP:C	1:E:355:PRO:HD3	2.44	0.42
1:F:309:PHE:N	1:F:310:PRO:CD	2.82	0.42
1:C:125:LEU:HD22	1:C:362:GLN:OE1	2.20	0.42
1:F:353:TRP:NE1	1:F:354:HIS:NE2	2.67	0.42
1:B:186:PHE:CE1	1:C:303:LEU:HD13	2.55	0.42
1:D:159:SER:HA	1:D:160:PRO:HD3	1.89	0.42
1:D:327:PHE:O	1:D:328:ALA:C	2.63	0.42
1:B:159:SER:HA	1:B:160:PRO:HD3	1.81	0.42
1:B:179:ILE:HG13	1:B:180:PHE:CD2	2.55	0.42
1:B:184:PHE:CD2	1:B:184:PHE:C	2.98	0.42
1:C:342:LEU:CD1	1:C:344:ASN:HB2	2.47	0.42
1:E:135:ARG:HD3	1:E:135:ARG:HA	1.82	0.42
1:E:382:GLU:HG2	5:E:16:HOH:O	2.18	0.41
1:B:182:LEU:O	1:B:183:PRO:C	2.61	0.41
1:B:206:PRO:HB2	1:B:211:TYR:CE2	2.55	0.41
1:B:393:LYS:O	1:B:394:LEU:O	2.38	0.41
1:D:316:LEU:HD11	1:D:341:LEU:HD23	2.01	0.41
1:E:159:SER:HA	1:E:160:PRO:HD3	1.91	0.41
1:A:207:ASN:N	1:A:210:HIS:CD2	2.70	0.41
1:A:214:ARG:HG3	1:A:386:LEU:HD21	2.02	0.41
1:A:224:ARG:HG3	1:A:225:LEU:N	2.35	0.41
1:C:150:THR:N	1:C:151:PRO:HD2	2.35	0.41
1:D:235:ARG:NH2	1:D:250:THR:HG21	2.35	0.41
1:F:219:LYS:HE3	1:F:382:GLU:OE1	2.21	0.41
1:F:338:VAL:HA	1:F:339:PRO:HD2	1.91	0.41
1:B:125:LEU:HD13	1:B:125:LEU:HA	1.73	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:253:SER:OG	1:B:290:ASP:OD2	2.31	0.41
1:B:344:ASN:O	1:B:363:LEU:HA	2.20	0.41
1:D:208:VAL:HG11	1:D:367:VAL:HG13	2.03	0.41
1:E:341:LEU:HD12	1:E:342:LEU:N	2.35	0.41
1:B:144:VAL:CB	1:B:148:ILE:HD13	2.47	0.41
1:E:261:ARG:HA	1:E:262:PRO:HD3	1.72	0.41
1:A:135:ARG:HH11	1:A:135:ARG:HG3	1.86	0.41
1:A:277:VAL:O	1:A:279:ARG:HG3	2.21	0.41
1:A:156:ASP:HB3	1:A:159:SER:HB2	2.02	0.41
1:D:200:TYR:HA	1:D:201:PRO:HD3	1.95	0.41
1:F:190:LYS:N	1:F:191:PRO:CD	2.84	0.41
1:F:216:LEU:HD12	1:F:221:LEU:HD12	2.03	0.41
1:A:200:TYR:CD2	1:A:201:PRO:HD2	2.55	0.41
1:A:345:ARG:NH1	1:A:365:ASP:HA	2.32	0.41
1:B:301:ARG:O	1:B:302:PHE:C	2.64	0.41
1:C:125:LEU:HD12	1:C:125:LEU:HA	1.91	0.41
1:D:208:VAL:HG13	1:D:209:THR:N	2.35	0.41
1:D:243:LYS:HD3	1:D:243:LYS:HA	1.90	0.41
1:F:229:ASN:HB3	1:F:231:ASP:OD2	2.21	0.41
1:F:298:LEU:HD23	1:F:298:LEU:HA	1.84	0.41
1:F:326:PRO:O	1:F:327:PHE:C	2.62	0.41
1:B:318:LEU:O	1:B:319:GLY:C	2.64	0.41
1:C:173:LEU:O	1:D:354:HIS:HE1	2.04	0.41
1:F:150:THR:HB	1:F:151:PRO:HD3	2.03	0.41
1:F:325:GLU:HB3	1:F:326:PRO:HA	2.02	0.41
1:A:205:LYS:HE3	1:A:394:LEU:HB3	2.01	0.40
1:A:213:LEU:HD13	1:A:225:LEU:HD21	2.03	0.40
1:B:160:PRO:HA	1:B:165:TYR:CG	2.55	0.40
1:C:139:ARG:N	1:C:313:ASP:OD2	2.46	0.40
1:C:277:VAL:O	1:C:279:ARG:HG3	2.21	0.40
1:C:363:LEU:HD23	1:C:363:LEU:HA	1.77	0.40
1:A:176:PRO:HD3	1:B:353:TRP:CE3	2.57	0.40
1:C:132:ILE:O	1:C:135:ARG:NH1	2.54	0.40
1:D:125:LEU:CD1	1:D:373:LEU:HD13	2.52	0.40
1:D:219:LYS:CD	1:D:379:TRP:CZ2	3.04	0.40
1:D:311:MET:HE3	1:D:311:MET:HB2	1.49	0.40
1:E:173:LEU:HD23	1:E:184:PHE:CE2	2.55	0.40
1:A:261:ARG:HB3	1:A:263:PHE:HE2	1.85	0.40
1:B:141:VAL:O	1:B:315:LEU:HD12	2.22	0.40
1:B:213:LEU:HD13	1:B:225:LEU:HD22	2.04	0.40
1:B:298:LEU:HD23	1:B:298:LEU:HA	1.84	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:386:LEU:C	1:C:388:GLN:H	2.29	0.40
1:A:140:VAL:HG23	1:A:221:LEU:O	2.21	0.40
1:B:128:VAL:C	1:B:130:GLU:H	2.29	0.40
1:F:208:VAL:HG11	1:F:367:VAL:HG13	2.03	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	271/285 (95%)	257 (95%)	13 (5%)	1 (0%)	30	54
1	B	270/285 (95%)	256 (95%)	14 (5%)	0	100	100
1	C	271/285 (95%)	256 (94%)	15 (6%)	0	100	100
1	D	272/285 (95%)	252 (93%)	16 (6%)	4 (2%)	8	22
1	E	272/285 (95%)	262 (96%)	9 (3%)	1 (0%)	30	54
1	F	270/285 (95%)	259 (96%)	11 (4%)	0	100	100
All	All	1626/1710 (95%)	1542 (95%)	78 (5%)	6 (0%)	30	54

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	322	LEU
1	D	324	VAL
1	D	290	ASP
1	E	290	ASP
1	D	147	GLY
1	A	392	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	237/246 (96%)	228 (96%)	9 (4%)	29	58
1	B	236/246 (96%)	219 (93%)	17 (7%)	13	32
1	C	237/246 (96%)	220 (93%)	17 (7%)	13	32
1	D	237/246 (96%)	220 (93%)	17 (7%)	13	32
1	E	237/246 (96%)	227 (96%)	10 (4%)	26	55
1	F	236/246 (96%)	219 (93%)	17 (7%)	13	32
All	All	1420/1476 (96%)	1333 (94%)	87 (6%)	17	40

All (87) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	122	LYS
1	A	135	ARG
1	A	154	ILE
1	A	200	TYR
1	A	257	THR
1	A	260	GLN
1	A	320	THR
1	A	345	ARG
1	A	389	ARG
1	B	125	LEU
1	B	126	GLN
1	B	131	LEU
1	B	170	GLN
1	B	194	THR
1	B	225	LEU
1	B	227	THR
1	B	306	VAL
1	B	318	LEU
1	B	320	THR
1	B	329	SER
1	B	332	GLU
1	B	345	ARG

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Mol	Chain	Res	Type
1	B	346	ASP
1	B	362	GLN
1	B	384	ARG
1	B	389	ARG
1	C	144	VAL
1	C	158	ARG
1	C	159	SER
1	C	166	SER
1	C	195	LEU
1	C	200	TYR
1	C	228	GLN
1	C	237	SER
1	C	248	HIS
1	C	250	THR
1	C	284	THR
1	C	306	VAL
1	C	337	SER
1	C	346	ASP
1	C	358	ARG
1	C	388	GLN
1	C	389	ARG
1	D	126	GLN
1	D	133	ARG
1	D	154	ILE
1	D	166	SER
1	D	169	GLN
1	D	175	TYR
1	D	179	ILE
1	D	200	TYR
1	D	216	LEU
1	D	231	ASP
1	D	267	ASP
1	D	300	GLN
1	D	351	LEU
1	D	374	VAL
1	D	376	LEU
1	D	381	GLU
1	D	390	GLU
1	E	122	LYS
1	E	154	ILE
1	E	159	SER
1	E	200	TYR

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Mol	Chain	Res	Type
1	E	275	ASP
1	E	279	ARG
1	E	284	THR
1	E	320	THR
1	E	346	ASP
1	E	370	VAL
1	F	138	GLN
1	F	149	SER
1	F	169	GLN
1	F	200	TYR
1	F	225	LEU
1	F	228	GLN
1	F	250	THR
1	F	284	THR
1	F	306	VAL
1	F	320	THR
1	F	329	SER
1	F	345	ARG
1	F	383	MET
1	F	384	ARG
1	F	385	ASP
1	F	389	ARG
1	F	391	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (36) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	169	GLN
1	A	210	HIS
1	A	217	HIS
1	B	126	GLN
1	B	138	GLN
1	B	167	ASN
1	B	169	GLN
1	B	170	GLN
1	B	210	HIS
1	B	228	GLN
1	B	248	HIS
1	B	354	HIS
1	C	126	GLN
1	C	169	GLN
1	C	210	HIS

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Mol	Chain	Res	Type
1	C	228	GLN
1	C	300	GLN
1	C	305	HIS
1	C	368	HIS
1	D	169	GLN
1	D	210	HIS
1	D	305	HIS
1	D	354	HIS
1	E	126	GLN
1	E	169	GLN
1	E	210	HIS
1	E	217	HIS
1	E	248	HIS
1	E	305	HIS
1	E	344	ASN
1	F	169	GLN
1	F	188	ASN
1	F	210	HIS
1	F	228	GLN
1	F	354	HIS
1	F	388	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 oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 9 ligands modelled in this entry, 6 are monoatomic - leaving 3 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The

Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
3	PGE	A	400	-	6,6,9	0.98	0	5,5,8	0.81	0
4	SO4	E	400	-	4,4,4	0.36	0	6,6,6	0.54	0
3	PGE	F	400	-	6,6,9	0.71	0	5,5,8	0.58	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	PGE	A	400	-	-	3/4/4/7	-
3	PGE	F	400	-	-	3/4/4/7	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (6) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	400	PGE	O1-C1-C2-O2
3	F	400	PGE	O3-C5-C6-O4
3	A	400	PGE	O2-C3-C4-O3
3	F	400	PGE	O2-C3-C4-O3
3	A	400	PGE	C4-C3-O2-C2
3	F	400	PGE	C3-C4-O3-C5

There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	E	400	SO4	1	0
3	F	400	PGE	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	273/285 (95%)	-0.32	2 (0%) 84 83	10, 23, 40, 49	5 (1%)
1	B	272/285 (95%)	-0.28	3 (1%) 78 76	11, 26, 49, 57	9 (3%)
1	C	273/285 (95%)	-0.39	2 (0%) 84 83	9, 23, 39, 53	9 (3%)
1	D	274/285 (96%)	-0.15	3 (1%) 78 76	17, 31, 52, 61	10 (3%)
1	E	274/285 (96%)	-0.38	0 100 100	12, 25, 37, 44	5 (1%)
1	F	272/285 (95%)	-0.33	4 (1%) 72 70	11, 25, 46, 69	6 (2%)
All	All	1638/1710 (95%)	-0.31	14 (0%) 81 80	9, 25, 45, 69	44 (2%)

All (14) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	368	HIS	4.4
1	A	388	GLN	2.6
1	D	184	PHE	2.5
1	F	385	ASP	2.5
1	C	394	LEU	2.4
1	B	313	ASP	2.4
1	A	161	GLY	2.4
1	F	388	GLN	2.4
1	D	380	THR	2.3
1	F	381	GLU	2.2
1	C	385	ASP	2.2
1	F	394	LEU	2.2
1	D	383	MET	2.2
1	B	387	VAL	2.2

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 oligosaccharides in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	PGE	A	400	7/10	0.90	0.13	23,24,24,25	0
4	SO4	E	400	5/5	0.91	0.11	50,51,53,54	5
3	PGE	F	400	7/10	0.94	0.09	19,21,22,22	0
2	ZN	A	2	1/1	0.98	0.06	38,38,38,38	0
2	ZN	B	4	1/1	0.99	0.02	22,22,22,22	0
2	ZN	D	6	1/1	0.99	0.03	36,36,36,36	0
2	ZN	E	1	1/1	0.99	0.02	32,32,32,32	0
2	ZN	F	3	1/1	1.00	0.02	20,20,20,20	0
2	ZN	C	5	1/1	1.00	0.01	15,15,15,15	0

6.5 Other polymers [i](#)

There are no such residues in this entry.