



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 12, 2026 – 06:19 AM UTC

PDB ID : 1LYW / pdb_00001lyw
Title : CATHEPSIN D AT PH 7.5
Authors : Lee, A.Y.; Gulnik, S.V.; Erickson, J.W.
Deposited on : 1998-06-30
Resolution : 2.50 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

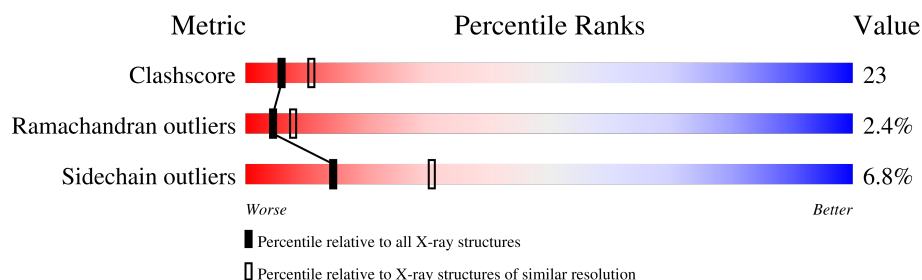
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.50 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	190562	6492 (2.50-2.50)
Ramachandran outliers	187476	6378 (2.50-2.50)
Sidechain outliers	187428	6380 (2.50-2.50)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	97	57% 34% 7% .
1	C	97	42% 54% . .
1	E	97	56% 37% 5% .
1	G	97	42% 47% 7% . .
2	B	241	54% 42% .
2	D	241	52% 41% 6%
2	F	241	45% 51% . .
2	H	241	50% 47% .

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	EPE	C	98	-	-	X	-
3	EPE	G	98	-	-	X	-

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 14242 atoms, of which 3296 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.

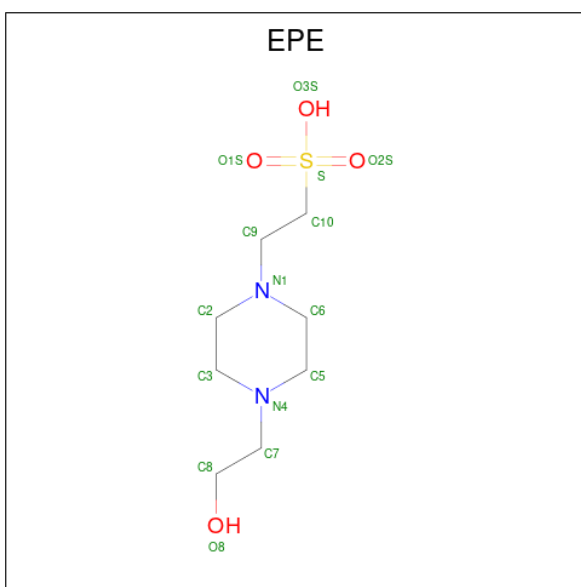
- Molecule 1 is a protein called CATHEPSIN D.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	95	Total	C	H	N	O	S	0	0	0
			890	471	153	117	144	5			
1	C	95	Total	C	H	N	O	S	0	0	0
			890	471	153	117	144	5			
1	E	95	Total	C	H	N	O	S	0	0	0
			890	471	153	117	144	5			
1	G	95	Total	C	H	N	O	S	0	0	0
			890	471	153	117	144	5			

- Molecule 2 is a protein called CATHEPSIN D.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
2	B	241	Total	C	H	N	O	S	0	0	0
			2235	1184	390	302	348	11			
2	D	241	Total	C	H	N	O	S	0	0	0
			2235	1184	390	302	348	11			
2	F	241	Total	C	H	N	O	S	0	0	0
			2235	1184	390	302	348	11			
2	H	241	Total	C	H	N	O	S	0	0	0
			2235	1184	390	302	348	11			

- Molecule 3 is 4-(2-HYDROXYETHYL)-1-PIPERAZINE ETHANESULFONIC ACID (CCD ID: EPE) (formula: C₈H₁₈N₂O₄S).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
3	A	1	Total	C	H	N	O	S	0	0
			17	8	2	2	4	1		
3	C	1	Total	C	H	N	O	S	0	0
			17	8	2	2	4	1		
3	E	1	Total	C	H	N	O	S	0	0
			17	8	2	2	4	1		
3	G	1	Total	C	H	N	O	S	0	0
			17	8	2	2	4	1		

- Molecule 4 is water.

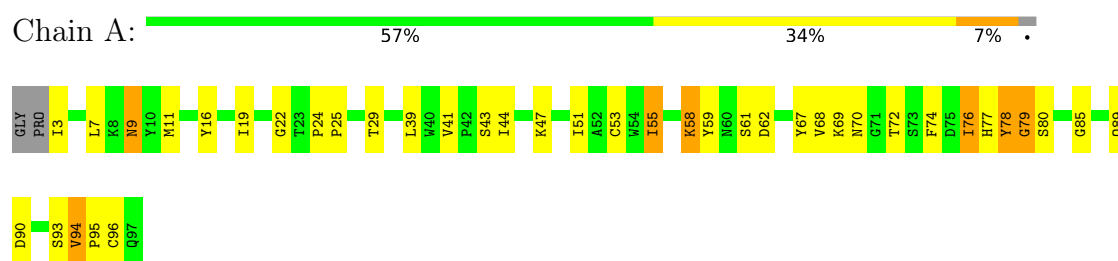
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	55	Total	H	O	0	0
			165	110	55		
4	B	110	Total	H	O	0	0
			330	220	110		
4	C	55	Total	H	O	0	0
			165	110	55		
4	D	78	Total	H	O	0	0
			234	156	78		
4	E	46	Total	H	O	0	0
			138	92	46		
4	F	90	Total	H	O	0	0
			270	180	90		
4	G	39	Total	H	O	0	0
			117	78	39		
4	H	85	Total	H	O	0	0
			255	170	85		

3 Residue-property plots [i](#)

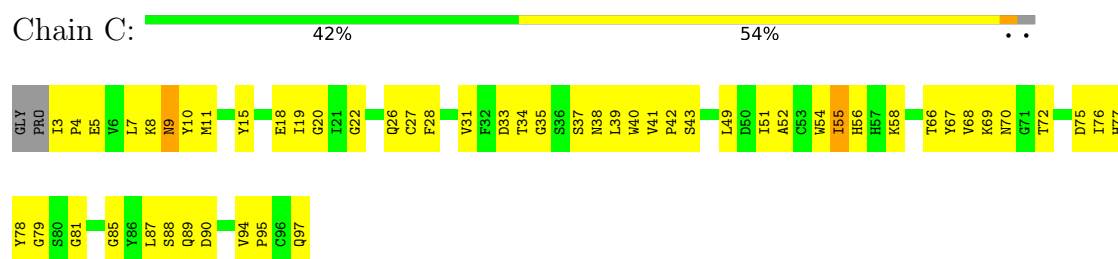
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded 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. 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.

Note EDS was not executed.

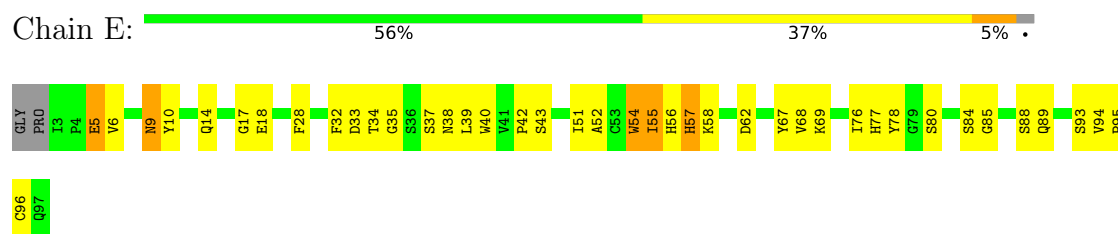
• Molecule 1: CATHEPSIN D



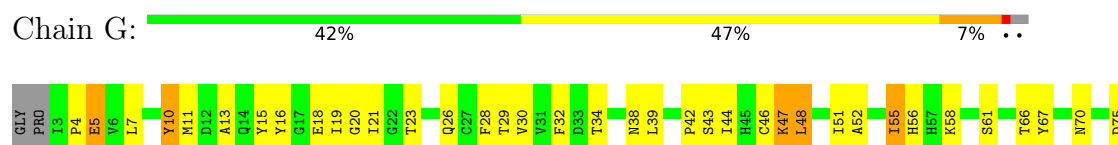
• Molecule 1: CATHEPSIN D



• Molecule 1: CATHEPSIN D



• Molecule 1: CATHEPSIN D





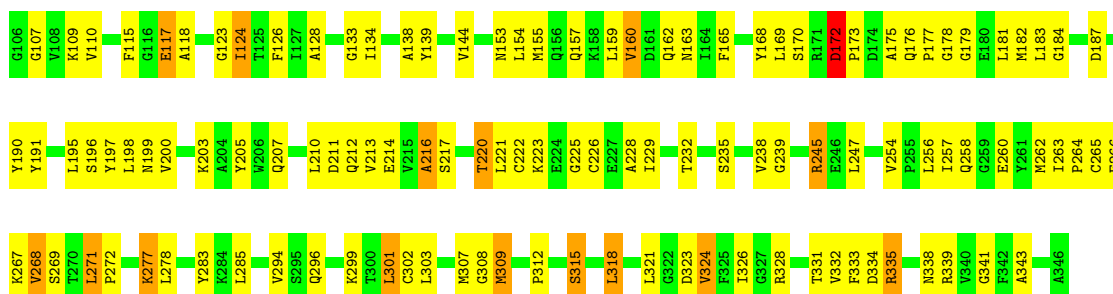
- Molecule 2: CATHEPSIN D

Chain B:  54% 42% .



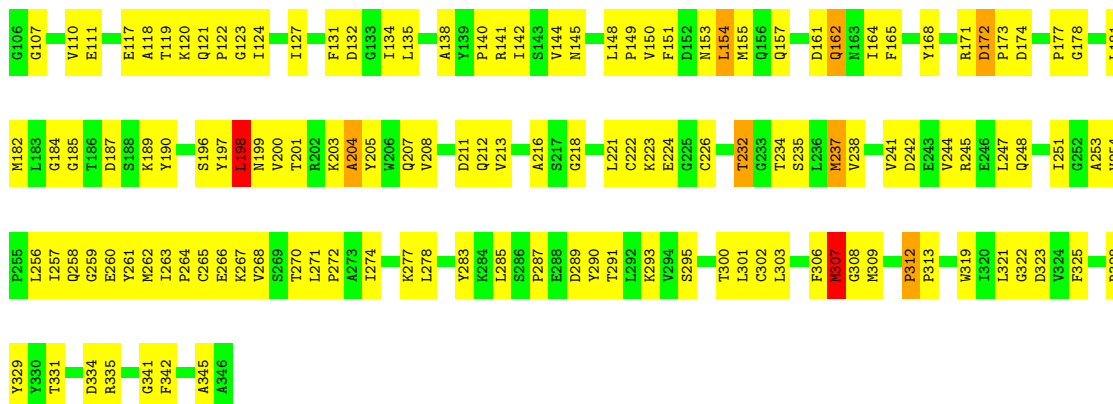
- Molecule 2: CATHEPSIN D

Chain D:  52% 41% 6%

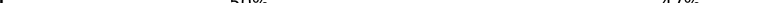


- Molecule 2: CATHEPSIN D

Chain F: 45% 51% .



- Molecule 2: CATHEPSIN D

Chain H:  50% 47%

E260	L181	G106	A345
Y261	M182	G107	A346
M262	L183	V108	
I263	G184	K109	
P264		V110	
C265	S188	E111	
E266		R112	
K267	Y191		
V288		F115	
	S196	G116	
L271	Y197	E117	
P272	L198	A118	
		T119	
K277	R202	K120	
L278		Q121	
G279	Y205	P122	
G280	W206	G123	
	Q207	I124	
Y283		T125	
K284	L210	F126	
L285	D211	I127	
	Q212	A128	
Y290		A129	
	V215		
L301	A216	D132	
G302		G133	
L303		I134	
	L219		
M307	T220	S143	
G308	L221	V144	
M309	C222	N145	
D310	K223	N146	
I311		V147	
P312	C226		
P313	E227	F151	
S314	A228	D152	
S315	I229	N153	
	V230	L154	
	D231	M155	
L318	T232	Q156	
W319	G233	Q157	
I320	T234	K158	
L321		L159	
G322	M237	V160	
D323	V238	D161	
V324		Q162	
F325	V241	N163	
I326	D242	I164	
	E243	F165	
Y330	V244	S166	
	R245	F167	
R335	E246	Y168	
D336	L247	L169	
N337	Q248		
N338	K249	A175	
R339		Q176	
V340	A253	P177	
G341	V254	G178	
F342	P255	G179	
A343	L256	E180	
E344			

4 Data and refinement statistics

Xtriage (Phenix) and EDS were not executed - this section is therefore incomplete.

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, α , β , γ	140.26 Å 136.80 Å 140.42 Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	8.00 – 2.50	Depositor
% Data completeness (in resolution range)	73.0 (8.00-2.50)	Depositor
R_{merge}	0.11	Depositor
R_{sym}	0.11	Depositor
Refinement program	X-PLOR 3.1	Depositor
R, R_{free}	0.195 , 0.257	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	14242	wwPDB-VP
Average B, all atoms (Å ²)	16.0	wwPDB-VP

5 Model quality

5.1 Standard geometry

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

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# $ Z > 5$	RMSZ	# $ Z > 5$
1	A	0.58	0/759	1.03	0/1034
1	C	0.57	0/759	1.03	2/1034 (0.2%)
1	E	0.62	0/759	1.03	2/1034 (0.2%)
1	G	0.64	0/759	1.08	5/1034 (0.5%)
2	B	0.66	0/1884	1.12	16/2551 (0.6%)
2	D	0.66	1/1884 (0.1%)	1.18	10/2551 (0.4%)
2	F	0.66	1/1884 (0.1%)	1.09	12/2551 (0.5%)
2	H	0.63	0/1884	1.07	8/2551 (0.3%)
All	All	0.64	2/10572 (0.0%)	1.10	55/14340 (0.4%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	335	ARG	CZ-NH1	6.44	1.41	1.32
2	F	335	ARG	CZ-NH1	5.53	1.40	1.32

All (55) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	257	ILE	N-CA-C	-8.27	100.87	110.21
1	E	57	HIS	N-CA-C	-7.56	100.77	110.53
2	D	123	GLY	N-CA-C	7.45	124.73	112.66
2	D	324	VAL	N-CA-C	-7.43	103.28	110.42
2	D	257	ILE	N-CA-C	7.40	118.13	110.36
2	D	312	PRO	CA-C-N	7.06	127.65	120.38
2	D	312	PRO	C-N-CA	7.06	127.65	120.38
2	B	237	MET	N-CA-C	-7.00	97.32	108.73
2	D	178	GLY	N-CA-C	-6.89	102.88	111.70
2	D	191	TYR	N-CA-C	6.74	119.65	109.95
2	H	205	TYR	N-CA-C	-6.66	100.93	110.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	222	CYS	N-CA-C	-6.62	102.25	111.39
2	D	205	TYR	N-CA-C	-6.58	100.47	109.95
2	B	315	SER	N-CA-C	-6.46	103.52	111.40
2	F	237	MET	N-CA-C	-6.22	99.09	109.24
2	F	312	PRO	CA-C-N	6.12	126.68	120.38
2	F	312	PRO	C-N-CA	6.12	126.68	120.38
2	H	223	LYS	N-CA-C	6.09	117.59	111.07
1	C	70	ASN	N-CA-C	-6.06	97.89	110.80
2	D	117	GLU	N-CA-C	-6.05	98.66	108.52
2	F	259	GLY	N-CA-C	5.89	119.88	113.58
2	B	205	TYR	N-CA-C	-5.86	101.28	110.36
2	H	207	GLN	N-CA-C	5.81	118.28	107.99
1	G	26	GLN	N-CA-C	-5.81	99.81	109.46
2	F	197	TYR	N-CA-C	5.77	118.65	109.24
2	F	198	LEU	N-CA-C	-5.73	102.05	110.52
2	D	254	VAL	N-CA-C	5.70	113.53	108.63
2	H	196	SER	N-CA-C	-5.67	101.05	110.17
2	F	254	VAL	N-CA-C	5.66	113.48	107.76
1	E	54	TRP	N-CA-C	5.66	117.13	110.97
2	H	319	TRP	N-CA-C	-5.65	100.50	109.76
1	G	46	CYS	N-CA-C	-5.64	101.55	109.96
2	B	191	TYR	N-CA-C	5.52	117.37	109.14
2	F	319	TRP	N-CA-C	-5.52	101.28	110.17
2	F	205	TYR	N-CA-C	-5.50	102.06	110.14
1	G	13	ALA	N-CA-C	-5.49	102.36	110.48
1	G	70	ASN	N-CA-C	-5.41	99.28	110.80
2	H	237	MET	N-CA-C	-5.41	96.40	107.70
2	B	201	THR	N-CA-C	5.37	118.29	111.69
2	B	259	GLY	N-CA-C	5.36	125.88	113.18
1	G	11	MET	N-CA-C	-5.32	98.58	107.99
2	B	206	TRP	N-CA-C	-5.31	101.66	109.62
2	F	307	MET	N-CA-C	5.30	117.14	108.55
2	B	121	GLN	CA-C-N	5.29	125.59	119.92
2	B	121	GLN	C-N-CA	5.29	125.59	119.92
2	B	268	VAL	N-CA-C	5.26	115.70	110.23
2	B	319	TRP	N-CA-C	-5.21	100.75	109.24
2	B	115	PHE	CA-C-N	-5.21	118.53	122.33
2	B	115	PHE	C-N-CA	-5.21	118.53	122.33
2	H	245	ARG	N-CA-C	-5.20	105.62	111.28
2	F	172	ASP	CA-C-N	5.12	125.03	119.76
2	F	172	ASP	C-N-CA	5.12	125.03	119.76
1	C	41	VAL	N-CA-C	-5.11	103.24	109.01

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	H	344	GLU	N-CA-C	-5.10	102.09	109.59
2	B	241	VAL	N-CA-C	5.09	115.81	110.62

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	737	153	690	40	0
1	C	737	153	690	59	0
1	E	737	153	690	43	0
1	G	737	153	690	51	0
2	B	1845	390	1850	92	0
2	D	1845	390	1850	88	0
2	F	1845	390	1850	92	0
2	H	1845	390	1850	94	0
3	A	15	2	18	4	0
3	C	15	2	18	8	0
3	E	15	2	18	2	0
3	G	15	2	18	11	0
4	A	55	110	0	0	0
4	B	110	220	0	0	0
4	C	55	110	0	2	0
4	D	78	156	0	0	0
4	E	46	92	0	0	0
4	F	90	180	0	2	0
4	G	39	78	0	0	0
4	H	85	170	0	2	0
All	All	10946	3296	10232	473	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 23.

All (473) 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:G:7:LEU:HD11	2:H:309:MET:HG2	1.29	1.05
2:H:253:ALA:HB1	2:H:261:TYR:HB3	1.39	1.04
1:E:43:SER:HB2	2:F:117:GLU:HG2	1.39	1.03
1:G:83:LEU:HD23	3:G:98:EPE:H92	1.42	1.02
2:B:172:ASP:HB2	2:B:173:PRO:HD3	1.44	1.00
2:F:293:LYS:HE2	2:F:302:CYS:SG	2.09	0.93
1:E:78:TYR:OH	2:F:122:PRO:HB3	1.77	0.85
1:A:7:LEU:HD22	2:B:307:MET:HG2	1.60	0.84
2:B:230:VAL:HG12	2:B:326:ILE:HD11	1.60	0.84
2:D:264:PRO:HD2	2:D:267:LYS:HD3	1.61	0.83
2:F:264:PRO:HB2	2:F:267:LYS:HG2	1.59	0.81
2:D:200:VAL:HG12	2:D:338:ASN:O	1.80	0.81
1:G:43:SER:HB2	2:H:117:GLU:HB3	1.63	0.81
2:F:263:ILE:HG21	2:F:271:LEU:HD11	1.63	0.80
1:E:68:VAL:HB	1:E:89:GLN:HB3	1.65	0.78
2:B:249:LYS:HE3	2:B:249:LYS:HA	1.66	0.77
2:F:221:LEU:HD11	2:F:247:LEU:HB2	1.67	0.77
2:B:263:ILE:HG21	2:B:271:LEU:HD11	1.66	0.77
1:E:78:TYR:HE1	1:E:80:SER:HB2	1.50	0.76
2:B:228:ALA:HB1	2:B:321:LEU:HD13	1.68	0.76
1:E:5:GLU:HG3	1:E:78:TYR:HB2	1.67	0.75
1:A:47:LYS:HD2	2:B:120:LYS:HE2	1.69	0.74
2:B:260:GLU:HG3	1:C:51:ILE:HD11	1.68	0.74
2:H:154:LEU:HD21	2:H:160:VAL:HG13	1.69	0.74
2:F:198:LEU:HD21	2:F:278:LEU:HD22	1.70	0.74
1:C:7:LEU:HD21	2:D:307:MET:SD	2.29	0.73
2:F:164:ILE:HG22	2:F:334:ASP:HA	1.70	0.72
1:G:76:ILE:HG13	3:G:98:EPE:H101	1.71	0.72
2:F:182:MET:HE3	2:F:190:TYR:HE2	1.55	0.72
1:A:53:CYS:SG	1:A:58:LYS:HE3	2.30	0.71
2:H:154:LEU:HD21	2:H:160:VAL:CG1	2.21	0.71
2:B:255:PRO:HB3	2:B:261:TYR:CZ	2.26	0.71
1:G:51:ILE:HG12	1:G:55:ILE:HD11	1.71	0.71
2:H:277:LYS:HZ3	2:H:280:GLY:HA2	1.56	0.71
1:E:78:TYR:CE1	1:E:80:SER:HB2	2.26	0.70
1:C:38:ASN:HB2	3:C:98:EPE:H91	1.74	0.70
2:D:139:TYR:CE2	2:D:203:LYS:HG2	2.27	0.70
1:A:19:ILE:HG22	1:A:94:VAL:HG13	1.74	0.69
2:B:271:LEU:HB2	2:B:287:PRO:HB3	1.73	0.69
2:H:277:LYS:NZ	2:H:280:GLY:HA2	2.07	0.69
1:A:62:ASP:HB3	1:E:62:ASP:O	1.91	0.69
2:H:256:LEU:HB2	2:H:260:GLU:HG3	1.74	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:161:ASP:O	2:F:162:GLN:HB2	1.92	0.68
2:H:255:PRO:HB3	2:H:261:TYR:CE2	2.28	0.68
2:D:154:LEU:HD12	2:D:159:LEU:HB2	1.75	0.68
2:D:239:GLY:O	2:D:308:GLY:HA2	1.94	0.68
2:B:169:LEU:HG	2:B:171:ARG:HB2	1.75	0.68
1:G:67:TYR:HE1	1:G:88:SER:HB3	1.58	0.68
2:D:182:MET:HE1	2:D:187:ASP:HB2	1.77	0.67
3:A:98:EPE:H82	2:B:115:PHE:HA	1.75	0.67
2:B:172:ASP:HB2	2:B:173:PRO:CD	2.24	0.67
2:B:281:LYS:HD3	2:B:282:GLY:N	2.10	0.67
2:H:108:VAL:HB	2:H:159:LEU:HD13	1.77	0.67
2:F:295:SER:HA	2:F:300:THR:HA	1.77	0.66
1:C:72:THR:HB	1:C:87:LEU:HD12	1.76	0.66
1:A:16:TYR:CD2	2:B:131:PHE:HE1	2.14	0.66
2:H:278:LEU:HB2	2:H:283:TYR:CE1	2.30	0.66
1:C:15:TYR:HD1	2:D:179:GLY:HA3	1.62	0.65
1:C:39:LEU:O	3:C:98:EPE:H81	1.96	0.65
1:A:11:MET:HE1	2:D:296:GLN:NE2	2.12	0.65
2:B:169:LEU:C	2:B:171:ARG:H	2.06	0.64
1:G:7:LEU:HD22	2:H:238:VAL:HG21	1.78	0.64
2:B:293:LYS:HE2	2:B:302:CYS:SG	2.37	0.64
1:C:7:LEU:HD22	2:D:238:VAL:HG21	1.79	0.64
1:G:83:LEU:HD23	3:G:98:EPE:C9	2.24	0.63
2:D:195:LEU:HD23	2:D:343:ALA:HB2	1.81	0.63
2:F:287:PRO:HA	2:F:290:TYR:CE2	2.34	0.63
2:F:212:GLN:HG2	2:F:223:LYS:HA	1.81	0.62
1:G:87:LEU:CD2	3:G:98:EPE:H71	2.29	0.62
2:H:210:LEU:HD23	2:H:226:CYS:SG	2.39	0.62
2:B:168:TYR:CE2	2:B:170:SER:HA	2.35	0.62
2:H:228:ALA:HB1	2:H:321:LEU:HD13	1.81	0.62
2:B:281:LYS:HD3	2:B:282:GLY:H	1.63	0.62
2:F:199:ASN:O	2:F:208:VAL:HG12	1.99	0.62
2:H:176:GLN:N	2:H:177:PRO:HD2	2.14	0.62
2:B:256:LEU:HD22	1:C:49:LEU:HG	1.82	0.62
2:B:278:LEU:HB2	2:B:283:TYR:CE1	2.35	0.62
1:G:16:TYR:HB2	1:G:30:VAL:O	2.00	0.62
2:H:248:GLN:HB3	2:H:253:ALA:HB3	1.82	0.61
2:F:151:PHE:O	2:F:155:MET:HG3	2.01	0.61
2:B:257:ILE:O	2:B:258:GLN:HB2	2.01	0.60
2:D:176:GLN:HG3	2:D:177:PRO:HD2	1.83	0.60
1:C:38:ASN:CG	3:C:98:EPE:H22	2.26	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:199:ASN:HA	2:D:339:ARG:HA	1.84	0.60
1:A:76:ILE:HD13	1:A:76:ILE:H	1.67	0.60
1:A:55:ILE:HD12	2:B:129:ALA:CB	2.32	0.60
2:F:162:GLN:O	2:F:184:GLY:HA2	2.01	0.59
1:G:39:LEU:HA	2:H:134:ILE:O	2.01	0.59
1:E:76:ILE:HD12	2:F:144:VAL:HG11	1.85	0.59
1:G:21:ILE:HG12	1:G:92:VAL:HG22	1.85	0.59
2:B:296:GLN:NE2	1:C:11:MET:HE1	2.18	0.59
1:C:15:TYR:CE1	2:D:169:LEU:HB2	2.38	0.59
2:F:248:GLN:HB3	2:F:261:TYR:CD2	2.38	0.59
1:G:42:PRO:HB2	1:G:58:LYS:HG3	1.85	0.59
3:C:98:EPE:H21	2:D:144:VAL:HB	1.85	0.59
1:E:5:GLU:CG	1:E:78:TYR:HB2	2.33	0.59
2:H:323:ASP:HA	2:H:326:ILE:HB	1.84	0.59
1:C:4:PRO:HG3	2:D:309:MET:SD	2.43	0.59
2:F:141:ARG:HD3	2:F:203:LYS:O	2.02	0.59
1:G:4:PRO:HD2	1:G:7:LEU:HD12	1.84	0.59
2:B:328:ARG:HD3	2:B:329:TYR:CE1	2.38	0.58
2:F:285:LEU:HD21	2:F:325:PHE:HD1	1.67	0.58
2:B:210:LEU:HD23	2:B:226:CYS:SG	2.44	0.58
2:B:215:VAL:HG21	2:B:219:LEU:HD23	1.84	0.58
2:D:235:SER:O	2:D:324:VAL:HG23	2.03	0.58
1:E:55:ILE:HD13	1:E:55:ILE:H	1.68	0.58
1:C:4:PRO:HG3	2:D:309:MET:HE1	1.84	0.58
2:D:264:PRO:HB2	2:D:267:LYS:HB3	1.86	0.58
2:D:238:VAL:HA	2:D:307:MET:O	2.04	0.58
1:E:67:TYR:HE1	1:E:88:SER:HB3	1.69	0.57
2:H:176:GLN:HE21	2:H:176:GLN:HA	1.68	0.57
1:G:5:GLU:HG3	2:H:126:PHE:HZ	1.69	0.57
2:B:170:SER:O	2:B:172:ASP:N	2.37	0.57
1:E:42:PRO:HG2	1:E:57:HIS:O	2.04	0.57
2:D:157:GLN:HB2	2:D:159:LEU:HG	1.84	0.57
2:D:265:CYS:O	2:D:268:VAL:HB	2.05	0.57
1:E:84:SER:O	2:F:118:ALA:HA	2.04	0.57
2:F:271:LEU:HB2	2:F:287:PRO:HB3	1.86	0.57
2:B:138:ALA:CB	2:B:142:ILE:HD11	2.35	0.56
1:G:7:LEU:O	2:H:234:THR:HG23	2.04	0.56
2:H:238:VAL:HG22	2:H:307:MET:HB3	1.88	0.56
2:B:207:GLN:HB2	2:B:229:ILE:HG22	1.86	0.56
1:A:44:ILE:HA	1:A:58:LYS:HD2	1.87	0.56
2:B:263:ILE:HD12	2:B:291:THR:HG23	1.87	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:40:TRP:HB3	3:E:98:EPE:H52	1.88	0.56
1:A:16:TYR:CD2	2:B:131:PHE:CE1	2.94	0.56
1:A:85:GLY:HA3	2:B:117:GLU:O	2.05	0.56
1:C:37:SER:OG	2:D:138:ALA:HB3	2.06	0.56
1:A:11:MET:HG2	2:B:126:PHE:O	2.06	0.56
2:F:198:LEU:HD23	2:F:208:VAL:HG21	1.87	0.56
2:F:258:GLN:HE21	2:F:258:GLN:HA	1.71	0.56
2:H:211:ASP:HB2	2:H:277:LYS:HB3	1.88	0.56
1:E:42:PRO:HD3	2:F:132:ASP:O	2.05	0.55
1:G:94:VAL:O	2:H:107:GLY:HA3	2.07	0.55
1:C:5:GLU:CD	1:C:5:GLU:H	2.14	0.55
2:D:256:LEU:HB2	2:D:260:GLU:HB2	1.87	0.55
2:D:220:THR:HG22	2:D:223:LYS:HG2	1.88	0.55
2:D:266:GLU:H	2:D:266:GLU:CD	2.13	0.55
1:G:83:LEU:CD2	3:G:98:EPE:H92	2.27	0.55
2:F:144:VAL:HG12	2:F:145:ASN:ND2	2.22	0.55
2:F:241:VAL:HG11	1:G:75:ASP:N	2.21	0.55
2:F:258:GLN:HA	2:F:258:GLN:NE2	2.20	0.55
2:H:133:GLY:C	2:H:134:ILE:HD13	2.32	0.55
2:B:263:ILE:CG2	2:B:271:LEU:HD11	2.36	0.55
1:G:51:ILE:HG23	1:G:52:ALA:N	2.21	0.55
2:B:164:ILE:HD11	2:B:185:GLY:HA2	1.88	0.54
2:D:155:MET:HG2	2:D:163:ASN:CG	2.32	0.54
2:D:211:ASP:HB2	2:D:277:LYS:O	2.08	0.54
1:C:77:HIS:HD2	1:C:79:GLY:H	1.55	0.54
2:H:278:LEU:HB2	2:H:283:TYR:HE1	1.71	0.54
2:B:238:VAL:HG22	2:B:307:MET:HB3	1.90	0.54
1:C:7:LEU:HD22	2:D:238:VAL:CG2	2.38	0.54
2:D:228:ALA:HB1	2:D:321:LEU:HD13	1.89	0.54
2:H:110:VAL:CG1	2:H:153:ASN:HB3	2.38	0.54
2:H:229:ILE:CG2	2:H:318:LEU:HD13	2.36	0.54
1:A:7:LEU:HD13	2:B:238:VAL:HG21	1.90	0.53
2:H:285:LEU:HD21	2:H:325:PHE:HA	1.90	0.53
2:F:200:VAL:HA	2:F:207:GLN:O	2.08	0.53
2:F:242:ASP:HA	2:F:245:ARG:NH1	2.24	0.53
1:G:5:GLU:HB3	2:H:126:PHE:CE2	2.43	0.53
2:H:151:PHE:O	2:H:155:MET:HG3	2.09	0.53
2:F:121:GLN:HB2	2:F:122:PRO:HD2	1.90	0.53
1:A:53:CYS:O	1:A:58:LYS:NZ	2.38	0.53
1:C:77:HIS:CD2	1:C:79:GLY:H	2.26	0.53
2:D:173:PRO:C	2:D:175:ALA:H	2.17	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:213:VAL:HB	2:D:221:LEU:HB2	1.90	0.53
1:E:84:SER:HB2	2:F:120:LYS:HB3	1.91	0.53
1:A:95:PRO:HD2	2:B:107:GLY:HA3	1.90	0.53
2:D:229:ILE:HG23	2:D:318:LEU:HD13	1.90	0.53
2:F:212:GLN:HA	2:F:222:CYS:O	2.09	0.53
1:C:95:PRO:HG2	1:C:97:GLN:OXT	2.10	0.52
1:C:15:TYR:CD1	2:D:179:GLY:HA3	2.43	0.52
1:C:18:GLU:HG3	1:C:28:PHE:O	2.09	0.52
1:C:38:ASN:CB	3:C:98:EPE:H22	2.38	0.52
2:H:256:LEU:HB2	2:H:260:GLU:CG	2.38	0.52
2:F:244:VAL:O	2:F:248:GLN:HG2	2.10	0.52
2:F:251:ILE:O	2:F:271:LEU:HD22	2.09	0.52
2:B:165:PHE:HA	2:B:182:MET:O	2.10	0.52
1:C:22:GLY:HA2	1:C:90:ASP:OD1	2.09	0.52
2:H:124:ILE:HA	2:H:127:ILE:O	2.10	0.52
2:H:144:VAL:O	2:H:147:VAL:HG23	2.09	0.52
1:C:4:PRO:HG2	1:C:7:LEU:HD12	1.92	0.52
2:H:268:VAL:HA	2:H:271:LEU:HD13	1.91	0.52
1:C:75:ASP:O	1:C:76:ILE:HD13	2.10	0.51
2:F:241:VAL:HG21	1:G:75:ASP:HB2	1.92	0.51
1:G:47:LYS:O	1:G:48:LEU:HD23	2.10	0.51
2:B:166:SER:O	2:B:181:LEU:HA	2.09	0.51
2:B:221:LEU:HD11	2:B:247:LEU:HB2	1.93	0.51
1:A:51:ILE:O	1:A:55:ILE:HG12	2.10	0.51
1:A:16:TYR:OH	2:B:177:PRO:HB2	2.11	0.51
1:A:55:ILE:HD12	2:B:129:ALA:HB1	1.92	0.51
2:B:297:ALA:HB3	2:D:128:ALA:HB1	1.92	0.51
2:F:148:LEU:HD23	2:F:153:ASN:OD1	2.11	0.51
2:F:293:LYS:CE	2:F:302:CYS:SG	2.93	0.51
2:F:328:ARG:HG3	2:F:329:TYR:CD2	2.46	0.51
3:C:98:EPE:C2	2:D:144:VAL:HB	2.40	0.51
2:B:148:LEU:HD12	2:B:149:PRO:HD2	1.92	0.51
1:E:52:ALA:O	1:E:56:HIS:HB2	2.10	0.51
3:A:98:EPE:H72	2:B:147:VAL:HG11	1.93	0.51
1:C:8:LYS:NZ	1:C:35:GLY:HA3	2.26	0.51
1:G:32:PHE:HB3	2:H:167:PHE:HE2	1.76	0.51
2:H:188:SER:HA	2:H:191:TYR:CE1	2.45	0.50
2:B:248:GLN:HB3	2:B:261:TYR:CD2	2.46	0.50
2:D:315:SER:O	2:D:318:LEU:HD23	2.10	0.50
1:G:82:SER:HB2	2:H:120:LYS:NZ	2.26	0.50
1:C:68:VAL:HB	1:C:89:GLN:HB3	1.94	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:39:LEU:HD12	1:E:40:TRP:H	1.76	0.50
2:F:278:LEU:HB2	2:F:283:TYR:CE1	2.47	0.50
2:B:166:SER:HB2	2:B:330:TYR:CE1	2.47	0.50
2:F:182:MET:CE	2:F:190:TYR:HE2	2.23	0.50
1:A:9:ASN:ND2	2:B:235:SER:HB2	2.27	0.49
2:B:249:LYS:HA	2:B:249:LYS:CE	2.40	0.49
2:B:284:LYS:HG2	2:B:285:LEU:N	2.26	0.49
1:G:38:ASN:OD1	2:H:143:SER:HA	2.12	0.49
2:B:148:LEU:HD11	2:B:152:ASP:HB3	1.93	0.49
2:B:192:LYS:HD2	2:B:344:GLU:CD	2.37	0.49
2:B:253:ALA:HB1	2:B:261:TYR:HB3	1.94	0.49
2:D:110:VAL:CG1	2:D:153:ASN:HB3	2.42	0.49
2:D:139:TYR:OH	2:D:200:VAL:HG11	2.12	0.49
2:F:237:MET:HE1	2:F:321:LEU:HD22	1.93	0.49
1:G:77:HIS:O	1:G:79:GLY:N	2.45	0.49
2:H:262:MET:SD	2:H:303:LEU:HB3	2.52	0.49
2:H:264:PRO:HB2	2:H:267:LYS:HB3	1.93	0.49
2:B:240:PRO:O	2:B:244:VAL:HG23	2.12	0.49
2:D:172:ASP:OD1	2:D:173:PRO:HD3	2.12	0.49
2:F:264:PRO:HB2	2:F:267:LYS:CG	2.36	0.49
2:F:234:THR:O	2:F:322:GLY:HA3	2.13	0.49
2:H:256:LEU:HD12	2:H:260:GLU:HG3	1.95	0.49
1:E:9:ASN:O	1:E:10:TYR:HB2	2.12	0.49
2:F:265:CYS:HA	2:F:268:VAL:HG23	1.94	0.49
1:G:87:LEU:HD21	3:G:98:EPE:H71	1.95	0.49
2:D:163:ASN:O	2:D:335:ARG:HB2	2.11	0.49
1:A:7:LEU:O	2:B:234:THR:HG23	2.13	0.49
2:D:271:LEU:HB3	2:D:272:PRO:HD2	1.95	0.49
2:D:323:ASP:HA	2:D:326:ILE:HB	1.95	0.49
1:E:85:GLY:HA3	2:F:117:GLU:O	2.13	0.49
2:F:164:ILE:HD11	2:F:185:GLY:HA2	1.94	0.49
1:C:5:GLU:HB2	2:D:126:PHE:CZ	2.48	0.48
2:D:221:LEU:HD11	2:D:247:LEU:HB2	1.95	0.48
1:G:10:TYR:N	1:G:10:TYR:CD1	2.80	0.48
2:H:157:GLN:O	2:H:159:LEU:N	2.46	0.48
2:D:212:GLN:HA	2:D:222:CYS:O	2.13	0.48
2:F:331:THR:HG23	2:F:342:PHE:CE1	2.48	0.48
2:B:311:ILE:O	2:B:316:GLY:HA3	2.13	0.48
1:C:9:ASN:O	1:C:10:TYR:HB2	2.13	0.48
2:D:278:LEU:HB2	2:D:283:TYR:CE1	2.47	0.48
1:E:77:HIS:CG	2:H:309:MET:HE1	2.49	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:228:ALA:HB1	2:B:321:LEU:CD1	2.43	0.48
1:E:14:GLN:HG2	2:F:323:ASP:OD2	2.13	0.48
3:C:98:EPE:H21	2:D:144:VAL:CB	2.42	0.48
2:D:168:TYR:OH	2:D:170:SER:HB3	2.13	0.48
2:D:264:PRO:O	2:D:267:LYS:HB3	2.14	0.48
1:E:5:GLU:CD	1:E:78:TYR:HB2	2.39	0.48
1:G:39:LEU:O	3:G:98:EPE:H52	2.13	0.48
1:A:19:ILE:C	1:A:96:CYS:HB2	2.38	0.48
1:A:39:LEU:O	3:A:98:EPE:H81	2.13	0.48
2:D:154:LEU:CD1	2:D:159:LEU:HB2	2.43	0.48
1:C:40:TRP:HB3	3:C:98:EPE:H52	1.95	0.48
1:C:67:TYR:CZ	1:C:69:LYS:HA	2.49	0.48
1:E:6:VAL:HG21	1:G:77:HIS:NE2	2.28	0.48
1:E:14:GLN:O	2:F:178:GLY:HA2	2.13	0.48
1:C:8:LYS:HZ1	1:C:35:GLY:HA3	1.79	0.48
2:D:211:ASP:O	2:D:225:GLY:HA2	2.13	0.48
2:H:330:TYR:HB3	2:H:343:ALA:HB3	1.95	0.47
1:C:4:PRO:HG3	2:D:309:MET:CE	2.44	0.47
1:C:87:LEU:HA	2:D:115:PHE:O	2.13	0.47
1:G:42:PRO:HD3	2:H:132:ASP:O	2.13	0.47
3:A:98:EPE:C8	2:B:115:PHE:HA	2.41	0.47
2:B:155:MET:HE3	2:B:163:ASN:ND2	2.28	0.47
2:B:229:ILE:O	2:B:229:ILE:HG13	2.13	0.47
2:F:253:ALA:HB1	2:F:261:TYR:HB3	1.95	0.47
1:G:5:GLU:HB3	2:H:126:PHE:HE2	1.79	0.47
2:H:196:SER:O	2:H:341:GLY:HA2	2.15	0.47
1:E:54:TRP:HD1	1:E:55:ILE:HG23	1.80	0.47
2:F:196:SER:O	2:F:341:GLY:HA2	2.14	0.47
2:F:278:LEU:HB2	2:F:283:TYR:CD1	2.50	0.47
1:A:9:ASN:C	1:A:11:MET:H	2.23	0.47
1:C:10:TYR:CD1	1:C:10:TYR:N	2.83	0.47
2:D:200:VAL:HA	2:D:207:GLN:O	2.14	0.47
1:C:5:GLU:HG3	1:C:78:TYR:O	2.15	0.47
2:H:263:ILE:HD13	2:H:271:LEU:HD21	1.96	0.47
1:C:34:THR:HG23	2:D:232:THR:OG1	2.15	0.47
1:E:40:TRP:HE1	2:F:134:ILE:HD12	1.79	0.47
2:F:211:ASP:HB2	2:F:277:LYS:O	2.15	0.47
2:F:274:ILE:HD12	2:F:306:PHE:CE2	2.50	0.47
1:A:68:VAL:HB	1:A:89:GLN:HB3	1.95	0.46
2:B:260:GLU:CD	2:B:260:GLU:H	2.24	0.46
2:D:262:MET:HE3	2:D:302:CYS:O	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:7:LEU:HD22	2:H:238:VAL:CG2	2.45	0.46
1:C:31:VAL:HB	2:D:134:ILE:HG13	1.97	0.46
2:D:334:ASP:HB3	2:D:339:ARG:HG2	1.96	0.46
2:H:229:ILE:HG21	2:H:318:LEU:HD13	1.97	0.46
1:A:3:ILE:HD13	2:B:205:TYR:CZ	2.50	0.46
2:F:110:VAL:HG22	2:F:154:LEU:HD12	1.97	0.46
2:B:244:VAL:O	2:B:248:GLN:HG2	2.15	0.46
2:H:230:VAL:HG21	2:H:340:VAL:HG11	1.98	0.46
1:A:61:SER:HB2	1:A:67:TYR:CD2	2.51	0.46
2:B:138:ALA:HB3	2:B:142:ILE:HD11	1.98	0.46
2:B:169:LEU:C	2:B:171:ARG:N	2.71	0.46
2:H:155:MET:SD	2:H:163:ASN:HB3	2.56	0.46
2:H:198:LEU:HD21	2:H:278:LEU:HB3	1.98	0.46
2:D:197:TYR:O	2:D:198:LEU:HD12	2.16	0.46
1:G:93:SER:HA	2:H:108:VAL:O	2.15	0.46
2:H:162:GLN:O	2:H:184:GLY:HA2	2.15	0.46
2:F:256:LEU:HG	2:F:262:MET:HG2	1.98	0.46
1:C:67:TYR:HE1	1:C:88:SER:HB3	1.81	0.45
2:F:247:LEU:HD11	2:F:274:ILE:HD13	1.97	0.45
1:G:85:GLY:HA2	2:H:119:THR:HG23	1.99	0.45
2:H:144:VAL:HG12	2:H:145:ASN:HD22	1.81	0.45
2:H:221:LEU:HD13	2:H:247:LEU:HD12	1.99	0.45
2:B:152:ASP:O	2:B:155:MET:HB2	2.16	0.45
1:G:15:TYR:OH	2:H:169:LEU:HB2	2.17	0.45
2:H:212:GLN:HA	2:H:222:CYS:HB3	1.98	0.45
2:H:265:CYS:HA	2:H:268:VAL:HG23	1.99	0.45
2:D:264:PRO:HB2	2:D:267:LYS:CB	2.46	0.45
2:F:165:PHE:HA	2:F:182:MET:O	2.17	0.45
1:G:19:ILE:HG22	1:G:94:VAL:HG12	1.97	0.45
1:G:34:THR:HG23	2:H:232:THR:OG1	2.15	0.45
1:A:69:LYS:HG3	1:A:70:ASN:N	2.32	0.45
2:B:169:LEU:O	2:B:171:ARG:N	2.50	0.45
1:C:42:PRO:HB2	1:C:58:LYS:HG2	1.98	0.45
2:H:216:ALA:HB3	2:H:272:PRO:HB2	1.98	0.45
1:A:43:SER:HB2	2:B:117:GLU:HB3	1.99	0.45
2:B:295:SER:HA	2:B:299:LYS:O	2.16	0.45
1:G:85:GLY:HA3	2:H:117:GLU:O	2.17	0.45
2:F:222:CYS:SG	2:F:226:CYS:N	2.90	0.45
2:F:224:GLU:HB2	4:F:371:HOH:O	2.16	0.45
1:A:19:ILE:O	1:A:96:CYS:HB2	2.17	0.45
1:A:55:ILE:HD12	2:B:129:ALA:HB2	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:8:LYS:HE3	4:C:476:HOH:O	2.17	0.45
2:D:196:SER:O	2:D:341:GLY:HA2	2.15	0.45
2:F:244:VAL:HG11	2:F:308:GLY:N	2.32	0.45
1:E:56:HIS:NE2	2:F:131:PHE:O	2.50	0.44
2:F:171:ARG:NH2	2:F:345:ALA:HB3	2.32	0.44
2:H:202:ARG:HH22	2:H:318:LEU:HD21	1.82	0.44
2:B:207:GLN:CB	2:B:229:ILE:HG22	2.46	0.44
1:A:59:TYR:CE2	2:B:115:PHE:HZ	2.35	0.44
2:D:197:TYR:C	2:D:198:LEU:HD12	2.43	0.44
3:G:98:EPE:C8	2:H:115:PHE:HA	2.47	0.44
1:C:11:MET:HB2	4:C:338:HOH:O	2.18	0.44
2:F:110:VAL:CG1	2:F:153:ASN:HB3	2.48	0.44
2:F:187:ASP:OD1	2:F:189:LYS:HG2	2.17	0.44
2:B:182:MET:HE3	2:B:190:TYR:HE2	1.83	0.44
1:E:37:SER:OG	2:F:138:ALA:HB3	2.17	0.44
1:C:54:TRP:CD1	1:C:55:ILE:HG23	2.53	0.44
2:D:216:ALA:HB3	2:D:272:PRO:HB2	1.99	0.44
1:E:9:ASN:ND2	2:F:235:SER:OG	2.51	0.44
1:E:76:ILE:CD1	2:F:144:VAL:HG11	2.47	0.44
1:C:94:VAL:HG11	2:D:183:LEU:HD11	1.99	0.44
2:F:182:MET:HE1	2:F:187:ASP:HB2	2.00	0.44
2:H:245:ARG:NH1	2:H:249:LYS:HE3	2.33	0.44
2:B:230:VAL:HG21	2:B:340:VAL:HG11	1.99	0.44
1:C:43:SER:HB2	2:D:117:GLU:HB2	2.00	0.44
1:G:15:TYR:HD1	2:H:179:GLY:HA3	1.83	0.44
2:H:152:ASP:O	2:H:156:GLN:HG3	2.18	0.44
2:H:315:SER:O	2:H:318:LEU:HG	2.18	0.44
2:D:299:LYS:HD2	2:D:299:LYS:HA	1.82	0.43
1:E:33:ASP:C	1:E:35:GLY:H	2.26	0.43
2:F:216:ALA:HB3	2:F:272:PRO:HB3	2.00	0.43
2:F:312:PRO:HA	2:F:313:PRO:HD3	1.71	0.43
1:G:56:HIS:HE1	4:H:350:HOH:O	2.00	0.43
2:B:182:MET:HE3	2:B:190:TYR:CE2	2.54	0.43
2:D:223:LYS:NZ	2:D:223:LYS:HB3	2.32	0.43
1:E:5:GLU:CD	1:E:5:GLU:H	2.26	0.43
2:F:307:MET:HE3	2:F:307:MET:HB2	1.96	0.43
1:G:51:ILE:CG2	1:G:52:ALA:N	2.81	0.43
1:C:33:ASP:C	1:C:35:GLY:H	2.26	0.43
2:D:162:GLN:HB2	2:D:184:GLY:O	2.19	0.43
2:D:165:PHE:HA	2:D:182:MET:O	2.18	0.43
2:F:213:VAL:O	2:F:221:LEU:N	2.51	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:176:GLN:N	2:H:177:PRO:CD	2.79	0.43
2:B:155:MET:HE3	2:B:163:ASN:HD22	1.83	0.43
2:D:210:LEU:HA	2:D:278:LEU:HD23	1.99	0.43
1:E:10:TYR:HB3	2:F:127:ILE:HA	2.00	0.43
1:G:18:GLU:HA	1:G:28:PHE:O	2.18	0.43
3:G:98:EPE:H61	3:G:98:EPE:S	2.58	0.43
2:H:202:ARG:HH22	2:H:318:LEU:HD11	1.82	0.43
1:G:77:HIS:HE1	1:G:80:SER:O	2.01	0.43
1:G:84:SER:OG	2:H:120:LYS:HB3	2.18	0.43
1:E:18:GLU:HA	1:E:28:PHE:O	2.19	0.43
2:H:202:ARG:NH2	2:H:318:LEU:HD11	2.33	0.43
2:B:182:MET:HE1	2:B:187:ASP:HB2	1.99	0.43
1:C:94:VAL:O	2:D:107:GLY:HA3	2.18	0.43
3:G:98:EPE:H81	2:H:115:PHE:HA	1.99	0.43
2:H:110:VAL:HG11	2:H:153:ASN:HB3	2.00	0.43
1:A:93:SER:HA	2:B:108:VAL:O	2.19	0.43
1:C:7:LEU:CD2	2:D:307:MET:SD	3.04	0.43
1:C:42:PRO:HG2	1:C:56:HIS:HB3	1.99	0.43
2:F:238:VAL:HA	2:F:307:MET:O	2.18	0.43
1:E:10:TYR:N	1:E:10:TYR:CD1	2.86	0.43
2:H:278:LEU:HD12	2:H:283:TYR:CD1	2.53	0.43
1:A:22:GLY:HA2	1:A:90:ASP:OD1	2.19	0.43
2:B:294:VAL:O	2:B:300:THR:HA	2.18	0.42
2:D:285:LEU:HD23	2:D:328:ARG:HD3	2.01	0.42
1:G:7:LEU:HD21	2:H:309:MET:HE2	2.01	0.42
2:H:238:VAL:HB	2:H:320:ILE:HB	2.02	0.42
1:C:20:GLY:HA2	1:C:26:GLN:O	2.19	0.42
2:F:235:SER:HA	2:F:323:ASP:H	1.85	0.42
2:F:256:LEU:HB2	2:F:260:GLU:OE2	2.19	0.42
2:H:337:ASN:O	2:H:338:ASN:C	2.63	0.42
2:B:283:TYR:CD1	2:B:283:TYR:N	2.87	0.42
1:E:85:GLY:HA2	2:F:119:THR:OG1	2.19	0.42
1:G:95:PRO:C	1:G:97:GLN:H	2.27	0.42
3:G:98:EPE:H22	3:G:98:EPE:O2S	2.19	0.42
2:H:221:LEU:HD23	2:H:243:GLU:HB3	2.02	0.42
2:B:263:ILE:O	2:B:302:CYS:HB2	2.19	0.42
1:C:19:ILE:HG22	1:C:94:VAL:HG22	1.99	0.42
1:C:85:GLY:HA3	2:D:118:ALA:HA	2.01	0.42
2:F:182:MET:CE	2:F:190:TYR:CE2	3.02	0.42
1:G:55:ILE:HG13	2:H:129:ALA:HB1	2.01	0.42
2:B:278:LEU:HD12	2:B:283:TYR:CD1	2.55	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:51:ILE:HD13	1:C:51:ILE:HA	1.92	0.42
1:C:78:TYR:N	1:C:81:GLY:O	2.53	0.42
2:F:111:GLU:N	2:F:157:GLN:HE22	2.18	0.42
2:H:219:LEU:HD12	2:H:220:THR:H	1.85	0.42
2:D:133:GLY:C	2:D:134:ILE:HD12	2.44	0.42
1:E:57:HIS:O	1:E:58:LYS:HG3	2.20	0.42
2:H:206:TRP:CH2	2:H:335:ARG:HD2	2.55	0.42
1:A:24:PRO:HA	1:A:25:PRO:HD3	1.92	0.42
2:D:154:LEU:HD11	2:D:160:VAL:HG13	2.02	0.42
1:G:5:GLU:HG2	1:G:78:TYR:C	2.45	0.42
2:H:312:PRO:HA	2:H:313:PRO:HD3	1.87	0.42
1:A:43:SER:C	1:A:58:LYS:HB3	2.45	0.41
2:B:142:ILE:HG23	2:B:204:ALA:HB1	2.01	0.41
2:D:182:MET:HE3	2:D:190:TYR:HE2	1.85	0.41
2:D:331:THR:HG22	2:D:332:VAL:N	2.35	0.41
2:D:333:PHE:CD1	2:D:333:PHE:N	2.89	0.41
2:D:181:LEU:HD21	2:D:183:LEU:HD21	2.01	0.41
1:C:52:ALA:O	1:C:56:HIS:HB2	2.20	0.41
2:D:262:MET:C	2:D:263:ILE:HG13	2.45	0.41
2:F:168:TYR:CD1	2:F:168:TYR:C	2.98	0.41
2:H:215:VAL:HB	2:H:219:LEU:HB3	2.03	0.41
2:D:222:CYS:SG	2:D:226:CYS:N	2.93	0.41
2:F:172:ASP:HA	2:F:173:PRO:HD3	1.91	0.41
1:G:20:GLY:O	1:G:92:VAL:HA	2.21	0.41
1:A:74:PHE:CD1	1:A:74:PHE:C	2.97	0.41
2:B:230:VAL:HG12	2:B:326:ILE:CD1	2.39	0.41
2:B:242:ASP:O	2:B:245:ARG:HG2	2.20	0.41
2:B:294:VAL:HG12	2:B:295:SER:N	2.35	0.41
2:B:295:SER:HA	2:B:300:THR:HA	2.03	0.41
2:F:122:PRO:HG2	2:F:127:ILE:HD12	2.02	0.41
2:F:201:THR:HG22	4:F:435:HOH:O	2.19	0.41
2:F:301:LEU:HD12	2:F:301:LEU:N	2.35	0.41
2:H:169:LEU:HD12	2:H:169:LEU:HA	1.83	0.41
1:C:10:TYR:N	1:C:10:TYR:HD1	2.17	0.41
1:C:19:ILE:O	1:C:27:CYS:HA	2.20	0.41
1:C:67:TYR:OH	1:C:69:LYS:HA	2.20	0.41
1:E:34:THR:HG23	2:F:232:THR:OG1	2.21	0.41
2:H:181:LEU:HD12	2:H:182:MET:H	1.84	0.41
1:E:51:ILE:O	1:E:55:ILE:HD13	2.20	0.41
1:A:55:ILE:HG12	1:A:55:ILE:H	1.69	0.41
2:D:256:LEU:HD11	2:D:262:MET:HG3	2.01	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:112:ARG:HB3	4:H:429:HOH:O	2.20	0.41
2:H:165:PHE:HA	2:H:182:MET:O	2.20	0.41
2:H:254:VAL:O	2:H:261:TYR:HA	2.21	0.41
2:D:162:GLN:O	2:D:184:GLY:HA2	2.21	0.41
2:D:245:ARG:HB3	2:D:245:ARG:NH1	2.36	0.41
1:E:17:GLY:N	1:E:32:PHE:CE2	2.89	0.41
2:F:289:ASP:OD2	2:F:328:ARG:HD2	2.21	0.41
1:A:77:HIS:O	1:A:79:GLY:N	2.54	0.40
2:B:337:ASN:O	2:B:338:ASN:HB2	2.21	0.40
1:C:3:ILE:HD11	2:D:229:ILE:CD1	2.52	0.40
2:B:266:GLU:HG2	2:B:267:LYS:N	2.34	0.40
1:E:94:VAL:HA	1:E:95:PRO:HA	1.77	0.40
2:H:175:ALA:C	2:H:177:PRO:HD2	2.46	0.40
1:A:9:ASN:O	1:A:11:MET:N	2.54	0.40
2:B:215:VAL:CG2	2:B:219:LEU:HD23	2.50	0.40
2:D:294:VAL:HG12	2:D:301:LEU:HD13	2.03	0.40
2:F:237:MET:HE1	2:F:321:LEU:CD2	2.51	0.40
2:H:271:LEU:HB3	2:H:290:TYR:OH	2.21	0.40
1:E:38:ASN:OD1	3:E:98:EPE:H22	2.22	0.40
2:F:140:PRO:HB3	2:F:149:PRO:HD2	2.04	0.40
2:F:142:ILE:HG23	2:F:204:ALA:HB1	2.03	0.40

There are no symmetry-related clashes.

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	93/97 (96%)	80 (86%)	10 (11%)	3 (3%)	3	4
1	C	93/97 (96%)	83 (89%)	9 (10%)	1 (1%)	11	22
1	E	93/97 (96%)	83 (89%)	9 (10%)	1 (1%)	11	22
1	G	93/97 (96%)	79 (85%)	12 (13%)	2 (2%)	5	9

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	B	239/241 (99%)	209 (87%)	23 (10%)	7 (3%)	3	5
2	D	239/241 (99%)	215 (90%)	18 (8%)	6 (2%)	4	7
2	F	239/241 (99%)	218 (91%)	13 (5%)	8 (3%)	3	4
2	H	239/241 (99%)	211 (88%)	24 (10%)	4 (2%)	7	13
All	All	1328/1352 (98%)	1178 (89%)	118 (9%)	32 (2%)	4	8

All (32) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	78	TYR
2	B	171	ARG
2	B	173	PRO
1	C	9	ASN
2	D	216	ALA
1	E	9	ASN
2	F	162	GLN
1	G	78	TYR
2	H	158	LYS
2	H	260	GLU
1	A	9	ASN
1	A	79	GLY
2	B	170	SER
2	B	172	ASP
2	D	124	ILE
2	D	268	VAL
2	F	107	GLY
2	F	123	GLY
2	D	172	ASP
2	D	269	SER
2	F	204	ALA
2	H	338	ASN
2	B	203	LYS
2	D	217	SER
2	F	174	ASP
1	G	10	TYR
2	H	123	GLY
2	B	107	GLY
2	B	218	GLY
2	F	257	ILE
2	F	218	GLY
2	F	150	VAL

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	84/86 (98%)	75 (89%)	9 (11%)	6	13
1	C	84/86 (98%)	82 (98%)	2 (2%)	43	70
1	E	84/86 (98%)	79 (94%)	5 (6%)	17	36
1	G	84/86 (98%)	71 (84%)	13 (16%)	2	5
2	B	199/199 (100%)	188 (94%)	11 (6%)	19	40
2	D	199/199 (100%)	184 (92%)	15 (8%)	12	26
2	F	199/199 (100%)	186 (94%)	13 (6%)	15	32
2	H	199/199 (100%)	190 (96%)	9 (4%)	24	49
All	All	1132/1140 (99%)	1055 (93%)	77 (7%)	14	31

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

Mol	Chain	Res	Type
1	A	29	THR
1	A	41	VAL
1	A	55	ILE
1	A	58	LYS
1	A	72	THR
1	A	76	ILE
1	A	78	TYR
1	A	80	SER
1	A	94	VAL
2	B	108	VAL
2	B	135	LEU
2	B	170	SER
2	B	199	ASN
2	B	217	SER
2	B	230	VAL
2	B	243	GLU
2	B	246	GLU
2	B	249	LYS
2	B	270	THR

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Mol	Chain	Res	Type
2	B	309	MET
1	C	55	ILE
1	C	66	THR
2	D	109	LYS
2	D	124	ILE
2	D	160	VAL
2	D	172	ASP
2	D	214	GLU
2	D	220	THR
2	D	245	ARG
2	D	258	GLN
2	D	271	LEU
2	D	277	LYS
2	D	301	LEU
2	D	303	LEU
2	D	309	MET
2	D	315	SER
2	D	318	LEU
1	E	5	GLU
1	E	55	ILE
1	E	69	LYS
1	E	93	SER
1	E	96	CYS
2	F	124	ILE
2	F	135	LEU
2	F	154	LEU
2	F	177	PRO
2	F	181	LEU
2	F	198	LEU
2	F	232	THR
2	F	266	GLU
2	F	270	THR
2	F	291	THR
2	F	303	LEU
2	F	307	MET
2	F	309	MET
1	G	5	GLU
1	G	23	THR
1	G	29	THR
1	G	44	ILE
1	G	47	LYS
1	G	48	LEU

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Mol	Chain	Res	Type
1	G	55	ILE
1	G	61	SER
1	G	66	THR
1	G	78	TYR
1	G	93	SER
1	G	94	VAL
1	G	96	CYS
2	H	121	GLN
2	H	122	PRO
2	H	154	LEU
2	H	162	GLN
2	H	241	VAL
2	H	266	GLU
2	H	301	LEU
2	H	303	LEU
2	H	310	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (20) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	89	GLN
2	B	162	GLN
2	B	199	ASN
2	B	338	ASN
1	C	77	HIS
1	C	89	GLN
2	D	153	ASN
2	D	337	ASN
1	E	9	ASN
1	E	57	HIS
2	F	121	GLN
2	F	145	ASN
2	F	162	GLN
2	F	258	GLN
1	G	56	HIS
2	H	145	ASN
2	H	176	GLN
2	H	199	ASN
2	H	337	ASN
2	H	338	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

4 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	EPE	A	98	-	15,15,15	1.18	2 (13%)	19,20,20	2.29	8 (42%)
3	EPE	G	98	-	15,15,15	0.86	1 (6%)	19,20,20	1.93	5 (26%)
3	EPE	E	98	-	15,15,15	1.23	2 (13%)	19,20,20	2.22	7 (36%)
3	EPE	C	98	-	15,15,15	1.34	2 (13%)	19,20,20	2.33	6 (31%)

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	EPE	A	98	-	-	1/9/19/19	0/1/1/1
3	EPE	G	98	-	-	1/9/19/19	0/1/1/1
3	EPE	E	98	-	-	4/9/19/19	0/1/1/1
3	EPE	C	98	-	-	6/9/19/19	0/1/1/1

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	98	EPE	O3S-S	3.59	1.60	1.47
3	C	98	EPE	C10-S	3.44	1.82	1.77
3	E	98	EPE	O3S-S	3.38	1.59	1.47
3	E	98	EPE	C10-S	2.91	1.81	1.77
3	A	98	EPE	O3S-S	2.69	1.57	1.47
3	A	98	EPE	C10-S	2.40	1.81	1.77
3	G	98	EPE	O3S-S	2.17	1.55	1.47

All (26) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	E	98	EPE	C5-N4-C3	-5.50	96.99	108.84
3	C	98	EPE	C5-N4-C3	-5.10	97.84	108.84
3	C	98	EPE	O3S-S-O2S	-4.51	100.11	111.40
3	C	98	EPE	C3-C2-N1	4.51	119.74	110.65
3	A	98	EPE	O3S-S-C10	3.98	113.80	106.00
3	E	98	EPE	C9-N1-C2	-3.90	100.86	111.24
3	G	98	EPE	C7-N4-C3	-3.87	100.92	111.24
3	A	98	EPE	C9-N1-C2	3.85	121.50	111.24
3	G	98	EPE	O1S-S-C10	3.78	112.44	106.73
3	A	98	EPE	O3S-S-O1S	-3.51	102.63	111.40
3	A	98	EPE	O1S-S-C10	3.38	111.84	106.73
3	E	98	EPE	C3-C2-N1	3.29	117.28	110.65
3	C	98	EPE	O3S-S-C10	3.24	112.34	106.00
3	C	98	EPE	C5-C6-N1	3.14	116.99	110.65
3	A	98	EPE	O3S-S-O2S	-3.11	103.62	111.40
3	A	98	EPE	C5-N4-C3	2.97	115.24	108.84
3	E	98	EPE	O3S-S-O1S	-2.87	104.21	111.40
3	E	98	EPE	O3S-S-C10	2.86	111.61	106.00
3	A	98	EPE	C7-N4-C5	-2.81	103.74	111.24
3	G	98	EPE	C6-N1-C2	2.67	114.59	108.84
3	A	98	EPE	C6-N1-C2	2.65	114.55	108.84
3	C	98	EPE	C9-N1-C2	-2.44	104.73	111.24
3	E	98	EPE	C5-C6-N1	2.34	115.38	110.65
3	G	98	EPE	C6-C5-N4	-2.32	105.97	110.65
3	G	98	EPE	O3S-S-O2S	-2.21	105.87	111.40
3	E	98	EPE	O1S-S-C10	2.11	109.91	106.73

There are no chirality outliers.

All (12) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	98	EPE	C10-C9-N1-C6
3	C	98	EPE	C9-C10-S-O2S
3	C	98	EPE	C9-C10-S-O3S
3	C	98	EPE	C8-C7-N4-C3
3	E	98	EPE	C9-C10-S-O3S
3	C	98	EPE	C9-C10-S-O1S
3	E	98	EPE	C9-C10-S-O1S
3	E	98	EPE	C9-C10-S-O2S
3	C	98	EPE	S-C10-C9-N1
3	E	98	EPE	C10-C9-N1-C6
3	G	98	EPE	C10-C9-N1-C2
3	C	98	EPE	C8-C7-N4-C5

There are no ring outliers.

4 monomers are involved in 25 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	98	EPE	4	0
3	G	98	EPE	11	0
3	E	98	EPE	2	0
3	C	98	EPE	8	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

EDS was not executed - this section is therefore empty.

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

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates

EDS was not executed - this section is therefore empty.

6.4 Ligands

EDS was not executed - this section is therefore empty.

6.5 Other polymers

EDS was not executed - this section is therefore empty.