



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 28, 2014 – 01:45 AM GMT

PDB ID : 1V02
Title : CRYSTAL STRUCTURE OF THE SORGHUM BICOLOR DHURRINASE 1
Authors : Moriniere, J.; Verdoucq, L.; Bevan, D.R.; Esen, A.; Henrissat, B.; Czjzek, M.
Deposited on : 2004-03-22
Resolution : 1.80 Å(reported)

This is a full wwPDB 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/ValidationPDFNotes.html>

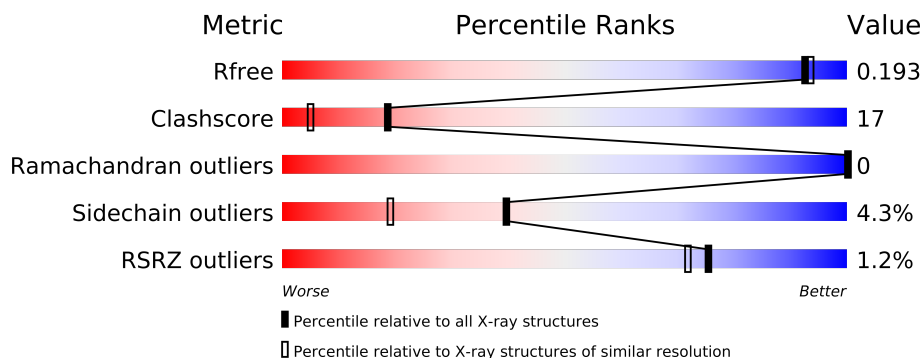
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.15 2013
Xtriage (Phenix) : dev-1323
EDS : stable22639
Percentile statistics : 21963
Refmac : 5.8.0049
CCP4 : 6.3.0 (Settle)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP) : stable22683

1 Overall quality at a glance

The reported resolution of this entry is 1.80 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}	66092	3513 (1.80-1.80)
Clashscore	79885	4461 (1.80-1.80)
Ramachandran outliers	78287	4404 (1.80-1.80)
Sidechain outliers	78261	4403 (1.80-1.80)
RSRZ outliers	66119	3515 (1.80-1.80)

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. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Mol	Chain	Length	Quality of chain
1	A	565	
1	B	565	
1	C	565	
1	D	565	
1	F	565	
2	E	565	

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 28327 atoms, of which 0 are hydrogen and 0 are deuterium.

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 DHURRINASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	484	Total	C	N	O	S	0	0	0
			3875	2476	652	728	19			
1	B	484	Total	C	N	O	S	0	0	0
			3875	2476	652	728	19			
1	C	484	Total	C	N	O	S	0	0	0
			3875	2476	652	728	19			
1	D	484	Total	C	N	O	S	0	0	0
			3875	2476	652	728	19			
1	F	484	Total	C	N	O	S	0	0	0
			3875	2476	652	728	19			

There are 20 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	119	ARG	GLY	CONFLICT	UNP Q41290
A	161	ARG	GLU	CONFLICT	UNP Q41290
A	162	ILE	ASP	CONFLICT	UNP Q41290
A	163	ILE	TYR	CONFLICT	UNP Q41290
B	119	ARG	GLY	CONFLICT	UNP Q41290
B	161	ARG	GLU	CONFLICT	UNP Q41290
B	162	ILE	ASP	CONFLICT	UNP Q41290
B	163	ILE	TYR	CONFLICT	UNP Q41290
C	119	ARG	GLY	CONFLICT	UNP Q41290
C	161	ARG	GLU	CONFLICT	UNP Q41290
C	162	ILE	ASP	CONFLICT	UNP Q41290
C	163	ILE	TYR	CONFLICT	UNP Q41290
D	119	ARG	GLY	CONFLICT	UNP Q41290
D	161	ARG	GLU	CONFLICT	UNP Q41290
D	162	ILE	ASP	CONFLICT	UNP Q41290
D	163	ILE	TYR	CONFLICT	UNP Q41290
F	119	ARG	GLY	CONFLICT	UNP Q41290
F	161	ARG	GLU	CONFLICT	UNP Q41290
F	162	ILE	ASP	CONFLICT	UNP Q41290

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
F	163	ILE	TYR	CONFLICT	UNP Q41290

- Molecule 2 is a protein called DHURRINASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	E	484	Total	C	N	O	S	0	0	0
			3884	2482	656	727	19			

There are 5 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
E	119	ARG	GLY	CONFLICT	UNP Q41290
E	161	ARG	GLU	CONFLICT	UNP Q41290
E	162	ILE	ASP	CONFLICT	UNP Q41290
E	163	ILE	TYR	CONFLICT	UNP Q41290
E	180	LYS	THR	CONFLICT	UNP Q41290

- Molecule 3 is water.

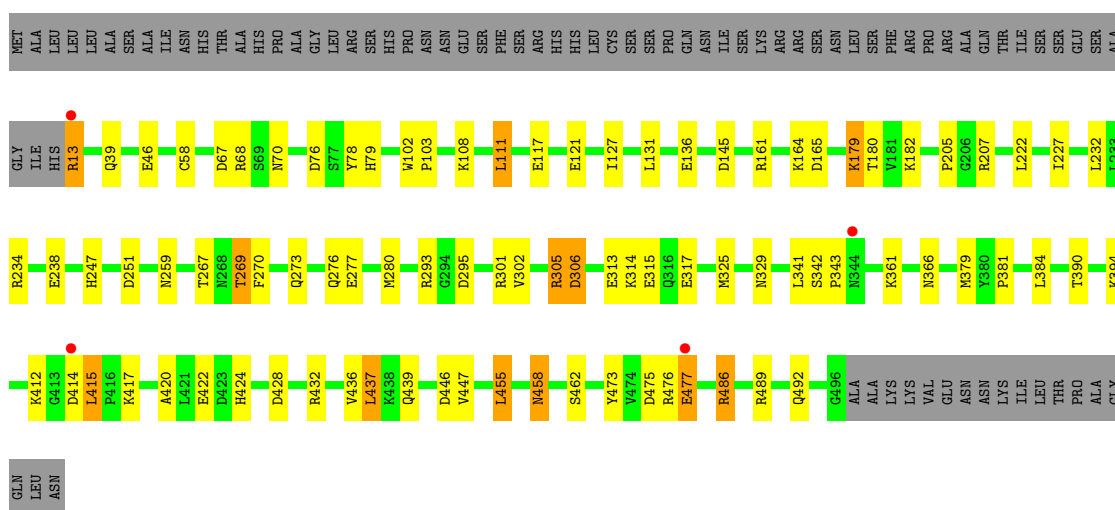
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	846	Total	O	0	0
			846	846		
3	B	860	Total	O	0	0
			860	860		
3	C	832	Total	O	0	0
			832	832		
3	D	827	Total	O	0	0
			827	827		
3	E	869	Total	O	0	0
			869	869		
3	F	834	Total	O	0	0
			834	834		

3 Residue-property plots

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.

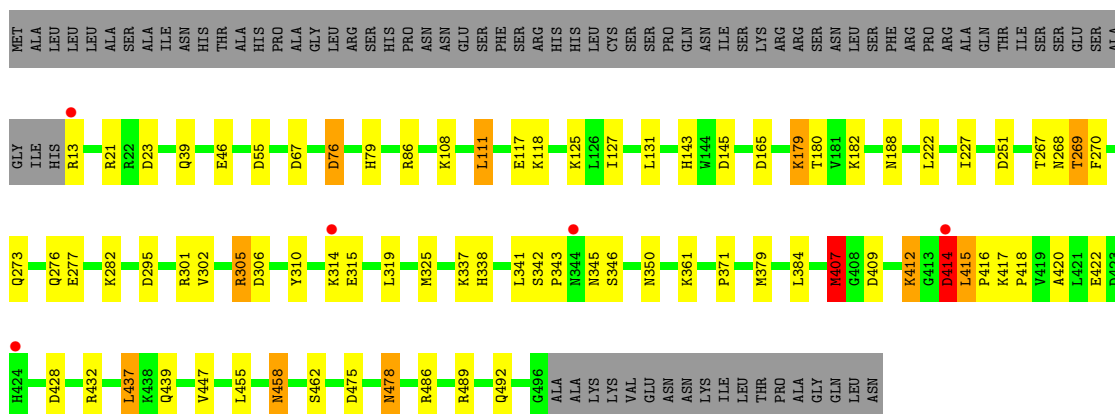
• Molecule 1: DHURRINASE

Chain A: 



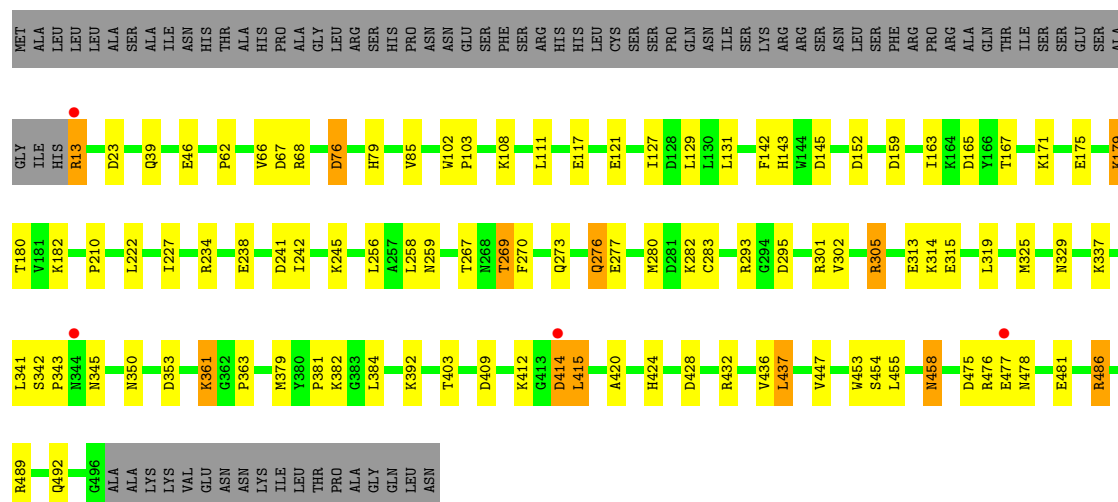
• Molecule 1: DHURRINASE

Chain B: 



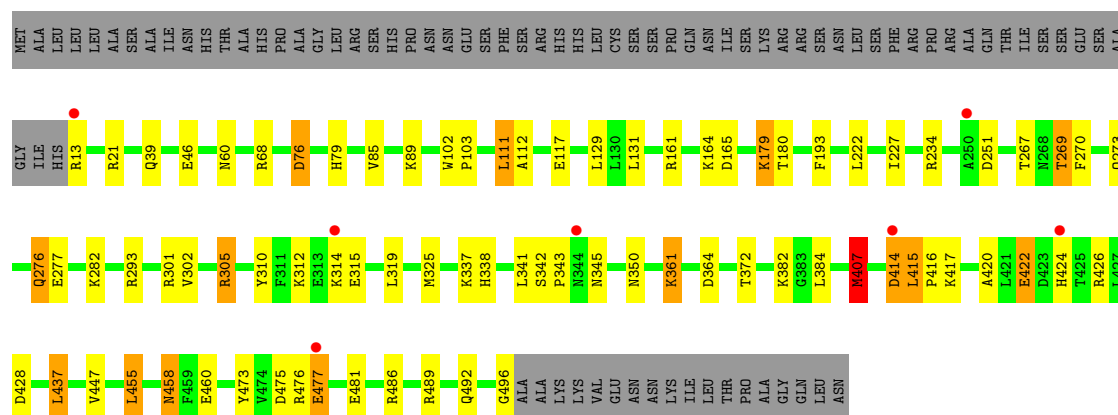
• Molecule 1: DHURRINASE

Chain C: 



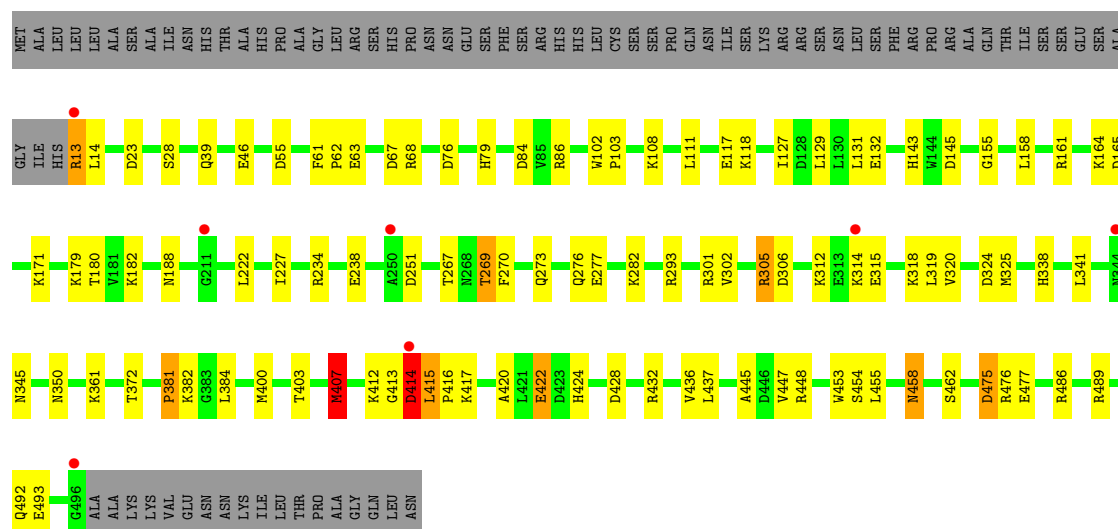
• Molecule 1: DHURRINASE

Chain D:



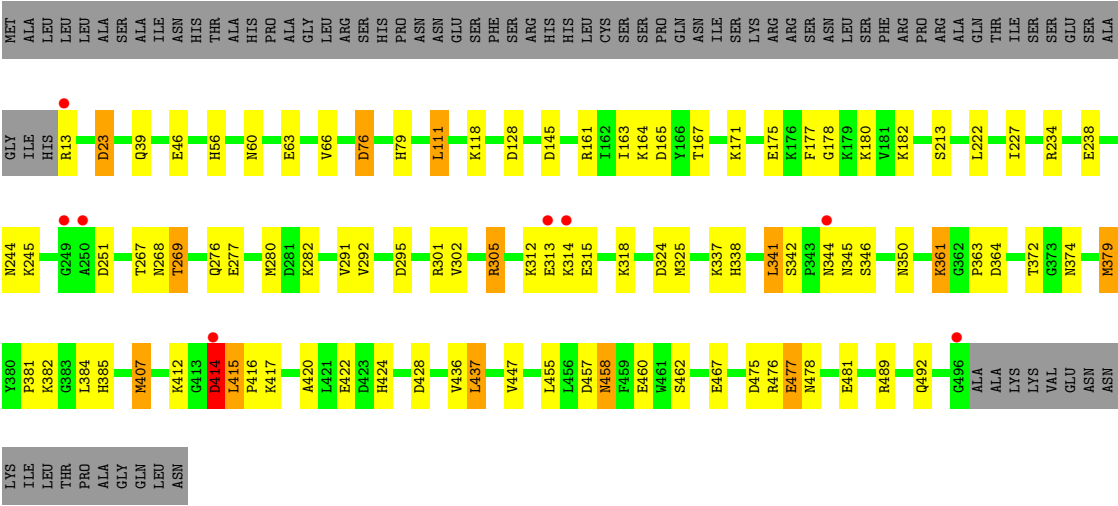
• Molecule 1: DHURRINASE

Chain F:



● Molecule 2: DHURRINASE

Chain E: 



4 Data and refinement statistics

Property	Value	Source
Space group	P 31	Depositor
Cell constants a, b, c, α , β , γ	101.05Å 101.05Å 279.05Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	30.00 – 1.80 19.92 – 1.80	Depositor EDS
% Data completeness (in resolution range)	98.6 (30.00-1.80) 98.6 (19.92-1.80)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.71 (at 1.80Å)	Xtriage
Refinement program	REFMAC 5.1.24	Depositor
R, R_{free}	0.172 , 0.210 0.152 , 0.193	Depositor DCC
R_{free} test set	14720 reflections (5.33%)	DCC
Wilson B-factor (Å ²)	17.3	Xtriage
Anisotropy	0.478	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.39 , 62.9	EDS
Estimated twinning fraction	0.000 for -h,-k,l 0.023 for h,-h-k,-l 0.013 for -k,-h,-l	Xtriage
L-test for twinning	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Outliers	0 of 291091 reflections	Xtriage
F_o, F_c correlation	0.97	EDS
Total number of atoms	28327	wwPDB-VP
Average B, all atoms (Å ²)	31.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 8.43% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

5 Model quality ⓘ

5.1 Standard geometry ⓘ

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	0.62	0/3990	0.80	10/5421 (0.2%)
1	B	0.62	2/3990 (0.1%)	0.80	12/5421 (0.2%)
1	C	0.61	0/3990	0.80	14/5421 (0.3%)
1	D	0.63	1/3990 (0.0%)	0.79	8/5421 (0.1%)
1	F	0.66	1/3990 (0.0%)	0.80	10/5421 (0.2%)
2	E	0.62	1/3999 (0.0%)	0.81	12/5431 (0.2%)
All	All	0.63	5/23949 (0.0%)	0.80	66/32536 (0.2%)

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	F	407	MET	SD-CE	-13.31	1.03	1.77
1	D	407	MET	SD-CE	-10.35	1.19	1.77
1	B	407	MET	SD-CE	-6.03	1.44	1.77
2	E	379	MET	CG-SD	-5.46	1.67	1.81
1	B	407	MET	CG-SD	-5.13	1.67	1.81

All (66) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	305	ARG	NE-CZ-NH1	9.27	124.93	120.30
2	E	305	ARG	NE-CZ-NH1	9.17	124.89	120.30
1	D	305	ARG	NE-CZ-NH1	9.05	124.82	120.30
1	B	305	ARG	NE-CZ-NH1	8.60	124.60	120.30
2	E	305	ARG	NE-CZ-NH2	-7.70	116.45	120.30
1	A	305	ARG	NE-CZ-NH1	7.41	124.01	120.30
1	F	305	ARG	NE-CZ-NH2	-7.17	116.71	120.30
1	B	305	ARG	NE-CZ-NH2	-6.93	116.83	120.30
1	A	165	ASP	CB-CG-OD2	6.84	124.46	118.30
2	E	165	ASP	CB-CG-OD2	6.83	124.45	118.30
1	C	305	ARG	NE-CZ-NH1	6.57	123.58	120.30
1	F	67	ASP	CB-CG-OD2	6.55	124.19	118.30
1	B	145	ASP	CB-CG-OD2	6.49	124.14	118.30

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	145	ASP	CB-CG-OD2	6.46	124.12	118.30
1	C	145	ASP	CB-CG-OD2	6.45	124.10	118.30
1	D	165	ASP	CB-CG-OD2	6.30	123.97	118.30
1	B	414	ASP	CB-CG-OD2	6.29	123.96	118.30
1	A	145	ASP	CB-CG-OD2	6.29	123.96	118.30
1	B	475	ASP	CB-CG-OD2	6.11	123.80	118.30
1	B	67	ASP	CB-CG-OD2	6.11	123.80	118.30
1	D	305	ARG	NE-CZ-NH2	-6.09	117.25	120.30
1	C	475	ASP	CB-CG-OD2	5.92	123.62	118.30
1	A	475	ASP	CB-CG-OD2	5.92	123.62	118.30
1	A	305	ARG	NE-CZ-NH2	-5.91	117.35	120.30
2	E	145	ASP	CB-CG-OD2	5.88	123.59	118.30
1	A	455	LEU	CB-CG-CD2	5.87	120.98	111.00
1	C	409	ASP	CB-CG-OD2	5.83	123.55	118.30
1	B	428	ASP	CB-CG-OD2	5.83	123.54	118.30
1	F	324	ASP	CB-CG-OD2	5.80	123.52	118.30
1	F	165	ASP	CB-CG-OD2	5.78	123.51	118.30
2	E	23	ASP	CB-CG-OD2	5.73	123.46	118.30
1	D	414	ASP	CB-CG-OD2	5.66	123.39	118.30
1	C	165	ASP	CB-CG-OD2	5.65	123.39	118.30
1	F	55	ASP	CB-CG-OD2	5.60	123.34	118.30
1	C	428	ASP	CB-CG-OD2	5.59	123.33	118.30
2	E	457	ASP	CB-CG-OD2	5.58	123.32	118.30
1	A	295	ASP	CB-CG-OD2	5.57	123.31	118.30
1	C	23	ASP	CB-CG-OD2	5.55	123.30	118.30
1	A	446	ASP	CB-CG-OD2	5.51	123.26	118.30
2	E	295	ASP	CB-CG-OD2	5.50	123.25	118.30
2	E	324	ASP	CB-CG-OD2	5.42	123.18	118.30
1	B	76	ASP	CB-CG-OD2	5.42	123.17	118.30
1	C	295	ASP	CB-CG-OD2	5.38	123.15	118.30
1	B	295	ASP	CB-CG-OD2	5.34	123.11	118.30
1	C	305	ARG	NE-CZ-NH2	-5.28	117.66	120.30
2	E	414	ASP	CB-CG-OD2	5.26	123.04	118.30
1	C	241	ASP	CB-CG-OD2	5.24	123.02	118.30
1	F	475	ASP	CB-CG-OD2	5.23	123.01	118.30
1	D	475	ASP	CB-CG-OD2	5.22	123.00	118.30
1	B	165	ASP	CB-CG-OD2	5.20	122.98	118.30
2	E	128	ASP	CB-CG-OD2	5.18	122.97	118.30
1	D	455	LEU	CB-CG-CD2	5.14	119.74	111.00
1	F	414	ASP	CB-CG-OD2	5.13	122.92	118.30
1	C	159	ASP	CB-CG-OD2	5.13	122.91	118.30
1	C	67	ASP	CB-CG-OD2	5.11	122.89	118.30

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	E	76	ASP	CB-CG-OD2	5.11	122.89	118.30
1	C	76	ASP	CB-CG-OD2	5.10	122.89	118.30
1	A	67	ASP	CB-CG-OD2	5.07	122.86	118.30
2	E	341	LEU	CA-CB-CG	5.06	126.95	115.30
1	B	409	ASP	CB-CG-OD2	5.06	122.85	118.30
1	D	364	ASP	CB-CG-OD2	5.05	122.85	118.30
1	B	55	ASP	CB-CG-OD2	5.03	122.83	118.30
1	D	76	ASP	CB-CG-OD2	5.03	122.83	118.30
1	C	353	ASP	CB-CG-OD2	5.00	122.80	118.30
1	A	306	ASP	CB-CG-OD2	5.00	122.80	118.30
1	F	84	ASP	CB-CG-OD2	5.00	122.80	118.30

There are no chirality outliers.

There are no planarity outliers.

5.2 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 hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3875	0	3686	124	0
1	B	3875	0	3686	102	0
1	C	3875	0	3686	129	0
1	D	3875	0	3686	115	0
1	F	3875	0	3686	155	0
2	E	3884	0	3704	137	1
3	A	846	0	0	75	2
3	B	860	0	0	71	1
3	C	832	0	0	86	3
3	D	827	0	0	71	2
3	E	869	0	0	99	2
3	F	834	0	0	110	1
All	All	28327	0	22134	757	6

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 17.

All (757) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:D:117:GLU:HB2	3:D:2299:HOH:O	1.22	1.39
2:E:372:THR:HB	2:E:407:MET:CE	1.51	1.39
1:F:277:GLU:HG3	3:F:2551:HOH:O	1.22	1.33
1:B:417:LYS:HB3	3:B:2765:HOH:O	1.22	1.31
1:D:407:MET:CE	1:D:407:MET:SD	1.19	1.28
1:A:462:SER:HB2	3:A:2792:HOH:O	1.16	1.28
1:B:462:SER:HB2	3:B:2815:HOH:O	1.17	1.28
1:C:277:GLU:HG3	3:C:2542:HOH:O	1.25	1.28
1:A:227:ILE:HG13	3:A:2255:HOH:O	1.14	1.27
1:C:245:LYS:HD3	3:C:2497:HOH:O	1.27	1.26
1:C:379:MET:HE2	3:C:2743:HOH:O	1.32	1.26
1:A:251:ASP:HB3	3:A:2532:HOH:O	1.30	1.26
1:B:407:MET:HE1	3:B:2709:HOH:O	1.27	1.25
1:F:227:ILE:HG13	3:F:2493:HOH:O	1.32	1.25
2:E:315:GLU:CD	3:E:2641:HOH:O	1.72	1.23
1:C:227:ILE:HG13	3:C:2240:HOH:O	1.30	1.23
1:C:171:LYS:HB2	3:C:2406:HOH:O	1.37	1.23
1:F:132:GLU:HB3	3:F:2314:HOH:O	1.38	1.22
2:E:372:THR:CB	2:E:407:MET:HE2	1.69	1.21
1:C:179:LYS:HE3	3:C:2434:HOH:O	1.41	1.20
2:E:422:GLU:HB2	3:E:2854:HOH:O	1.38	1.19
1:D:424:HIS:HB2	3:D:2740:HOH:O	1.39	1.19
1:F:422:GLU:HB2	3:F:2819:HOH:O	1.39	1.19
1:A:424:HIS:ND1	3:A:2751:HOH:O	1.73	1.19
2:E:23:ASP:HB3	3:E:2040:HOH:O	1.42	1.18
1:D:68:ARG:CA	3:D:2181:HOH:O	1.88	1.18
2:E:424:HIS:ND1	3:E:2779:HOH:O	1.78	1.17
1:F:407:MET:CE	1:F:407:MET:CG	2.22	1.17
1:A:13:ARG:CG	1:A:432:ARG:HH21	1.57	1.17
2:E:251:ASP:HB3	3:E:2559:HOH:O	1.43	1.16
1:B:345:ASN:OD1	3:B:2666:HOH:O	1.61	1.16
1:F:182:LYS:HG2	3:F:2518:HOH:O	1.46	1.15
2:E:462:SER:HB2	3:E:2822:HOH:O	0.98	1.14
1:B:182:LYS:HG2	3:B:2455:HOH:O	1.47	1.14
2:E:407:MET:SD	3:E:2759:HOH:O	2.04	1.14
1:F:227:ILE:CG1	3:F:2493:HOH:O	1.88	1.14
1:A:422:GLU:HB2	3:A:2828:HOH:O	1.46	1.13
1:D:131:LEU:HD11	1:D:180:THR:HG22	1.29	1.13
1:F:407:MET:SD	1:F:407:MET:CE	1.03	1.12
1:D:407:MET:SD	1:D:407:MET:HE1	1.77	1.12
1:C:179:LYS:HB2	1:C:179:LYS:HZ3	1.10	1.12
1:F:477:GLU:HB3	3:F:2799:HOH:O	1.46	1.12

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:D:234:ARG:NH2	3:D:2492:HOH:O	1.83	1.12
1:C:179:LYS:HB2	1:C:179:LYS:NZ	1.65	1.11
2:E:277:GLU:HG3	3:E:2303:HOH:O	1.48	1.10
2:E:269:THR:CG2	3:E:2576:HOH:O	2.00	1.10
1:A:227:ILE:CG1	3:A:2255:HOH:O	1.73	1.10
2:E:318:LYS:HD2	3:E:2540:HOH:O	1.52	1.10
1:A:131:LEU:HD11	1:A:180:THR:CG2	1.81	1.10
2:E:269:THR:HG23	3:E:2576:HOH:O	1.50	1.10
1:D:407:MET:SD	1:D:407:MET:HE2	1.77	1.09
1:F:86:ARG:HG3	3:F:2117:HOH:O	1.52	1.09
1:F:129:LEU:HA	3:F:2314:HOH:O	1.51	1.08
1:C:345:ASN:OD1	3:C:2625:HOH:O	1.67	1.08
1:D:407:MET:SD	1:D:407:MET:HE3	1.77	1.08
1:F:161:ARG:HD3	3:F:2400:HOH:O	1.51	1.08
1:B:407:MET:SD	3:B:2709:HOH:O	2.04	1.08
1:A:13:ARG:HG2	1:A:432:ARG:HH21	0.96	1.07
1:C:227:ILE:CG1	3:C:2240:HOH:O	1.90	1.07
1:D:312:LYS:NZ	3:D:2588:HOH:O	1.72	1.07
2:E:111:LEU:HG	3:E:2449:HOH:O	1.52	1.07
1:A:13:ARG:HA	3:A:2005:HOH:O	1.52	1.07
1:B:23:ASP:HB3	3:B:2039:HOH:O	1.54	1.07
1:C:131:LEU:HD11	1:C:180:THR:HG23	1.35	1.06
2:E:56:HIS:CE1	3:E:2160:HOH:O	2.08	1.06
2:E:372:THR:CB	2:E:407:MET:CE	2.30	1.06
1:F:361:LYS:HD2	3:F:2654:HOH:O	1.55	1.06
1:A:108:LYS:HE3	3:A:2294:HOH:O	1.55	1.05
1:C:131:LEU:CD1	1:C:180:THR:HG23	1.86	1.05
1:D:407:MET:CE	1:D:407:MET:CG	2.34	1.05
2:E:313:GLU:OE1	3:E:2633:HOH:O	1.72	1.04
2:E:417:LYS:HB3	3:E:2483:HOH:O	1.57	1.04
1:D:338:HIS:HD2	3:D:2616:HOH:O	1.40	1.03
1:D:131:LEU:HD11	1:D:180:THR:CG2	1.87	1.03
1:D:234:ARG:CZ	3:D:2492:HOH:O	2.07	1.03
2:E:227:ILE:HG13	3:E:2275:HOH:O	0.85	1.03
1:F:407:MET:HE3	1:F:407:MET:SD	1.63	1.01
2:E:313:GLU:HB2	3:E:2634:HOH:O	1.59	1.01
1:F:407:MET:HE1	1:F:407:MET:SD	1.63	1.01
1:B:227:ILE:HG13	3:B:2515:HOH:O	0.85	1.01
1:C:131:LEU:HD11	1:C:180:THR:CG2	1.90	1.00
2:E:291:VAL:HG23	3:E:2601:HOH:O	1.58	1.00
1:F:407:MET:HE2	1:F:407:MET:SD	1.63	1.00
1:D:227:ILE:HG13	3:D:2252:HOH:O	0.84	1.00

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:118:LYS:HG2	3:B:2314:HOH:O	1.61	1.00
1:D:282:LYS:HG2	3:D:2638:HOH:O	1.60	0.99
1:D:179:LYS:HZ2	1:D:179:LYS:HB2	1.28	0.98
1:D:111:LEU:HG	3:D:2412:HOH:O	1.62	0.98
1:A:13:ARG:HG2	1:A:432:ARG:NH2	1.77	0.98
1:B:346:SER:HB3	3:B:2667:HOH:O	1.62	0.97
1:C:392:LYS:HD3	3:C:2694:HOH:O	1.65	0.97
1:F:382:LYS:HE3	3:F:2684:HOH:O	1.63	0.96
1:A:131:LEU:CD1	1:A:180:THR:HG23	1.94	0.96
1:A:131:LEU:CD1	1:A:180:THR:CG2	2.44	0.96
2:E:56:HIS:ND1	3:E:2160:HOH:O	1.95	0.95
2:E:312:LYS:NZ	3:E:2629:HOH:O	1.98	0.95
1:D:179:LYS:NZ	1:D:179:LYS:HB2	1.82	0.95
1:A:277:GLU:CD	3:A:2559:HOH:O	2.04	0.95
1:F:117:GLU:HB2	3:F:2287:HOH:O	1.67	0.95
2:E:345:ASN:OD1	3:E:2673:HOH:O	1.84	0.94
1:A:394:LYS:HB2	3:A:2709:HOH:O	1.67	0.94
2:E:56:HIS:CG	3:E:2160:HOH:O	2.19	0.94
1:B:118:LYS:HD3	3:B:2311:HOH:O	1.65	0.94
1:D:422:GLU:HG2	3:D:2733:HOH:O	1.66	0.94
1:F:63:GLU:OE1	3:F:2157:HOH:O	1.86	0.94
1:D:131:LEU:CD1	1:D:180:THR:CG2	2.47	0.93
1:F:131:LEU:HD11	1:F:180:THR:CG2	1.98	0.93
1:F:447:VAL:HG23	3:F:2771:HOH:O	1.68	0.93
2:E:56:HIS:HD2	2:E:60:ASN:HD22	1.14	0.92
2:E:56:HIS:HD2	2:E:60:ASN:ND2	1.67	0.92
1:F:462:SER:HB2	3:F:2782:HOH:O	0.75	0.92
1:D:486:ARG:NH1	3:D:2811:HOH:O	1.78	0.91
1:A:131:LEU:HD11	1:A:180:THR:HG23	1.48	0.91
1:B:118:LYS:CG	3:B:2314:HOH:O	2.17	0.91
1:C:182:LYS:HE3	3:C:2438:HOH:O	1.70	0.91
1:D:164:LYS:HE2	3:D:2401:HOH:O	1.71	0.90
1:A:379:MET:HG2	3:A:2008:HOH:O	1.70	0.90
2:E:238:GLU:HG3	3:E:2541:HOH:O	1.70	0.90
1:A:238:GLU:OE2	3:A:2511:HOH:O	1.88	0.90
2:E:56:HIS:CD2	2:E:60:ASN:ND2	2.40	0.90
1:C:258:LEU:HG	3:C:2512:HOH:O	1.70	0.89
1:C:293:ARG:NE	3:C:2557:HOH:O	1.66	0.89
1:F:238:GLU:HG3	3:F:2504:HOH:O	1.70	0.89
1:F:417:LYS:HD3	3:F:2447:HOH:O	1.72	0.89
1:D:112:ALA:HB3	3:D:2288:HOH:O	1.73	0.89
1:B:108:LYS:HG2	3:B:2138:HOH:O	1.72	0.89

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:179:LYS:HZ2	1:A:179:LYS:HB2	1.37	0.89
1:A:179:LYS:HB2	1:A:179:LYS:NZ	1.86	0.88
1:F:407:MET:HE2	1:F:407:MET:CG	1.94	0.88
1:F:413:GLY:HA2	3:F:2724:HOH:O	1.72	0.88
1:C:280:MET:HG3	3:C:2543:HOH:O	1.74	0.88
1:F:400:MET:HE3	3:F:2771:HOH:O	1.72	0.88
1:C:179:LYS:CB	1:C:179:LYS:NZ	2.38	0.87
1:F:117:GLU:HG3	3:F:2286:HOH:O	1.73	0.87
1:F:158:LEU:HB2	3:F:2379:HOH:O	1.72	0.87
1:F:118:LYS:HG3	3:F:2295:HOH:O	1.74	0.86
1:C:293:ARG:NH2	3:C:2557:HOH:O	2.06	0.86
1:F:118:LYS:CG	3:F:2295:HOH:O	2.23	0.86
1:A:477:GLU:HB3	3:A:2810:HOH:O	1.76	0.86
1:F:13:ARG:HD2	3:F:2018:HOH:O	1.76	0.85
1:F:131:LEU:HD11	1:F:180:THR:HG23	1.55	0.85
1:C:171:LYS:HD2	3:C:2187:HOH:O	1.74	0.85
1:F:182:LYS:HE3	3:F:2203:HOH:O	1.76	0.85
1:B:314:LYS:HB2	3:B:2620:HOH:O	1.76	0.84
1:A:131:LEU:HD11	1:A:180:THR:HG22	1.59	0.84
1:C:379:MET:CE	3:C:2743:HOH:O	2.01	0.84
1:F:422:GLU:HG2	3:F:2740:HOH:O	1.76	0.84
1:F:131:LEU:CD1	1:F:180:THR:HG23	2.06	0.84
1:A:46:GLU:HG3	3:A:2126:HOH:O	1.78	0.84
1:B:46:GLU:HB3	3:B:2129:HOH:O	1.78	0.84
1:F:412:LYS:HB2	3:F:2720:HOH:O	1.77	0.83
1:B:277:GLU:CD	3:B:2579:HOH:O	2.16	0.83
1:B:131:LEU:CD1	1:B:180:THR:HG23	2.08	0.83
1:F:415:LEU:HD13	1:F:420:ALA:HB2	1.59	0.83
1:A:476:ARG:HD3	3:A:2807:HOH:O	1.78	0.82
1:B:125:LYS:HD3	3:B:2324:HOH:O	1.78	0.82
1:B:478:ASN:CG	3:B:2832:HOH:O	2.18	0.82
1:B:131:LEU:CD1	1:B:180:THR:CG2	2.57	0.82
2:E:417:LYS:HE2	2:E:477:GLU:OE1	1.79	0.82
1:D:277:GLU:HG3	3:D:2553:HOH:O	1.79	0.81
2:E:280:MET:HE2	3:E:2304:HOH:O	1.80	0.81
1:A:314:LYS:HE3	3:A:2615:HOH:O	1.78	0.81
1:D:312:LYS:HE3	3:D:2492:HOH:O	1.79	0.81
1:D:76:ASP:OD1	1:D:79:HIS:HD2	1.63	0.81
1:C:68:ARG:CA	3:C:2170:HOH:O	2.28	0.81
2:E:417:LYS:HD2	3:E:2483:HOH:O	1.81	0.81
1:C:280:MET:HE2	3:C:2690:HOH:O	1.81	0.81
1:C:117:GLU:HG3	3:C:2284:HOH:O	1.79	0.81

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:C:379:MET:HG2	3:C:2743:HOH:O	1.78	0.81
1:C:131:LEU:CD1	1:C:180:THR:CG2	2.55	0.81
1:A:394:LYS:CB	3:A:2709:HOH:O	2.25	0.81
1:A:489:ARG:HH11	1:A:492:GLN:HE22	1.28	0.81
1:F:417:LYS:HE3	3:F:2803:HOH:O	1.79	0.80
1:F:489:ARG:HH11	1:F:492:GLN:HE22	1.25	0.80
1:B:417:LYS:HD2	3:B:2410:HOH:O	1.80	0.80
1:A:280:MET:HE3	3:A:2568:HOH:O	1.81	0.80
1:F:306:ASP:HB2	3:F:2582:HOH:O	1.82	0.80
1:C:13:ARG:CG	3:C:2753:HOH:O	2.30	0.80
1:D:46:GLU:HG3	3:D:2128:HOH:O	1.80	0.80
1:F:417:LYS:HE2	1:F:475:ASP:OD1	1.82	0.80
2:E:338:HIS:HB3	3:E:2577:HOH:O	1.81	0.79
1:B:131:LEU:HD11	1:B:180:THR:CG2	2.13	0.79
1:B:111:LEU:HG	3:B:2431:HOH:O	1.82	0.79
1:A:13:ARG:CG	1:A:432:ARG:NH2	2.42	0.78
1:D:486:ARG:HD2	3:D:2735:HOH:O	1.83	0.78
1:B:117:GLU:OE1	3:B:2307:HOH:O	2.01	0.78
1:B:23:ASP:CG	1:F:448:ARG:HH22	1.86	0.78
1:A:13:ARG:CA	3:A:2005:HOH:O	2.20	0.78
1:C:13:ARG:N	3:C:2001:HOH:O	2.17	0.78
1:F:407:MET:CE	3:F:2669:HOH:O	2.32	0.78
1:B:314:LYS:HE3	3:B:2621:HOH:O	1.82	0.78
1:A:462:SER:CB	3:A:2792:HOH:O	1.90	0.77
1:C:382:LYS:HE2	3:C:2682:HOH:O	1.83	0.77
2:E:111:LEU:CG	3:E:2449:HOH:O	2.19	0.77
1:F:61:PHE:HA	1:F:63:GLU:OE2	1.84	0.77
2:E:467:GLU:OE1	3:E:2828:HOH:O	2.02	0.77
1:C:337:LYS:NZ	3:C:2609:HOH:O	2.13	0.77
2:E:280:MET:CE	3:E:2304:HOH:O	2.33	0.77
1:D:361:LYS:HD3	3:D:2343:HOH:O	1.85	0.77
1:C:13:ARG:NH1	3:C:2002:HOH:O	2.18	0.77
1:B:412:LYS:HE3	3:B:2402:HOH:O	1.84	0.77
1:F:413:GLY:CA	3:F:2724:HOH:O	2.32	0.76
1:B:306:ASP:HB2	3:B:2609:HOH:O	1.84	0.76
1:A:277:GLU:OE1	3:A:2559:HOH:O	2.01	0.76
2:E:372:THR:HB	2:E:407:MET:HE2	0.79	0.76
1:C:489:ARG:HH11	1:C:492:GLN:HE22	1.31	0.76
1:A:477:GLU:CB	3:A:2810:HOH:O	2.32	0.76
1:F:345:ASN:OD1	3:F:2626:HOH:O	2.03	0.75
2:E:76:ASP:OD1	2:E:79:HIS:HD2	1.70	0.75
1:A:68:ARG:CA	3:A:2185:HOH:O	2.34	0.75

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:D:21:ARG:NH2	3:D:2032:HOH:O	2.18	0.75
1:A:13:ARG:NH2	3:A:2009:HOH:O	2.20	0.74
1:C:476:ARG:HG2	3:C:2196:HOH:O	1.87	0.74
1:B:46:GLU:OE2	3:B:2129:HOH:O	2.05	0.74
1:D:89:LYS:HD2	3:D:2246:HOH:O	1.88	0.74
1:B:462:SER:CB	3:B:2815:HOH:O	1.93	0.74
2:E:292:VAL:HG23	3:E:2601:HOH:O	1.88	0.74
1:F:164:LYS:HE3	3:F:2189:HOH:O	1.87	0.74
1:B:46:GLU:CG	3:B:2129:HOH:O	2.36	0.74
1:C:238:GLU:OE1	3:C:2487:HOH:O	2.05	0.74
1:F:171:LYS:HE3	3:F:2421:HOH:O	1.89	0.73
1:C:76:ASP:OD1	1:C:79:HIS:HD2	1.70	0.73
1:F:314:LYS:CE	3:F:2604:HOH:O	2.35	0.73
1:D:422:GLU:HB2	3:D:2811:HOH:O	1.87	0.73
2:E:489:ARG:HH11	2:E:492:GLN:HE22	1.36	0.73
1:B:422:GLU:OE1	1:B:486:ARG:NH1	2.22	0.73
1:F:131:LEU:CD1	1:F:180:THR:CG2	2.64	0.73
1:C:13:ARG:HG2	3:C:2753:HOH:O	1.87	0.73
1:C:127:ILE:HG22	1:C:180:THR:HG21	1.70	0.73
1:F:314:LYS:HD2	3:F:2604:HOH:O	1.88	0.73
1:C:242:ILE:HD11	3:C:2405:HOH:O	1.88	0.73
2:E:182:LYS:HG2	3:E:2469:HOH:O	1.88	0.72
1:F:23:ASP:HB3	3:F:2036:HOH:O	1.88	0.72
1:D:407:MET:CE	3:D:2672:HOH:O	2.36	0.72
1:F:424:HIS:HB2	3:F:2743:HOH:O	1.90	0.72
1:D:179:LYS:HD2	3:D:2209:HOH:O	1.89	0.72
2:E:227:ILE:CG1	3:E:2275:HOH:O	1.66	0.72
1:F:422:GLU:O	1:F:422:GLU:HG2	1.90	0.72
1:C:108:LYS:NZ	3:C:2264:HOH:O	2.23	0.71
1:F:227:ILE:HD11	3:F:2296:HOH:O	1.89	0.71
1:B:346:SER:CB	3:B:2667:HOH:O	2.27	0.71
1:F:302:VAL:O	1:F:305:ARG:HD3	1.91	0.71
1:D:407:MET:CG	1:D:407:MET:HE2	2.10	0.70
1:C:127:ILE:CG2	1:C:180:THR:HG21	2.21	0.70
1:F:179:LYS:HG3	3:F:2437:HOH:O	1.91	0.70
2:E:372:THR:CG2	2:E:407:MET:CE	2.70	0.70
1:F:108:LYS:NZ	3:F:2263:HOH:O	2.22	0.70
1:F:314:LYS:CD	3:F:2604:HOH:O	2.40	0.70
1:B:131:LEU:HD11	1:B:180:THR:HG22	1.74	0.70
2:E:417:LYS:CB	3:E:2483:HOH:O	2.26	0.70
1:A:476:ARG:NH2	3:A:2809:HOH:O	2.25	0.69
1:D:417:LYS:HG2	1:D:473:TYR:OH	1.91	0.69

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:C:171:LYS:HE3	3:C:2419:HOH:O	1.92	0.69
1:D:112:ALA:CB	3:D:2288:HOH:O	2.35	0.69
1:F:493:GLU:OE1	3:F:2828:HOH:O	2.09	0.69
1:D:302:VAL:O	1:D:305:ARG:HD3	1.92	0.69
2:E:313:GLU:HB3	3:E:2630:HOH:O	1.91	0.69
2:E:182:LYS:HE3	3:E:2476:HOH:O	1.92	0.69
1:B:337:LYS:NZ	3:B:2648:HOH:O	2.14	0.69
1:B:108:LYS:NZ	3:B:2280:HOH:O	2.25	0.69
1:B:131:LEU:HD12	1:B:180:THR:CG2	2.21	0.69
1:B:227:ILE:HD11	3:B:2319:HOH:O	1.92	0.69
1:C:280:MET:CE	3:C:2690:HOH:O	2.39	0.69
1:F:424:HIS:ND1	3:F:2741:HOH:O	2.26	0.68
2:E:462:SER:CB	3:E:2822:HOH:O	1.79	0.68
1:D:293:ARG:NH1	3:D:2560:HOH:O	1.80	0.68
2:E:477:GLU:CB	3:E:2838:HOH:O	2.41	0.68
2:E:244:ASN:CG	3:E:2548:HOH:O	2.31	0.68
1:F:28:SER:HB3	3:F:2060:HOH:O	1.94	0.68
1:B:46:GLU:HG3	3:B:2130:HOH:O	1.94	0.68
1:D:489:ARG:HH11	1:D:492:GLN:HE22	1.42	0.68
1:B:13:ARG:NH2	3:B:2008:HOH:O	2.26	0.68
1:C:238:GLU:HG3	3:C:2487:HOH:O	1.94	0.68
1:B:46:GLU:CB	3:B:2129:HOH:O	2.37	0.67
1:F:179:LYS:HD3	3:F:2199:HOH:O	1.94	0.67
2:E:315:GLU:OE2	3:E:2641:HOH:O	1.91	0.67
1:F:76:ASP:OD1	1:F:79:HIS:HD2	1.78	0.67
2:E:111:LEU:HD13	3:E:2148:HOH:O	1.92	0.67
1:D:13:ARG:HD2	3:D:2006:HOH:O	1.93	0.67
1:F:314:LYS:HD3	3:F:2303:HOH:O	1.95	0.67
1:A:280:MET:CE	3:A:2568:HOH:O	2.42	0.66
1:A:13:ARG:CG	3:A:2005:HOH:O	2.43	0.66
2:E:164:LYS:HE2	3:E:2228:HOH:O	1.94	0.66
1:C:412:LYS:NZ	3:C:2722:HOH:O	2.10	0.66
1:C:415:LEU:HD13	1:C:420:ALA:HB2	1.78	0.66
1:A:117:GLU:OE1	3:A:2300:HOH:O	2.13	0.66
1:A:366:ASN:ND2	3:A:2680:HOH:O	2.28	0.66
1:B:371:PRO:O	3:B:2707:HOH:O	2.14	0.66
1:B:302:VAL:O	1:B:305:ARG:HD3	1.95	0.66
1:F:417:LYS:HG3	3:F:2735:HOH:O	1.94	0.66
1:D:312:LYS:HE2	3:D:2589:HOH:O	1.95	0.66
1:B:361:LYS:HD2	3:B:2695:HOH:O	1.94	0.66
2:E:477:GLU:HB3	3:E:2838:HOH:O	1.96	0.66
2:E:56:HIS:CD2	3:E:2160:HOH:O	2.43	0.66

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:179:LYS:NZ	1:A:179:LYS:CB	2.59	0.66
1:F:227:ILE:HG12	3:F:2493:HOH:O	1.73	0.65
1:F:117:GLU:OE2	3:F:2286:HOH:O	2.13	0.65
1:D:417:LYS:HE3	3:D:2731:HOH:O	1.96	0.65
1:F:117:GLU:CG	3:F:2286:HOH:O	2.38	0.65
1:A:117:GLU:O	1:A:121:GLU:HG3	1.96	0.65
2:E:302:VAL:O	2:E:305:ARG:HD3	1.95	0.65
1:D:338:HIS:CD2	3:D:2616:HOH:O	2.27	0.65
1:C:277:GLU:CD	3:C:2539:HOH:O	2.35	0.65
1:C:182:LYS:HD3	3:C:2507:HOH:O	1.97	0.65
1:D:417:LYS:HB3	3:D:2440:HOH:O	1.96	0.65
1:F:486:ARG:NH1	3:F:2819:HOH:O	2.28	0.65
2:E:363:PRO:HD2	3:E:2704:HOH:O	1.97	0.65
1:B:21:ARG:NH2	3:B:2028:HOH:O	1.96	0.64
2:E:227:ILE:HD12	3:E:2277:HOH:O	1.97	0.64
1:F:476:ARG:NH2	3:F:2795:HOH:O	2.30	0.64
1:C:477:GLU:HG3	3:C:2802:HOH:O	1.97	0.64
1:F:417:LYS:HD2	3:F:2736:HOH:O	1.96	0.64
1:F:46:GLU:HG3	3:F:2119:HOH:O	1.98	0.64
2:E:412:LYS:HE2	3:E:2767:HOH:O	1.98	0.64
2:E:227:ILE:HD12	3:E:2276:HOH:O	1.98	0.64
1:B:489:ARG:HH11	1:B:492:GLN:HE22	1.45	0.64
1:A:417:LYS:HB3	3:A:2453:HOH:O	1.96	0.64
1:F:13:ARG:HB2	3:F:2001:HOH:O	1.97	0.64
2:E:314:LYS:HD2	3:E:2635:HOH:O	1.97	0.64
2:E:314:LYS:CD	3:E:2635:HOH:O	2.46	0.64
1:F:117:GLU:CD	3:F:2286:HOH:O	2.36	0.63
1:C:13:ARG:O	3:C:2004:HOH:O	2.15	0.63
1:A:205:PRO:HB2	3:A:2473:HOH:O	1.97	0.63
1:F:413:GLY:O	3:F:2724:HOH:O	2.15	0.63
1:A:302:VAL:O	1:A:305:ARG:HD3	1.97	0.63
1:B:76:ASP:OD1	1:B:79:HIS:HD2	1.81	0.63
1:F:171:LYS:HD2	3:F:2187:HOH:O	1.98	0.63
1:A:13:ARG:CB	3:A:2005:HOH:O	2.44	0.63
1:F:63:GLU:H	1:F:63:GLU:CD	2.01	0.63
1:B:131:LEU:HD12	1:B:180:THR:HG23	1.80	0.63
1:A:13:ARG:NH1	1:A:428:ASP:OD2	2.32	0.63
1:C:13:ARG:HB3	3:C:2753:HOH:O	1.98	0.63
1:D:314:LYS:HE3	3:D:2593:HOH:O	1.99	0.63
1:B:407:MET:CE	3:B:2709:HOH:O	1.90	0.62
1:D:179:LYS:HD2	3:D:2103:HOH:O	1.99	0.62
1:D:424:HIS:CB	3:D:2740:HOH:O	2.16	0.62

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:F:422:GLU:CG	1:F:422:GLU:O	2.48	0.62
2:E:213:SER:HB2	3:E:2510:HOH:O	1.99	0.62
1:C:302:VAL:O	1:C:305:ARG:HD3	1.99	0.62
1:A:390:THR:HG23	3:A:2709:HOH:O	1.98	0.62
1:C:242:ILE:CD1	3:C:2405:HOH:O	2.46	0.62
1:F:407:MET:HE1	3:F:2669:HOH:O	1.99	0.61
2:E:412:LYS:HA	3:E:2765:HOH:O	1.99	0.61
1:F:417:LYS:HB3	3:F:2447:HOH:O	2.00	0.61
1:C:167:THR:CB	3:C:2405:HOH:O	2.49	0.61
1:C:108:LYS:HG2	3:C:2063:HOH:O	1.99	0.61
2:E:111:LEU:CD1	3:E:2148:HOH:O	2.47	0.61
1:F:413:GLY:C	3:F:2724:HOH:O	2.39	0.61
1:D:345:ASN:OD1	3:D:2631:HOH:O	2.16	0.61
1:B:379:MET:CE	1:B:432:ARG:HD2	2.31	0.61
2:E:13:ARG:HA	3:E:2003:HOH:O	1.99	0.60
1:B:416:PRO:HD3	3:B:2762:HOH:O	2.02	0.60
2:E:478:ASN:HB3	3:E:2843:HOH:O	2.00	0.60
1:F:13:ARG:NH1	3:F:2004:HOH:O	2.34	0.60
1:D:417:LYS:HD3	1:D:473:TYR:CE2	2.36	0.60
1:C:13:ARG:HH11	1:C:13:ARG:CG	2.13	0.60
1:F:108:LYS:NZ	3:F:2262:HOH:O	2.20	0.60
1:A:227:ILE:HD11	3:A:2311:HOH:O	2.01	0.60
1:D:276:GLN:NE2	3:D:2547:HOH:O	0.75	0.60
1:F:131:LEU:HD11	1:F:180:THR:HG22	1.81	0.60
1:A:136:GLU:HG2	3:A:2348:HOH:O	2.02	0.60
1:C:486:ARG:HD3	3:C:2817:HOH:O	2.02	0.59
1:B:127:ILE:HG22	1:B:180:THR:HG21	1.84	0.59
1:D:415:LEU:HD13	1:D:420:ALA:HB2	1.84	0.59
1:B:315:GLU:HG3	3:B:2626:HOH:O	2.02	0.59
1:C:179:LYS:HB2	1:C:179:LYS:HZ2	1.64	0.59
1:F:164:LYS:CE	3:F:2189:HOH:O	2.48	0.59
2:E:382:LYS:HG3	3:E:2731:HOH:O	2.01	0.59
1:F:238:GLU:CG	3:F:2504:HOH:O	2.40	0.59
1:F:171:LYS:CE	3:F:2420:HOH:O	2.51	0.59
1:A:111:LEU:HG	3:A:2422:HOH:O	2.03	0.59
1:A:317:GLU:HB3	3:A:2616:HOH:O	2.01	0.59
1:A:13:ARG:HG3	1:A:432:ARG:HH21	1.59	0.58
1:A:207:ARG:HG3	3:A:2473:HOH:O	2.02	0.58
1:A:486:ARG:NH1	3:A:2828:HOH:O	2.29	0.58
1:F:476:ARG:NH1	3:F:2797:HOH:O	2.18	0.58
1:B:417:LYS:CD	3:B:2410:HOH:O	2.47	0.58
1:F:407:MET:HE2	1:F:407:MET:HG2	1.82	0.58

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:C:171:LYS:O	1:C:175:GLU:HG3	2.03	0.57
2:E:417:LYS:HG3	3:E:2773:HOH:O	2.03	0.57
1:C:13:ARG:HG3	1:C:13:ARG:HH11	1.68	0.57
1:B:417:LYS:HG3	3:B:2767:HOH:O	2.04	0.57
1:F:475:ASP:OD2	1:F:477:GLU:HG2	2.04	0.57
1:A:476:ARG:NH1	3:A:2803:HOH:O	2.26	0.57
1:F:179:LYS:HE2	3:F:2095:HOH:O	2.05	0.57
1:D:407:MET:HE1	3:D:2672:HOH:O	2.03	0.57
1:D:227:ILE:HD11	3:D:2307:HOH:O	2.03	0.57
1:C:283:CYS:HB2	3:C:2521:HOH:O	2.05	0.57
1:D:422:GLU:O	1:D:422:GLU:CG	2.52	0.57
1:A:131:LEU:HD12	1:A:180:THR:CG2	2.33	0.57
1:A:476:ARG:HH21	1:A:476:ARG:HG2	1.69	0.57
1:C:13:ARG:CB	3:C:2753:HOH:O	2.53	0.57
1:D:337:LYS:NZ	3:D:2615:HOH:O	2.24	0.57
1:D:117:GLU:HG3	3:D:2297:HOH:O	2.03	0.56
1:D:417:LYS:HD3	1:D:473:TYR:HE2	1.68	0.56
1:D:13:ARG:NH2	3:D:2005:HOH:O	2.24	0.56
1:B:268:ASN:ND2	3:B:2564:HOH:O	2.38	0.56
2:E:161:ARG:NH1	3:E:2428:HOH:O	2.38	0.56
1:A:317:GLU:HG2	3:A:2616:HOH:O	2.05	0.56
2:E:161:ARG:CZ	3:E:2428:HOH:O	2.53	0.56
1:A:161:ARG:NH2	1:C:152:ASP:O	2.38	0.56
1:C:314:LYS:HG2	3:C:2588:HOH:O	2.04	0.56
2:E:234:ARG:NE	2:E:315:GLU:OE2	2.31	0.56
1:D:301:ARG:O	1:D:305:ARG:HD2	2.05	0.56
2:E:382:LYS:HE3	3:E:2387:HOH:O	2.05	0.56
1:A:293:ARG:NH1	3:A:2572:HOH:O	2.25	0.56
1:A:68:ARG:CA	3:A:2186:HOH:O	2.53	0.56
1:D:417:LYS:HD2	3:D:2440:HOH:O	2.05	0.56
1:C:424:HIS:HB2	3:C:2736:HOH:O	2.06	0.56
2:E:244:ASN:ND2	3:E:2548:HOH:O	2.37	0.56
2:E:422:GLU:O	2:E:422:GLU:HG2	2.06	0.56
2:E:227:ILE:CD1	3:E:2276:HOH:O	2.54	0.56
1:A:164:LYS:HE3	3:A:2411:HOH:O	2.06	0.56
2:E:385:HIS:CE1	3:E:2730:HOH:O	2.58	0.56
1:D:179:LYS:NZ	1:D:179:LYS:CB	2.60	0.56
1:F:171:LYS:HE2	3:F:2420:HOH:O	2.05	0.56
2:E:379:MET:HE2	3:E:2008:HOH:O	2.06	0.56
1:C:13:ARG:HD2	3:C:2005:HOH:O	2.06	0.56
1:A:13:ARG:HB3	1:A:428:ASP:OD1	2.06	0.55
1:B:314:LYS:HD2	3:B:2625:HOH:O	2.05	0.55

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:C:256:LEU:O	3:C:2512:HOH:O	2.17	0.55
1:C:117:GLU:O	1:C:121:GLU:HG3	2.05	0.55
1:C:167:THR:HB	3:C:2405:HOH:O	2.06	0.55
1:F:320:VAL:HG21	3:F:2600:HOH:O	2.06	0.55
1:A:182:LYS:HE3	3:A:2446:HOH:O	2.05	0.55
1:B:269:THR:HA	3:B:2565:HOH:O	2.06	0.55
1:C:315:GLU:HG3	3:C:2592:HOH:O	2.06	0.55
1:D:476:ARG:NH2	3:D:2789:HOH:O	2.39	0.55
1:C:127:ILE:CG2	1:C:180:THR:CG2	2.84	0.55
1:D:477:GLU:HB3	3:D:2794:HOH:O	2.05	0.55
1:D:76:ASP:OD1	1:D:79:HIS:CD2	2.53	0.55
1:B:179:LYS:HA	1:B:179:LYS:HE3	1.88	0.55
1:F:171:LYS:CD	3:F:2187:HOH:O	2.54	0.55
1:D:13:ARG:NH1	1:D:428:ASP:OD2	2.40	0.55
1:B:343:PRO:HB2	3:B:2659:HOH:O	2.06	0.55
1:C:227:ILE:HD11	3:C:2297:HOH:O	2.07	0.55
1:A:267:THR:OG1	1:A:269:THR:HB	2.07	0.55
2:E:374:ASN:ND2	3:E:2828:HOH:O	2.39	0.54
1:C:167:THR:HG21	3:C:2405:HOH:O	2.07	0.54
3:B:2008:HOH:O	2:E:364:ASP:HA	2.06	0.54
1:B:414:ASP:HB2	3:B:2754:HOH:O	2.07	0.54
1:F:118:LYS:HE3	3:F:2295:HOH:O	2.06	0.54
1:A:313:GLU:HB2	3:C:2155:HOH:O	2.07	0.54
1:A:314:LYS:HE2	3:A:2609:HOH:O	2.07	0.54
2:E:13:ARG:NH1	2:E:428:ASP:OD2	2.40	0.54
2:E:337:LYS:NZ	3:E:2660:HOH:O	2.25	0.54
1:A:13:ARG:HB2	3:A:2003:HOH:O	2.07	0.54
1:B:39:GLN:O	1:B:458:ASN:HB2	2.08	0.54
1:F:422:GLU:HG3	1:F:424:HIS:CE1	2.42	0.54
1:A:179:LYS:HE3	1:A:179:LYS:HA	1.90	0.54
1:A:227:ILE:HG12	3:A:2255:HOH:O	1.66	0.54
2:E:267:THR:OG1	2:E:269:THR:HB	2.08	0.54
1:D:417:LYS:HG2	1:D:473:TYR:CZ	2.43	0.53
1:A:417:LYS:CD	3:A:2453:HOH:O	2.56	0.53
1:F:414:ASP:CB	3:F:2725:HOH:O	2.56	0.53
1:F:414:ASP:HB3	3:F:2725:HOH:O	2.07	0.53
1:F:445:ALA:HB1	3:F:2771:HOH:O	2.06	0.53
1:F:68:ARG:CA	3:F:2169:HOH:O	2.56	0.53
1:D:424:HIS:CE1	3:D:2735:HOH:O	2.60	0.53
1:C:432:ARG:NH2	3:C:2753:HOH:O	1.72	0.53
1:D:21:ARG:HD2	3:D:2041:HOH:O	2.07	0.53
1:D:13:ARG:NH2	3:D:2001:HOH:O	2.29	0.53

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:439:GLN:HG2	3:B:2789:HOH:O	2.07	0.53
1:A:182:LYS:HD3	3:A:2529:HOH:O	2.08	0.53
1:F:338:HIS:HD2	3:F:2259:HOH:O	1.90	0.53
2:E:227:ILE:HD11	3:E:2332:HOH:O	2.09	0.53
2:E:372:THR:HB	2:E:407:MET:HE1	1.73	0.53
1:C:39:GLN:O	1:C:458:ASN:HB2	2.08	0.53
1:B:118:LYS:HG3	3:B:2314:HOH:O	1.94	0.53
1:B:127:ILE:CG2	1:B:180:THR:HG21	2.39	0.53
2:E:164:LYS:NZ	3:E:2437:HOH:O	2.30	0.53
1:D:496:GLY:C	3:D:2818:HOH:O	2.47	0.53
1:D:315:GLU:HG3	3:D:2595:HOH:O	2.09	0.53
1:A:78:TYR:HB3	3:A:2213:HOH:O	2.09	0.53
1:D:382:LYS:HE3	3:D:2694:HOH:O	2.08	0.53
1:B:21:ARG:HD3	3:B:2040:HOH:O	2.09	0.52
1:F:338:HIS:CD2	3:F:2259:HOH:O	2.62	0.52
1:D:417:LYS:CE	3:D:2731:HOH:O	2.55	0.52
3:A:2571:HOH:O	1:B:338:HIS:CE1	2.63	0.52
1:A:343:PRO:HD3	1:B:310:TYR:CZ	2.45	0.52
1:D:85:VAL:HG11	1:D:129:LEU:HG	1.91	0.52
1:A:317:GLU:CG	3:A:2616:HOH:O	2.58	0.52
1:C:66:VAL:HG21	3:C:2198:HOH:O	2.08	0.52
1:B:118:LYS:CD	3:B:2311:HOH:O	2.39	0.52
2:E:476:ARG:HD2	3:E:2234:HOH:O	2.10	0.52
2:E:39:GLN:O	2:E:458:ASN:HB2	2.09	0.51
2:E:182:LYS:NZ	3:E:2475:HOH:O	2.43	0.51
1:D:314:LYS:CE	3:D:2599:HOH:O	2.58	0.51
1:D:345:ASN:ND2	3:D:2631:HOH:O	2.38	0.51
2:E:379:MET:HG2	2:E:381:PRO:HD3	1.91	0.51
1:F:267:THR:OG1	1:F:269:THR:HB	2.11	0.51
1:D:60:ASN:HB3	3:D:2160:HOH:O	2.09	0.51
2:E:118:LYS:HG3	3:E:2324:HOH:O	2.10	0.51
2:E:227:ILE:HG23	3:E:2277:HOH:O	2.11	0.51
2:E:164:LYS:CE	3:E:2228:HOH:O	2.54	0.51
1:A:437:LEU:HD21	1:A:447:VAL:HG11	1.92	0.51
1:D:269:THR:HG21	3:D:2536:HOH:O	2.11	0.51
1:D:193:PHE:HA	3:D:2451:HOH:O	2.09	0.51
1:C:337:LYS:NZ	3:C:2608:HOH:O	2.17	0.51
1:F:14:LEU:HD21	3:F:2026:HOH:O	2.11	0.51
1:D:267:THR:OG1	1:D:269:THR:HB	2.11	0.51
2:E:182:LYS:HD3	3:E:2470:HOH:O	2.10	0.51
1:F:312:LYS:HE2	3:F:2175:HOH:O	2.10	0.51
1:C:227:ILE:HG12	3:C:2240:HOH:O	1.83	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:C:301:ARG:O	1:C:305:ARG:HD2	2.11	0.50
1:A:293:ARG:NH2	3:A:2571:HOH:O	2.44	0.50
2:E:415:LEU:HD13	2:E:420:ALA:HB2	1.93	0.50
1:C:478:ASN:HB3	3:C:2804:HOH:O	2.10	0.50
1:C:131:LEU:HD12	1:C:180:THR:HG23	1.85	0.50
1:F:301:ARG:O	1:F:305:ARG:HD2	2.11	0.50
1:B:301:ARG:O	1:B:305:ARG:HD2	2.11	0.50
1:A:39:GLN:O	1:A:458:ASN:HB2	2.11	0.50
1:B:414:ASP:HB3	3:B:2762:HOH:O	2.10	0.50
1:A:306:ASP:HB2	3:A:2312:HOH:O	2.12	0.50
1:F:345:ASN:ND2	3:F:2626:HOH:O	2.44	0.50
1:A:317:GLU:CB	3:A:2616:HOH:O	2.60	0.50
1:A:269:THR:HG21	3:A:2280:HOH:O	2.11	0.50
2:E:342:SER:HB2	3:E:2669:HOH:O	2.11	0.50
1:F:171:LYS:HE3	3:F:2420:HOH:O	2.12	0.50
1:D:422:GLU:O	1:D:422:GLU:HG2	2.10	0.50
1:B:86:ARG:CZ	3:B:2247:HOH:O	2.59	0.49
1:D:424:HIS:CG	3:D:2735:HOH:O	2.65	0.49
1:A:381:PRO:HB2	1:A:436:VAL:HG21	1.94	0.49
1:F:428:ASP:OD1	3:F:2748:HOH:O	2.20	0.49
1:D:282:LYS:NZ	1:D:350:ASN:HD22	2.11	0.49
1:F:400:MET:CE	3:F:2771:HOH:O	2.43	0.49
1:A:476:ARG:NE	3:A:2803:HOH:O	2.32	0.49
1:C:476:ARG:HD2	3:C:2796:HOH:O	2.12	0.49
1:A:417:LYS:HG2	1:A:473:TYR:CZ	2.46	0.49
1:B:267:THR:OG1	1:B:269:THR:HB	2.11	0.49
1:A:234:ARG:NE	1:A:315:GLU:OE2	2.41	0.49
1:D:131:LEU:CD1	1:D:180:THR:HG23	2.42	0.49
1:A:301:ARG:O	1:A:305:ARG:HD2	2.13	0.49
1:D:314:LYS:HD3	3:D:2592:HOH:O	2.12	0.49
1:B:417:LYS:CB	3:B:2410:HOH:O	2.60	0.49
1:D:131:LEU:HD12	1:D:180:THR:CG2	2.41	0.49
1:D:476:ARG:HD3	3:D:2790:HOH:O	2.13	0.49
1:C:210:PRO:CG	3:C:2231:HOH:O	2.60	0.49
1:F:234:ARG:NE	1:F:315:GLU:OE2	2.35	0.49
1:F:227:ILE:HD12	3:F:2168:HOH:O	2.13	0.49
1:B:227:ILE:HD12	3:B:2185:HOH:O	2.12	0.49
1:A:417:LYS:HG2	1:A:473:TYR:OH	2.12	0.49
1:B:282:LYS:NZ	1:B:350:ASN:HD22	2.11	0.49
2:E:56:HIS:CD2	2:E:60:ASN:HD22	2.04	0.49
1:F:372:THR:HB	1:F:407:MET:HE1	1.94	0.49
2:E:268:ASN:ND2	3:E:2572:HOH:O	2.44	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:E:171:LYS:NZ	2:E:175:GLU:OE2	2.42	0.48
1:A:422:GLU:HG2	3:A:2749:HOH:O	2.13	0.48
1:B:361:LYS:HE2	1:B:361:LYS:HB3	1.67	0.48
2:E:46:GLU:HG3	3:E:2130:HOH:O	2.14	0.48
1:B:417:LYS:N	1:B:418:PRO:CD	2.75	0.48
1:F:447:VAL:CG2	3:F:2771:HOH:O	2.40	0.48
2:E:460:GLU:HG3	2:E:460:GLU:O	2.13	0.48
2:E:178:GLY:O	3:E:2468:HOH:O	2.20	0.48
1:F:238:GLU:OE1	3:F:2504:HOH:O	2.19	0.48
1:B:227:ILE:CG1	3:B:2515:HOH:O	1.74	0.48
1:D:314:LYS:HD2	3:D:2599:HOH:O	2.13	0.48
1:C:227:ILE:HD12	3:C:2169:HOH:O	2.14	0.48
1:F:477:GLU:CB	3:F:2799:HOH:O	2.27	0.48
2:E:381:PRO:HB2	2:E:436:VAL:HG21	1.96	0.48
1:D:437:LEU:HD21	1:D:447:VAL:HG11	1.96	0.48
1:B:131:LEU:HD11	1:B:180:THR:HG23	1.84	0.47
1:A:270:PHE:HA	1:A:273:GLN:HE21	1.79	0.47
1:A:313:GLU:HB3	3:A:2610:HOH:O	2.13	0.47
2:E:346:SER:CB	3:E:2675:HOH:O	2.62	0.47
1:A:76:ASP:OD1	1:A:79:HIS:HD2	1.98	0.47
2:E:314:LYS:NZ	3:E:2637:HOH:O	2.46	0.47
1:C:210:PRO:HG3	3:C:2231:HOH:O	2.14	0.47
1:A:415:LEU:HD13	1:A:420:ALA:HB2	1.97	0.47
1:A:127:ILE:HG22	1:A:180:THR:HG21	1.95	0.47
1:C:142:PHE:O	3:C:2340:HOH:O	2.20	0.47
1:A:13:ARG:HD2	3:A:2005:HOH:O	2.13	0.47
1:B:108:LYS:HE2	3:B:2138:HOH:O	2.13	0.47
1:C:13:ARG:NH1	1:C:13:ARG:CG	2.73	0.47
2:E:76:ASP:OD1	2:E:79:HIS:CD2	2.60	0.47
2:E:282:LYS:NZ	2:E:350:ASN:HD22	2.13	0.47
1:C:131:LEU:HD11	1:C:180:THR:HG22	1.84	0.47
1:F:164:LYS:NZ	3:F:2405:HOH:O	2.47	0.47
1:C:167:THR:CG2	3:C:2405:HOH:O	2.62	0.47
1:B:379:MET:HE2	1:B:432:ARG:HD2	1.96	0.47
2:E:161:ARG:CD	3:E:2428:HOH:O	2.62	0.47
1:F:282:LYS:NZ	1:F:350:ASN:HD22	2.12	0.47
1:C:267:THR:OG1	1:C:269:THR:HB	2.15	0.47
1:B:417:LYS:CB	3:B:2765:HOH:O	2.09	0.47
2:E:379:MET:CE	3:E:2008:HOH:O	2.62	0.47
3:B:2011:HOH:O	2:E:269:THR:HG21	2.14	0.47
1:A:127:ILE:CG2	1:A:180:THR:HG21	2.46	0.46
1:D:111:LEU:CG	3:D:2412:HOH:O	2.41	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:476:ARG:CD	3:A:2801:HOH:O	2.61	0.46
1:A:476:ARG:CD	3:A:2807:HOH:O	2.51	0.46
1:C:108:LYS:CE	3:C:2264:HOH:O	2.61	0.46
1:F:486:ARG:CZ	3:F:2821:HOH:O	2.63	0.46
1:F:155:GLY:HA3	3:F:2379:HOH:O	2.14	0.46
1:F:381:PRO:HB2	1:F:436:VAL:HG21	1.98	0.46
1:C:276:GLN:HE21	1:C:276:GLN:HB3	1.55	0.46
2:E:313:GLU:CB	3:E:2634:HOH:O	2.37	0.46
1:B:314:LYS:HG2	3:B:2623:HOH:O	2.15	0.46
1:D:342:SER:HB2	3:D:2624:HOH:O	2.16	0.46
2:E:163:ILE:O	2:E:167:THR:HG23	2.16	0.46
1:D:496:GLY:HA2	3:D:2819:HOH:O	2.15	0.46
1:F:118:LYS:HE3	3:F:2291:HOH:O	2.15	0.46
1:C:238:GLU:CG	3:C:2487:HOH:O	2.58	0.46
1:F:62:PRO:HA	3:F:2176:HOH:O	2.15	0.46
1:C:270:PHE:HA	1:C:273:GLN:HE21	1.80	0.46
1:F:414:ASP:O	3:F:2730:HOH:O	2.21	0.46
1:A:415:LEU:HD23	3:A:2394:HOH:O	2.16	0.46
1:C:171:LYS:O	1:C:175:GLU:CG	2.64	0.45
1:C:62:PRO:HB3	3:C:2145:HOH:O	2.15	0.45
1:B:314:LYS:CD	3:B:2625:HOH:O	2.62	0.45
2:E:314:LYS:CE	3:E:2635:HOH:O	2.65	0.45
1:A:342:SER:HA	1:B:310:TYR:OH	2.16	0.45
1:A:379:MET:CE	1:A:432:ARG:HD2	2.46	0.45
1:F:238:GLU:OE1	1:F:318:LYS:NZ	2.36	0.45
1:F:179:LYS:CD	3:F:2199:HOH:O	2.60	0.45
1:D:117:GLU:CB	3:D:2299:HOH:O	2.09	0.45
2:E:437:LEU:HD21	2:E:447:VAL:HG11	1.98	0.45
1:D:117:GLU:OE2	3:D:2297:HOH:O	2.21	0.45
2:E:346:SER:HB3	3:E:2675:HOH:O	2.17	0.45
1:C:102:TRP:HB3	1:C:103:PRO:HD3	1.99	0.45
1:A:315:GLU:HG3	3:A:2613:HOH:O	2.16	0.45
2:E:305:ARG:HB3	3:E:2616:HOH:O	2.16	0.45
2:E:238:GLU:CG	3:E:2541:HOH:O	2.46	0.44
1:F:458:ASN:HD22	1:F:458:ASN:C	2.20	0.44
1:C:179:LYS:CE	3:C:2434:HOH:O	2.24	0.44
1:B:270:PHE:HA	1:B:273:GLN:HE21	1.82	0.44
2:E:13:ARG:HD2	3:E:2018:HOH:O	2.17	0.44
1:A:477:GLU:HB2	3:A:2810:HOH:O	2.07	0.44
1:C:414:ASP:HB2	3:C:2721:HOH:O	2.17	0.44
1:D:270:PHE:HA	1:D:273:GLN:HE21	1.83	0.44
1:B:379:MET:HE1	1:B:432:ARG:HD2	1.98	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:182:LYS:HE2	1:B:182:LYS:HB2	1.77	0.44
2:E:301:ARG:O	2:E:305:ARG:HD2	2.17	0.44
1:B:415:LEU:HD13	1:B:420:ALA:HB2	2.00	0.44
1:D:39:GLN:O	1:D:458:ASN:HB2	2.17	0.44
1:B:13:ARG:HB2	3:B:2009:HOH:O	2.16	0.44
1:B:143:HIS:CE1	1:B:188:ASN:ND2	2.86	0.44
1:D:407:MET:SD	1:D:426:ARG:HA	2.58	0.44
1:D:343:PRO:HA	3:D:2628:HOH:O	2.18	0.44
1:D:161:ARG:HD3	3:D:2396:HOH:O	2.18	0.44
1:B:179:LYS:HB2	3:B:2456:HOH:O	2.17	0.44
1:C:282:LYS:NZ	1:C:350:ASN:HD22	2.16	0.44
1:A:102:TRP:HB3	1:A:103:PRO:HD3	1.99	0.44
1:C:179:LYS:CA	1:C:179:LYS:HZ2	2.31	0.43
1:C:382:LYS:CE	3:C:2682:HOH:O	2.51	0.43
1:C:381:PRO:HB2	1:C:436:VAL:HG21	2.00	0.43
2:E:372:THR:CB	2:E:407:MET:HE1	2.37	0.43
2:E:251:ASP:OD1	2:E:251:ASP:N	2.50	0.43
2:E:475:ASP:OD2	2:E:477:GLU:CD	2.56	0.43
1:D:131:LEU:HD12	1:D:180:THR:HG21	2.00	0.43
1:C:314:LYS:HE3	3:C:2590:HOH:O	2.17	0.43
1:B:342:SER:HB2	3:B:2164:HOH:O	2.18	0.43
2:E:13:ARG:N	3:E:2007:HOH:O	2.51	0.43
1:C:234:ARG:NE	1:C:315:GLU:OE2	2.47	0.43
1:C:313:GLU:HB3	3:C:2589:HOH:O	2.19	0.43
1:A:394:LYS:HB3	3:A:2709:HOH:O	2.06	0.43
1:D:361:LYS:HB3	1:D:361:LYS:HE2	1.62	0.43
1:F:476:ARG:NE	3:F:2797:HOH:O	2.47	0.43
1:F:414:ASP:O	1:F:416:PRO:HD3	2.19	0.43
1:F:129:LEU:CA	3:F:2314:HOH:O	2.31	0.43
1:F:475:ASP:OD2	1:F:477:GLU:CD	2.57	0.43
1:C:437:LEU:HD21	1:C:447:VAL:HG11	2.00	0.43
1:C:293:ARG:CZ	3:C:2557:HOH:O	2.12	0.43
1:A:182:LYS:HB2	1:A:182:LYS:HE2	1.82	0.43
1:A:247:HIS:HD2	3:A:2430:HOH:O	2.01	0.43
1:A:422:GLU:HG2	1:A:422:GLU:O	2.19	0.43
1:D:234:ARG:NE	3:D:2492:HOH:O	2.34	0.43
1:D:460:GLU:HG3	1:D:460:GLU:O	2.18	0.43
1:A:476:ARG:HD2	3:A:2801:HOH:O	2.19	0.43
1:C:46:GLU:OE2	1:C:79:HIS:HE1	2.01	0.43
1:B:437:LEU:HD21	1:B:447:VAL:HG11	2.00	0.43
1:F:102:TRP:HB3	1:F:103:PRO:HD3	2.01	0.43
1:D:414:ASP:O	1:D:416:PRO:HD3	2.18	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:F:422:GLU:HG3	1:F:424:HIS:ND1	2.34	0.42
1:C:363:PRO:HD2	3:C:2660:HOH:O	2.18	0.42
1:D:417:LYS:NZ	3:D:2731:HOH:O	2.52	0.42
1:B:179:LYS:NZ	3:B:2456:HOH:O	2.50	0.42
2:E:177:PHE:C	3:E:2468:HOH:O	2.57	0.42
1:F:39:GLN:O	1:F:458:ASN:HB2	2.18	0.42
1:C:343:PRO:HA	3:C:2620:HOH:O	2.18	0.42
1:F:345:ASN:CG	3:F:2626:HOH:O	2.54	0.42
1:C:85:VAL:HG11	1:C:129:LEU:HG	2.01	0.42
1:F:251:ASP:N	1:F:251:ASP:OD1	2.52	0.42
2:E:361:LYS:HB3	2:E:361:LYS:HE2	1.25	0.42
2:E:238:GLU:OE1	3:E:2541:HOH:O	2.21	0.42
2:E:63:GLU:HB3	3:E:2205:HOH:O	2.19	0.42
1:F:314:LYS:HE3	3:F:2604:HOH:O	2.13	0.42
1:B:417:LYS:HB3	3:B:2410:HOH:O	2.19	0.42
1:C:337:LYS:CE	3:C:2608:HOH:O	2.62	0.42
1:B:412:LYS:NZ	3:B:2757:HOH:O	2.53	0.42
1:F:320:VAL:CG2	3:F:2600:HOH:O	2.65	0.42
1:F:143:HIS:CE1	1:F:188:ASN:ND2	2.88	0.42
1:F:13:ARG:HB3	1:F:432:ARG:HH21	1.84	0.42
1:F:314:LYS:HB2	3:F:2303:HOH:O	2.20	0.42
1:A:111:LEU:HD22	1:A:111:LEU:HA	1.91	0.42
1:F:270:PHE:HA	1:F:273:GLN:HE21	1.84	0.42
1:A:361:LYS:HE2	1:A:361:LYS:HB3	1.74	0.42
2:E:292:VAL:CG2	3:E:2601:HOH:O	2.56	0.42
1:A:476:ARG:HH21	1:A:476:ARG:CG	2.33	0.42
2:E:314:LYS:HD3	3:E:2631:HOH:O	2.19	0.42
1:F:453:TRP:HA	1:F:454:SER:HA	1.83	0.42
1:A:439:GLN:CD	3:A:2772:HOH:O	2.57	0.42
1:F:422:GLU:CB	3:F:2819:HOH:O	2.25	0.42
1:F:417:LYS:CB	3:F:2447:HOH:O	2.63	0.42
1:F:412:LYS:NZ	3:F:2721:HOH:O	2.52	0.42
1:C:259:ASN:HA	1:C:329:ASN:HB2	2.02	0.42
1:D:131:LEU:CD1	1:D:180:THR:HG21	2.41	0.42
1:F:462:SER:CB	3:F:2782:HOH:O	1.63	0.42
1:D:345:ASN:CG	3:D:2631:HOH:O	2.58	0.42
1:C:453:TRP:HA	1:C:454:SER:HA	1.81	0.42
1:D:251:ASP:OD1	1:D:251:ASP:N	2.52	0.42
1:D:111:LEU:HA	1:D:111:LEU:HD22	1.83	0.41
1:D:314:LYS:CD	3:D:2599:HOH:O	2.67	0.41
1:D:102:TRP:HB3	1:D:103:PRO:HD3	2.02	0.41
1:A:179:LYS:HA	1:A:179:LYS:CE	2.50	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:C:46:GLU:HG3	3:C:2115:HOH:O	2.20	0.41
1:A:412:LYS:HE2	3:A:2737:HOH:O	2.20	0.41
1:C:412:LYS:HE2	3:C:2378:HOH:O	2.19	0.41
1:B:269:THR:HG21	3:B:2566:HOH:O	2.20	0.41
1:B:417:LYS:CE	3:B:2824:HOH:O	2.69	0.41
1:D:372:THR:HB	1:D:407:MET:HE1	2.02	0.41
1:A:13:ARG:HG3	3:A:2005:HOH:O	2.14	0.41
1:C:342:SER:HA	1:D:310:TYR:OH	2.21	0.41
1:A:117:GLU:HG2	3:A:2150:HOH:O	2.20	0.41
1:A:259:ASN:HA	1:A:329:ASN:HB2	2.02	0.41
2:E:245:LYS:HE3	3:E:2544:HOH:O	2.21	0.41
1:C:131:LEU:HD12	1:C:180:THR:CG2	2.43	0.41
2:E:227:ILE:HD13	2:E:227:ILE:HA	1.83	0.41
1:C:432:ARG:NE	3:C:2753:HOH:O	2.52	0.41
1:C:238:GLU:CD	3:C:2487:HOH:O	2.56	0.41
1:B:46:GLU:CD	3:B:2129:HOH:O	2.52	0.41
1:C:108:LYS:HE3	3:C:2264:HOH:O	2.21	0.41
1:C:143:HIS:HD2	3:C:2072:HOH:O	2.03	0.41
1:C:361:LYS:HE2	1:C:361:LYS:HB3	1.45	0.41
1:F:293:ARG:HD2	3:F:2563:HOH:O	2.20	0.41
1:A:232:LEU:C	1:A:232:LEU:HD23	2.41	0.41
2:E:315:GLU:HA	3:E:2540:HOH:O	2.21	0.41
1:C:171:LYS:HD3	3:C:2418:HOH:O	2.21	0.41
2:E:111:LEU:CD1	3:E:2449:HOH:O	2.60	0.41
1:F:171:LYS:HE2	3:F:2512:HOH:O	2.21	0.41
1:F:179:LYS:NZ	1:F:179:LYS:HB3	2.35	0.41
2:E:314:LYS:CG	3:E:2647:HOH:O	2.69	0.41
2:E:414:ASP:O	2:E:416:PRO:HD3	2.21	0.41
2:E:372:THR:HG21	2:E:407:MET:HE3	2.02	0.40
1:C:163:ILE:O	1:C:167:THR:HG23	2.21	0.40
1:A:366:ASN:CG	3:A:2680:HOH:O	2.58	0.40
1:C:314:LYS:NZ	3:C:2590:HOH:O	2.54	0.40
1:B:251:ASP:OD1	1:B:251:ASP:N	2.54	0.40
1:F:108:LYS:CE	3:F:2263:HOH:O	2.65	0.40
2:E:344:ASN:ND2	3:E:2670:HOH:O	2.54	0.40
1:A:58:CYS:HB3	1:A:70:ASN:HB3	2.02	0.40
1:F:127:ILE:HG22	1:F:180:THR:HG21	2.01	0.40
1:C:76:ASP:OD1	1:C:79:HIS:CD2	2.61	0.40
1:C:108:LYS:HE2	3:C:2032:HOH:O	2.21	0.40
1:A:417:LYS:HD3	3:A:2453:HOH:O	2.21	0.40
1:A:251:ASP:OD1	1:A:251:ASP:N	2.53	0.40
2:E:315:GLU:OE1	3:E:2641:HOH:O	2.04	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:F:475:ASP:OD2	1:F:477:GLU:CG	2.68	0.40

All (6) 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	Distance(Å)	Clash(Å)
3:B:2759:HOH:O	3:D:2088:HOH:O[1_655]	1.87	0.33
3:A:2416:HOH:O	3:C:2368:HOH:O[1_545]	1.89	0.31
3:D:2376:HOH:O	3:F:2409:HOH:O[1_565]	2.13	0.07
3:C:2589:HOH:O	3:E:2173:HOH:O[1_455]	2.15	0.05
2:E:314:LYS:CB	3:A:2168:HOH:O[1_655]	2.16	0.04
3:C:2569:HOH:O	3:E:2518:HOH:O[1_455]	2.18	0.02

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	482/565 (85%)	468 (97%)	14 (3%)	0	100	100
1	B	482/565 (85%)	467 (97%)	15 (3%)	0	100	100
1	C	482/565 (85%)	466 (97%)	16 (3%)	0	100	100
1	D	482/565 (85%)	468 (97%)	14 (3%)	0	100	100
1	F	482/565 (85%)	469 (97%)	13 (3%)	0	100	100
2	E	482/565 (85%)	470 (98%)	12 (2%)	0	100	100
All	All	2892/3390 (85%)	2808 (97%)	84 (3%)	0	100	100

There are no Ramachandran outliers to report.

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	412/482 (86%)	396 (96%)	16 (4%)	43	23
1	B	412/482 (86%)	395 (96%)	17 (4%)	41	21
1	C	412/482 (86%)	393 (95%)	19 (5%)	37	17
1	D	412/482 (86%)	394 (96%)	18 (4%)	39	18
1	F	412/482 (86%)	394 (96%)	18 (4%)	39	18
2	E	413/482 (86%)	395 (96%)	18 (4%)	39	18
All	All	2473/2892 (86%)	2367 (96%)	106 (4%)	40	19

All (106) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	13	ARG
1	A	111	LEU
1	A	179	LYS
1	A	222	LEU
1	A	269	THR
1	A	276	GLN
1	A	325	MET
1	A	341	LEU
1	A	384	LEU
1	A	414	ASP
1	A	415	LEU
1	A	437	LEU
1	A	455	LEU
1	A	458	ASN
1	A	477	GLU
1	A	486	ARG
1	B	111	LEU
1	B	179	LYS
1	B	222	LEU
1	B	269	THR
1	B	276	GLN
1	B	319	LEU
1	B	325	MET
1	B	341	LEU
1	B	384	LEU
1	B	407	MET
1	B	412	LYS
1	B	414	ASP
1	B	415	LEU
1	B	437	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	455	LEU
1	B	458	ASN
1	B	478	ASN
1	C	13	ARG
1	C	111	LEU
1	C	179	LYS
1	C	222	LEU
1	C	269	THR
1	C	276	GLN
1	C	319	LEU
1	C	325	MET
1	C	341	LEU
1	C	361	LYS
1	C	384	LEU
1	C	403	THR
1	C	414	ASP
1	C	415	LEU
1	C	437	LEU
1	C	455	LEU
1	C	458	ASN
1	C	481	GLU
1	C	486	ARG
1	D	111	LEU
1	D	179	LYS
1	D	222	LEU
1	D	269	THR
1	D	276	GLN
1	D	319	LEU
1	D	325	MET
1	D	341	LEU
1	D	361	LYS
1	D	384	LEU
1	D	407	MET
1	D	415	LEU
1	D	422	GLU
1	D	437	LEU
1	D	455	LEU
1	D	458	ASN
1	D	477	GLU
1	D	481	GLU
2	E	66	VAL
2	E	111	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	E	180	LYS
2	E	222	LEU
2	E	269	THR
2	E	276	GLN
2	E	325	MET
2	E	341	LEU
2	E	361	LYS
2	E	384	LEU
2	E	407	MET
2	E	414	ASP
2	E	415	LEU
2	E	437	LEU
2	E	455	LEU
2	E	458	ASN
2	E	477	GLU
2	E	481	GLU
1	F	13	ARG
1	F	111	LEU
1	F	222	LEU
1	F	269	THR
1	F	276	GLN
1	F	319	LEU
1	F	325	MET
1	F	341	LEU
1	F	381	PRO
1	F	384	LEU
1	F	403	THR
1	F	407	MET
1	F	414	ASP
1	F	415	LEU
1	F	422	GLU
1	F	437	LEU
1	F	455	LEU
1	F	458	ASN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (69) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	133	ASN
1	A	244	ASN
1	A	247	HIS
1	A	268	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	273	GLN
1	A	274	GLN
1	A	276	GLN
1	A	316	GLN
1	A	458	ASN
1	A	492	GLN
1	B	79	HIS
1	B	133	ASN
1	B	244	ASN
1	B	268	ASN
1	B	273	GLN
1	B	276	GLN
1	B	316	GLN
1	B	350	ASN
1	B	458	ASN
1	B	492	GLN
1	C	79	HIS
1	C	133	ASN
1	C	143	HIS
1	C	244	ASN
1	C	247	HIS
1	C	268	ASN
1	C	273	GLN
1	C	274	GLN
1	C	276	GLN
1	C	316	GLN
1	C	350	ASN
1	C	458	ASN
1	C	492	GLN
1	D	79	HIS
1	D	133	ASN
1	D	244	ASN
1	D	268	ASN
1	D	273	GLN
1	D	274	GLN
1	D	276	GLN
1	D	316	GLN
1	D	350	ASN
1	D	458	ASN
1	D	492	GLN
2	E	56	HIS
2	E	60	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	E	79	HIS
2	E	133	ASN
2	E	148	GLN
2	E	244	ASN
2	E	268	ASN
2	E	273	GLN
2	E	274	GLN
2	E	276	GLN
2	E	316	GLN
2	E	350	ASN
2	E	458	ASN
2	E	492	GLN
1	F	79	HIS
1	F	133	ASN
1	F	244	ASN
1	F	268	ASN
1	F	273	GLN
1	F	274	GLN
1	F	276	GLN
1	F	316	GLN
1	F	350	ASN
1	F	458	ASN
1	F	492	GLN

5.3.3 RNA ⓘ

There are no RNA chains in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry ⓘ

There are no ligands in this entry.

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	484/565 (85%)	-0.47	4 (0%)	83 81	20, 26, 37, 53	1 (0%)
1	B	484/565 (85%)	-0.50	5 (1%)	79 76	20, 26, 37, 52	1 (0%)
1	C	484/565 (85%)	-0.48	4 (0%)	83 81	20, 26, 37, 52	1 (0%)
1	D	484/565 (85%)	-0.49	7 (1%)	72 68	20, 26, 37, 54	1 (0%)
1	F	484/565 (85%)	-0.49	7 (1%)	72 68	19, 25, 36, 54	1 (0%)
2	E	484/565 (85%)	-0.47	8 (1%)	67 62	19, 25, 37, 51	1 (0%)
All	All	2904/3390 (85%)	-0.48	35 (1%)	75 72	19, 26, 37, 54	6 (0%)

All (35) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	344	ASN	5.1
1	F	344	ASN	4.4
1	D	344	ASN	4.0
1	D	13	ARG	3.9
1	A	414	ASP	3.8
1	F	13	ARG	3.6
1	C	414	ASP	3.5
2	E	313	GLU	3.5
2	E	344	ASN	3.4
2	E	249	GLY	3.3
2	E	414	ASP	3.3
1	A	344	ASN	3.2
1	F	414	ASP	3.0
1	B	13	ARG	2.9
1	A	13	ARG	2.9
1	F	211	GLY	2.8
1	D	250	ALA	2.8
1	C	344	ASN	2.8
1	B	414	ASP	2.7

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	D	414	ASP	2.7
1	F	314	LYS	2.7
1	C	13	ARG	2.6
2	E	250	ALA	2.6
1	D	424	HIS	2.5
2	E	13	ARG	2.5
1	F	496	GLY	2.5
1	A	477	GLU	2.3
2	E	314	LYS	2.3
1	C	477	GLU	2.3
2	E	496	GLY	2.3
1	D	477	GLU	2.2
1	F	250	ALA	2.1
1	B	424	HIS	2.1
1	D	314	LYS	2.1
1	B	314	LYS	2.1

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 ⓘ

There are no carbohydrates in this entry.

6.4 Ligands ⓘ

There are no ligands in this entry.

6.5 Other polymers ⓘ

There are no such residues in this entry.