Full wwPDB X-ray Structure Validation Report ⓘ

Dec 10, 2022 – 02:04 PM EST

PDB ID	:	1KBW
Title	:	CRYSTAL STRUCTURE OF THE SOLUBLE DOMAIN OF ANIA FROM NEISSERIA GONORRHOEAE
Authors	:	Boulanger, M.J.; Murphy, M.E.P.
Deposited on	:	2001-11-06
Resolution	:	2.40 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:

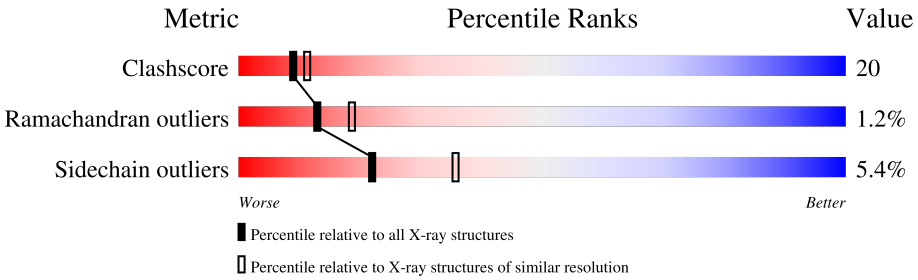
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.31.2

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 2.40 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	141614	4398 (2.40-2.40)
Ramachandran outliers	138981	4318 (2.40-2.40)
Sidechain outliers	138945	4319 (2.40-2.40)

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 <=5%

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	327	61% 28% • 8%
1	B	327	63% 27% • 8%
1	C	327	62% 27% • 8%
1	D	327	64% 26% • 8%
1	E	327	64% 25% • 8%
1	F	327	64% 24% • 8%

2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 14902 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called Major outer membrane protein PAN 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	302	Total	C	N	O	S	0	0	0
			2291	1461	385	435	10			
1	B	302	Total	C	N	O	S	0	0	0
			2291	1461	385	435	10			
1	C	302	Total	C	N	O	S	0	0	0
			2291	1461	385	435	10			
1	D	302	Total	C	N	O	S	0	0	0
			2291	1461	385	435	10			
1	E	302	Total	C	N	O	S	0	0	0
			2291	1461	385	435	10			
1	F	302	Total	C	N	O	S	0	0	0
			2291	1461	385	435	10			

There are 48 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1	MET	-	initiating methionine	UNP Q02219
A	209	ALA	SER	SEE REMARK 999	UNP Q02219
A	210	LEU	ILE	SEE REMARK 999	UNP Q02219
A	211	THR	ALA	SEE REMARK 999	UNP Q02219
A	283	ASN	SER	SEE REMARK 999	UNP Q02219
A	325	VAL	-	cloning artifact	UNP Q02219
A	326	PRO	-	cloning artifact	UNP Q02219
A	327	ARG	-	cloning artifact	UNP Q02219
B	1	MET	-	initiating methionine	UNP Q02219
B	209	ALA	SER	SEE REMARK 999	UNP Q02219
B	210	LEU	ILE	SEE REMARK 999	UNP Q02219
B	211	THR	ALA	SEE REMARK 999	UNP Q02219
B	283	ASN	SER	SEE REMARK 999	UNP Q02219
B	325	VAL	-	cloning artifact	UNP Q02219
B	326	PRO	-	cloning artifact	UNP Q02219
B	327	ARG	-	cloning artifact	UNP Q02219
C	1	MET	-	initiating methionine	UNP Q02219

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Chain	Residue	Modelled	Actual	Comment	Reference
C	209	ALA	SER	SEE REMARK 999	UNP Q02219
C	210	LEU	ILE	SEE REMARK 999	UNP Q02219
C	211	THR	ALA	SEE REMARK 999	UNP Q02219
C	283	ASN	SER	SEE REMARK 999	UNP Q02219
C	325	VAL	-	cloning artifact	UNP Q02219
C	326	PRO	-	cloning artifact	UNP Q02219
C	327	ARG	-	cloning artifact	UNP Q02219
D	1	MET	-	initiating methionine	UNP Q02219
D	209	ALA	SER	SEE REMARK 999	UNP Q02219
D	210	LEU	ILE	SEE REMARK 999	UNP Q02219
D	211	THR	ALA	SEE REMARK 999	UNP Q02219
D	283	ASN	SER	SEE REMARK 999	UNP Q02219
D	325	VAL	-	cloning artifact	UNP Q02219
D	326	PRO	-	cloning artifact	UNP Q02219
D	327	ARG	-	cloning artifact	UNP Q02219
E	1	MET	-	initiating methionine	UNP Q02219
E	209	ALA	SER	SEE REMARK 999	UNP Q02219
E	210	LEU	ILE	SEE REMARK 999	UNP Q02219
E	211	THR	ALA	SEE REMARK 999	UNP Q02219
E	283	ASN	SER	SEE REMARK 999	UNP Q02219
E	325	VAL	-	cloning artifact	UNP Q02219
E	326	PRO	-	cloning artifact	UNP Q02219
E	327	ARG	-	cloning artifact	UNP Q02219
F	1	MET	-	initiating methionine	UNP Q02219
F	209	ALA	SER	SEE REMARK 999	UNP Q02219
F	210	LEU	ILE	SEE REMARK 999	UNP Q02219
F	211	THR	ALA	SEE REMARK 999	UNP Q02219
F	283	ASN	SER	SEE REMARK 999	UNP Q02219
F	325	VAL	-	cloning artifact	UNP Q02219
F	326	PRO	-	cloning artifact	UNP Q02219
F	327	ARG	-	cloning artifact	UNP Q02219

- Molecule 2 is COPPER (II) ION (three-letter code: CU) (formula: Cu).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	2	Total Cu 2 2	0	0
2	B	2	Total Cu 2 2	0	0
2	C	2	Total Cu 2 2	0	0
2	D	2	Total Cu 2 2	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	E	2	Total Cu 2 2	0	0
2	F	2	Total Cu 2 2	0	0

- Molecule 3 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	221	Total O 221 221	0	0
3	B	183	Total O 183 183	0	0
3	C	182	Total O 182 182	0	0
3	D	210	Total O 210 210	0	0
3	E	192	Total O 192 192	0	0
3	F	156	Total O 156 156	0	0

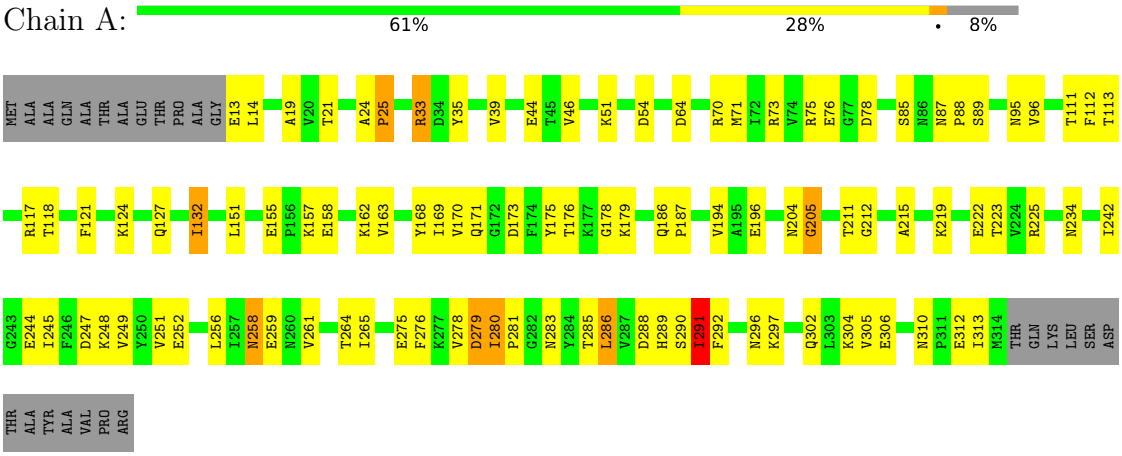
3 Residue-property plots (i)

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

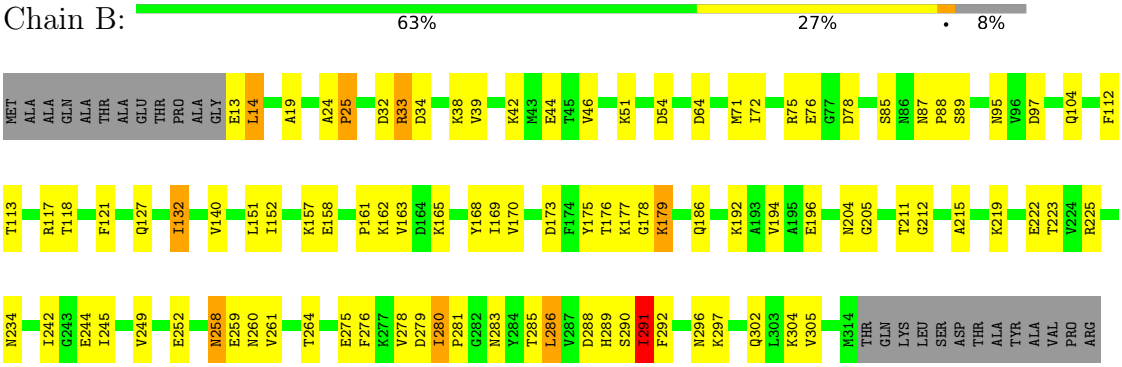
• Molecule 1: Major outer membrane protein PAN 1

Chain A:



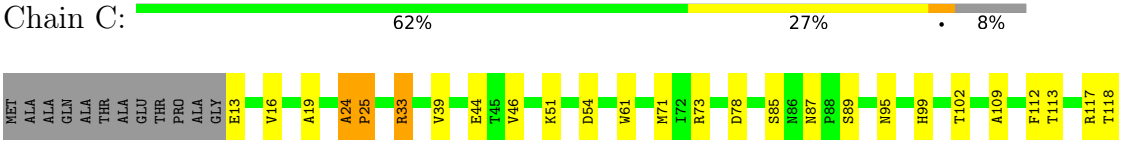
• Molecule 1: Major outer membrane protein PAN 1

Chain B:



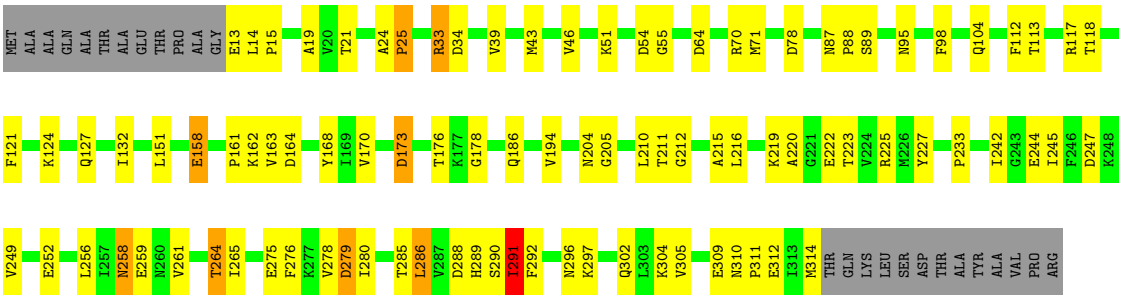
• Molecule 1: Major outer membrane protein PAN 1

Chain C:



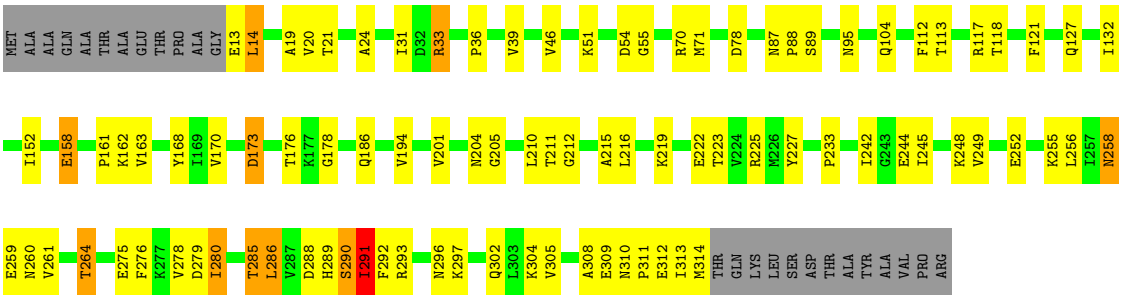
• Molecule 1: Major outer membrane protein PAN 1

Chain D:



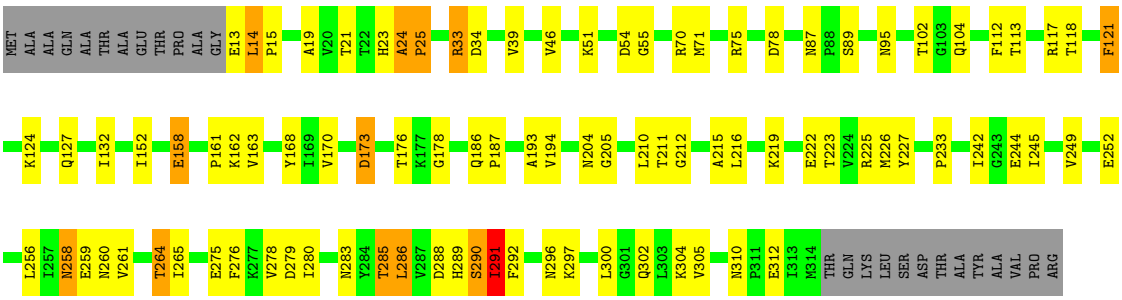
• Molecule 1: Major outer membrane protein PAN 1

Chain E:



• Molecule 1: Major outer membrane protein PAN 1

Chain F:



4 Data and refinement statistics (i)

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

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α, β, γ	66.23Å 99.55Å 103.71Å 83.55° 73.70° 73.01°	Depositor
Resolution (Å)	50.00 – 2.40	Depositor
% Data completeness (in resolution range)	80.7 (50.00-2.40)	Depositor
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	CNS 1.0	Depositor
R, R_{free}	0.211 , 0.234	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	14902	wwPDB-VP
Average B, all atoms (Å^2)	27.0	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: CU

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	0.39	0/2346	0.90	7/3185 (0.2%)
1	B	0.38	0/2346	0.90	7/3185 (0.2%)
1	C	0.39	0/2346	0.90	7/3185 (0.2%)
1	D	0.39	0/2346	0.90	6/3185 (0.2%)
1	E	0.40	0/2346	0.84	6/3185 (0.2%)
1	F	0.39	0/2346	0.89	7/3185 (0.2%)
All	All	0.39	0/14076	0.89	40/19110 (0.2%)

There are no bond length outliers.

All (40) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	24	ALA	C-N-CD	-20.91	74.60	120.60
1	A	24	ALA	C-N-CD	-20.51	75.47	120.60
1	C	24	ALA	C-N-CD	-20.11	76.35	120.60
1	D	24	ALA	C-N-CD	-19.77	77.11	120.60
1	F	24	ALA	C-N-CD	-19.55	77.60	120.60
1	E	24	ALA	C-N-CD	-14.02	89.75	120.60
1	F	24	ALA	C-N-CA	13.74	179.72	122.00
1	D	24	ALA	C-N-CA	13.65	179.35	122.00
1	C	24	ALA	C-N-CA	13.46	178.54	122.00
1	A	24	ALA	C-N-CA	13.06	176.87	122.00
1	B	24	ALA	C-N-CA	12.94	176.34	122.00
1	E	24	ALA	C-N-CA	9.39	161.42	122.00
1	F	290	SER	N-CA-C	-7.41	90.99	111.00
1	A	290	SER	N-CA-C	-7.31	91.27	111.00
1	C	290	SER	N-CA-C	-7.26	91.41	111.00
1	E	290	SER	N-CA-C	-7.20	91.57	111.00
1	B	290	SER	N-CA-C	-7.17	91.65	111.00
1	D	290	SER	N-CA-C	-7.14	91.72	111.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	25	PRO	CA-N-CD	-6.88	101.87	111.50
1	E	288	ASP	N-CA-C	-6.83	92.55	111.00
1	F	288	ASP	N-CA-C	-6.78	92.71	111.00
1	D	288	ASP	N-CA-C	-6.72	92.85	111.00
1	B	288	ASP	N-CA-C	-6.72	92.86	111.00
1	F	25	PRO	CA-N-CD	-6.68	102.15	111.50
1	C	288	ASP	N-CA-C	-6.61	93.16	111.00
1	D	25	PRO	CA-N-CD	-6.57	102.30	111.50
1	C	25	PRO	CA-N-CD	-6.55	102.33	111.50
1	B	25	PRO	CA-N-CD	-6.54	102.34	111.50
1	A	288	ASP	N-CA-C	-6.51	93.42	111.00
1	A	205	GLY	N-CA-C	6.07	128.27	113.10
1	D	205	GLY	N-CA-C	6.04	128.21	113.10
1	F	205	GLY	N-CA-C	5.92	127.91	113.10
1	C	205	GLY	N-CA-C	5.87	127.77	113.10
1	E	205	GLY	N-CA-C	5.79	127.58	113.10
1	B	205	GLY	N-CA-C	5.50	126.85	113.10
1	B	291	ILE	N-CA-C	5.50	125.84	111.00
1	C	291	ILE	N-CA-C	5.21	125.07	111.00
1	F	291	ILE	N-CA-C	5.15	124.90	111.00
1	E	291	ILE	N-CA-C	5.13	124.86	111.00
1	A	291	ILE	N-CA-C	5.12	124.83	111.00

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts (i)

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	2291	0	2234	106	0
1	B	2291	0	2234	96	0
1	C	2291	0	2234	101	0
1	D	2291	0	2234	94	0
1	E	2291	0	2234	95	0
1	F	2291	0	2234	106	0
2	A	2	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	B	2	0	0	0	0
2	C	2	0	0	0	0
2	D	2	0	0	0	0
2	E	2	0	0	0	0
2	F	2	0	0	0	0
3	A	221	0	0	28	0
3	B	183	0	0	28	0
3	C	182	0	0	19	0
3	D	210	0	0	17	0
3	E	192	0	0	21	0
3	F	156	0	0	24	0
All	All	14902	0	13404	549	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 20.

All (549) 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:C:278:VAL:HG11	1:C:305:VAL:HG21	1.24	1.17
1:E:201:VAL:HB	3:E:679:HOH:O	1.46	1.14
1:D:264:THR:HG22	1:F:252:GLU:OE1	1.50	1.12
1:A:264:THR:HG22	1:C:252:GLU:OE1	1.48	1.12
1:A:278:VAL:HG11	1:A:305:VAL:HG21	1.37	1.05
1:F:278:VAL:HG11	1:F:305:VAL:HG21	1.37	1.04
1:B:34:ASP:HA	3:B:662:HOH:O	1.57	1.03
1:B:278:VAL:HG11	1:B:305:VAL:HG21	1.40	1.01
1:F:297:LYS:HE2	3:F:640:HOH:O	1.62	0.99
1:D:252:GLU:OE1	1:E:264:THR:HG22	1.62	0.97
1:A:252:GLU:OE1	1:B:264:THR:HG22	1.64	0.97
1:B:252:GLU:OE1	1:C:264:THR:HG22	1.63	0.97
1:C:33:ARG:HB2	3:C:676:HOH:O	1.63	0.97
1:D:13:GLU:HA	3:D:530:HOH:O	1.66	0.95
1:E:278:VAL:HG11	1:E:305:VAL:HG21	1.49	0.94
1:B:297:LYS:HE2	3:B:657:HOH:O	1.66	0.93
1:C:249:VAL:HG11	1:C:264:THR:HG21	1.51	0.92
1:A:280:ILE:HB	3:A:695:HOH:O	1.69	0.92
1:F:13:GLU:HA	3:F:637:HOH:O	1.71	0.91
3:A:696:HOH:O	1:C:99:HIS:CE1	2.25	0.91
1:B:249:VAL:HG11	1:B:264:THR:HG21	1.50	0.90
1:D:264:THR:CG2	1:F:252:GLU:OE1	2.19	0.90

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:249:VAL:HG11	1:A:264:THR:HG21	1.52	0.90
1:A:35:TYR:CZ	3:A:690:HOH:O	2.25	0.89
1:E:252:GLU:OE1	1:F:264:THR:HG22	1.72	0.87
1:B:258:ASN:HD22	1:B:259:GLU:H	1.23	0.87
1:E:54:ASP:HB2	3:E:611:HOH:O	1.75	0.86
1:E:249:VAL:HG11	1:E:264:THR:HG21	1.58	0.86
1:D:249:VAL:HG11	1:D:264:THR:HG21	1.57	0.86
1:F:34:ASP:OD1	3:F:645:HOH:O	1.95	0.85
1:D:278:VAL:HG11	1:D:305:VAL:HG21	1.58	0.83
1:F:249:VAL:HG11	1:F:264:THR:HG21	1.59	0.82
1:A:87:ASN:HD22	1:A:89:SER:H	1.28	0.82
1:D:297:LYS:HE2	3:D:693:HOH:O	1.79	0.82
1:D:13:GLU:HB3	3:D:685:HOH:O	1.79	0.82
1:F:87:ASN:HD22	1:F:89:SER:H	1.26	0.82
1:F:51:LYS:HE2	1:F:54:ASP:HA	1.62	0.82
1:E:225:ARG:NH2	3:E:682:HOH:O	2.00	0.81
1:E:51:LYS:HE2	1:E:54:ASP:HA	1.61	0.80
1:D:51:LYS:HE2	1:D:54:ASP:HA	1.62	0.80
1:F:33:ARG:HB2	3:F:652:HOH:O	1.80	0.80
1:D:87:ASN:HD22	1:D:89:SER:H	1.30	0.80
1:C:306:GLU:HG3	3:C:665:HOH:O	1.80	0.80
1:C:176:THR:HG23	1:C:186:GLN:HB3	1.64	0.80
1:B:176:THR:HG23	1:B:186:GLN:HB3	1.63	0.79
1:A:51:LYS:HE2	1:A:54:ASP:HA	1.65	0.79
1:A:176:THR:HG23	1:A:186:GLN:HB3	1.63	0.79
1:B:87:ASN:HD22	1:B:89:SER:H	1.31	0.78
1:C:51:LYS:HE2	1:C:54:ASP:HA	1.66	0.78
1:F:13:GLU:OE1	3:F:533:HOH:O	2.02	0.78
1:C:87:ASN:HD22	1:C:89:SER:H	1.30	0.78
1:C:258:ASN:HD22	1:C:259:GLU:H	1.31	0.78
1:E:87:ASN:HD22	1:E:89:SER:H	1.30	0.78
1:B:51:LYS:HE2	1:B:54:ASP:HA	1.65	0.78
1:E:176:THR:HG23	1:E:186:GLN:HB3	1.66	0.77
1:A:258:ASN:HD22	1:A:259:GLU:H	1.30	0.77
1:A:33:ARG:HD2	3:A:690:HOH:O	1.84	0.76
1:B:177:LYS:HA	3:B:678:HOH:O	1.84	0.76
1:A:111:THR:HB	3:A:576:HOH:O	1.86	0.76
1:D:176:THR:HG23	1:D:186:GLN:HB3	1.67	0.76
1:F:51:LYS:HE3	3:F:590:HOH:O	1.85	0.76
1:A:289:HIS:NE2	3:A:696:HOH:O	2.18	0.75
1:A:304:LYS:HE3	3:A:700:HOH:O	1.85	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:278:VAL:HG11	1:F:305:VAL:CG2	2.14	0.74
1:F:176:THR:HG23	1:F:186:GLN:HB3	1.70	0.74
1:F:19:ALA:HB2	1:F:39:VAL:CG1	2.16	0.74
1:D:21:THR:OG1	1:D:70:ARG:HD3	1.86	0.74
1:C:297:LYS:HE2	3:C:667:HOH:O	1.88	0.73
1:F:258:ASN:HD22	1:F:259:GLU:H	1.36	0.73
1:E:258:ASN:HD22	1:E:259:GLU:H	1.36	0.72
1:B:242:ILE:HG12	3:B:682:HOH:O	1.89	0.72
1:E:176:THR:HG22	1:E:178:GLY:O	1.90	0.72
1:D:117:ARG:HD3	3:D:701:HOH:O	1.90	0.71
1:B:211:THR:HG22	1:B:212:GLY:N	2.05	0.71
1:A:211:THR:HG22	1:A:212:GLY:N	2.04	0.71
1:B:75:ARG:NH2	3:B:662:HOH:O	2.23	0.71
1:C:211:THR:HG22	1:C:212:GLY:N	2.06	0.70
1:D:127:GLN:HE21	1:E:260:ASN:HD22	1.39	0.70
1:D:176:THR:HG22	1:D:178:GLY:O	1.91	0.70
1:C:16:VAL:O	3:C:655:HOH:O	2.10	0.70
1:A:35:TYR:OH	3:A:690:HOH:O	2.08	0.69
1:D:311:PRO:HG3	3:D:654:HOH:O	1.91	0.69
1:E:51:LYS:CE	1:E:54:ASP:HA	2.22	0.69
1:B:38:LYS:HE2	3:B:600:HOH:O	1.92	0.69
1:B:158:GLU:CD	1:B:158:GLU:H	1.94	0.69
1:C:13:GLU:N	3:C:595:HOH:O	2.26	0.69
1:C:158:GLU:H	1:C:158:GLU:CD	1.93	0.69
1:F:285:THR:OG1	3:F:643:HOH:O	2.09	0.69
1:A:158:GLU:H	1:A:158:GLU:CD	1.95	0.69
1:E:252:GLU:OE1	1:F:264:THR:CG2	2.41	0.69
1:B:176:THR:HG22	1:B:178:GLY:O	1.93	0.69
1:F:13:GLU:N	3:F:637:HOH:O	2.26	0.69
1:D:211:THR:HG22	1:D:212:GLY:N	2.08	0.68
1:F:13:GLU:CA	3:F:637:HOH:O	2.35	0.68
1:F:176:THR:HG22	1:F:178:GLY:O	1.93	0.68
1:D:258:ASN:HD22	1:D:259:GLU:H	1.41	0.68
1:A:176:THR:HG22	1:A:178:GLY:O	1.93	0.67
1:D:51:LYS:CE	1:D:54:ASP:HA	2.22	0.67
1:F:300:LEU:HG	3:F:643:HOH:O	1.94	0.67
1:B:244:GLU:HG2	1:B:276:PHE:CD1	2.29	0.67
1:F:219:LYS:O	1:F:222:GLU:HG3	1.94	0.67
1:F:51:LYS:CE	1:F:54:ASP:HA	2.24	0.67
1:F:211:THR:HG22	1:F:212:GLY:N	2.09	0.66
1:C:217:LYS:HE3	3:C:626:HOH:O	1.94	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:33:ARG:HD3	3:F:512:HOH:O	1.95	0.66
1:A:127:GLN:HE21	1:B:260:ASN:HD22	1.41	0.66
1:F:124:LYS:HE3	3:F:642:HOH:O	1.95	0.66
1:A:19:ALA:HB2	1:A:39:VAL:CG1	2.26	0.66
1:D:64:ASP:OD1	3:D:684:HOH:O	2.14	0.66
1:E:309:GLU:O	1:E:311:PRO:HD3	1.96	0.66
1:E:211:THR:HG22	1:E:212:GLY:N	2.10	0.66
1:A:211:THR:HG22	1:A:212:GLY:H	1.61	0.65
1:A:96:VAL:HG12	3:A:576:HOH:O	1.96	0.65
1:E:158:GLU:CD	1:E:158:GLU:H	1.99	0.65
1:E:117:ARG:HG2	1:E:118:THR:N	2.12	0.65
1:A:194:VAL:O	1:B:297:LYS:NZ	2.30	0.65
1:F:211:THR:HG23	1:F:302:GLN:CD	2.17	0.65
1:B:258:ASN:HD22	1:B:259:GLU:N	1.92	0.65
1:D:117:ARG:HG2	1:D:118:THR:N	2.12	0.65
1:C:176:THR:HG22	1:C:178:GLY:O	1.96	0.64
1:F:117:ARG:HG2	1:F:118:THR:N	2.10	0.64
1:F:158:GLU:CD	1:F:158:GLU:H	2.00	0.64
1:F:283:ASN:HB3	3:F:604:HOH:O	1.97	0.64
1:E:211:THR:HG23	1:E:302:GLN:CD	2.18	0.64
1:E:308:ALA:HB3	3:E:610:HOH:O	1.97	0.64
1:C:297:LYS:NZ	3:C:667:HOH:O	2.30	0.64
1:D:158:GLU:CD	1:D:158:GLU:H	1.99	0.63
1:B:211:THR:HG22	1:B:212:GLY:H	1.63	0.63
1:D:220:ALA:HB1	3:D:690:HOH:O	1.97	0.63
1:E:278:VAL:HG11	1:E:305:VAL:CG2	2.26	0.63
1:A:244:GLU:HG2	1:A:276:PHE:CD1	2.32	0.63
1:F:211:THR:HG23	1:F:302:GLN:OE1	1.98	0.63
1:C:244:GLU:HG2	1:C:276:PHE:CD1	2.33	0.63
1:D:219:LYS:O	1:D:222:GLU:HG3	1.98	0.63
1:D:252:GLU:OE1	1:E:264:THR:CG2	2.44	0.62
1:A:54:ASP:HB2	3:A:699:HOH:O	2.00	0.62
1:C:117:ARG:HG2	1:C:118:THR:N	2.14	0.62
1:D:279:ASP:OD2	1:F:102:THR:HG21	1.98	0.62
1:C:213:ASP:HB3	3:C:666:HOH:O	1.98	0.62
1:C:278:VAL:HG11	1:C:305:VAL:CG2	2.16	0.62
1:C:117:ARG:HG3	3:C:663:HOH:O	1.98	0.62
3:E:693:HOH:O	1:F:242:ILE:HG12	2.00	0.62
1:C:297:LYS:CE	3:C:667:HOH:O	2.46	0.61
1:B:261:VAL:HG11	1:B:264:THR:HG23	1.82	0.61
1:E:215:ALA:HB3	1:E:304:LYS:HD2	1.81	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:13:GLU:O	1:A:13:GLU:HG3	1.99	0.61
1:A:51:LYS:CE	1:A:54:ASP:HA	2.31	0.61
1:B:194:VAL:O	1:C:297:LYS:NZ	2.32	0.61
1:D:304:LYS:HE3	3:D:707:HOH:O	2.00	0.61
1:C:51:LYS:CE	1:C:54:ASP:HA	2.30	0.61
1:D:19:ALA:HB2	1:D:39:VAL:CG1	2.30	0.61
1:E:219:LYS:O	1:E:222:GLU:HG3	1.99	0.61
1:C:19:ALA:HB2	1:C:39:VAL:CG1	2.31	0.61
1:D:13:GLU:O	1:D:14:LEU:HB2	2.01	0.61
1:B:140:VAL:HG23	3:B:664:HOH:O	2.00	0.60
1:E:211:THR:HG23	1:E:302:GLN:OE1	2.01	0.60
1:F:113:THR:HG23	1:F:117:ARG:HD2	1.84	0.60
1:F:285:THR:CB	3:F:643:HOH:O	2.48	0.60
1:E:54:ASP:OD2	3:E:611:HOH:O	2.16	0.60
1:B:19:ALA:HB2	1:B:39:VAL:CG1	2.31	0.60
1:D:113:THR:HG23	1:D:117:ARG:HD2	1.83	0.60
1:E:278:VAL:CG1	1:E:305:VAL:HG11	2.31	0.60
1:E:293:ARG:HB3	3:E:679:HOH:O	2.01	0.60
1:A:117:ARG:HG2	1:A:118:THR:N	2.16	0.60
1:F:87:ASN:ND2	1:F:89:SER:H	1.98	0.60
1:A:75:ARG:NH1	3:A:503:HOH:O	2.31	0.60
1:B:51:LYS:CE	1:B:54:ASP:HA	2.32	0.60
1:C:258:ASN:ND2	1:C:259:GLU:H	2.00	0.60
1:B:192:LYS:CE	3:B:678:HOH:O	2.50	0.60
1:B:258:ASN:ND2	1:B:259:GLU:H	1.95	0.60
1:D:210:LEU:HD22	1:D:216:LEU:HD21	1.83	0.60
1:D:211:THR:HG23	1:D:302:GLN:CD	2.21	0.60
1:D:215:ALA:HB3	1:D:304:LYS:HD2	1.82	0.59
1:F:215:ALA:HB3	1:F:304:LYS:HD2	1.83	0.59
1:A:258:ASN:HD22	1:A:259:GLU:N	1.99	0.59
1:C:258:ASN:HD22	1:C:259:GLU:N	1.99	0.59
1:C:117:ARG:CG	3:C:663:HOH:O	2.49	0.59
1:F:244:GLU:HG2	1:F:276:PHE:CD1	2.37	0.59
1:B:117:ARG:HG2	1:B:118:THR:N	2.16	0.59
1:E:14:LEU:N	3:E:614:HOH:O	2.35	0.59
1:D:244:GLU:HG2	1:D:276:PHE:CD1	2.38	0.59
1:A:258:ASN:ND2	1:A:259:GLU:H	1.98	0.59
1:C:211:THR:HG22	1:C:212:GLY:H	1.65	0.59
1:D:162:LYS:HE2	1:D:162:LYS:HA	1.84	0.59
1:C:244:GLU:HG3	1:C:245:ILE:H	1.67	0.58
1:C:261:VAL:HG11	1:C:264:THR:HG23	1.85	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:306:GLU:HG3	3:A:673:HOH:O	2.03	0.58
1:C:225:ARG:HG3	1:C:275:GLU:CG	2.34	0.58
1:D:278:VAL:HG11	1:D:305:VAL:CG2	2.33	0.58
1:B:280:ILE:HD11	3:B:669:HOH:O	2.02	0.58
1:E:162:LYS:HA	1:E:162:LYS:HE2	1.85	0.58
1:A:113:THR:HG23	1:A:117:ARG:HD2	1.85	0.58
1:A:261:VAL:HG11	1:A:264:THR:HG23	1.86	0.58
1:D:256:LEU:H	1:E:258:ASN:HD21	1.52	0.58
1:D:211:THR:CG2	1:D:212:GLY:N	2.67	0.58
1:B:244:GLU:HG3	1:B:245:ILE:H	1.69	0.58
1:E:244:GLU:HG2	1:E:276:PHE:CD1	2.39	0.58
1:F:21:THR:OG1	1:F:70:ARG:HD3	2.04	0.58
1:E:87:ASN:ND2	1:E:89:SER:H	2.00	0.57
1:C:113:THR:HG23	1:C:117:ARG:HD2	1.87	0.57
1:C:132:ILE:HD12	1:C:151:LEU:CD2	2.34	0.57
1:A:13:GLU:O	1:A:13:GLU:CG	2.52	0.57
1:F:211:THR:CG2	1:F:212:GLY:N	2.67	0.57
1:A:225:ARG:HG3	1:A:275:GLU:CG	2.35	0.57
1:A:248:LYS:HE2	3:A:553:HOH:O	2.03	0.57
1:B:192:LYS:HE3	3:B:678:HOH:O	2.03	0.57
1:F:162:LYS:HE2	1:F:162:LYS:HA	1.85	0.57
1:F:278:VAL:CG1	1:F:305:VAL:HG11	2.35	0.57
1:E:19:ALA:HB2	1:E:39:VAL:CG1	2.35	0.57
1:D:211:THR:HG23	1:D:302:GLN:OE1	2.04	0.57
1:E:113:THR:HG23	1:E:117:ARG:HD2	1.87	0.56
1:E:297:LYS:HB2	3:E:679:HOH:O	2.03	0.56
1:E:248:LYS:NZ	3:E:542:HOH:O	2.39	0.56
1:A:244:GLU:HG3	1:A:245:ILE:H	1.69	0.56
1:F:117:ARG:HD3	3:F:651:HOH:O	2.05	0.56
1:A:127:GLN:HE21	1:B:260:ASN:ND2	2.02	0.56
1:C:51:LYS:HG3	3:C:668:HOH:O	2.04	0.56
1:D:87:ASN:ND2	1:D:89:SER:H	2.00	0.56
1:F:23:HIS:CE1	3:F:639:HOH:O	2.58	0.56
1:F:278:VAL:CG1	1:F:305:VAL:HG21	2.26	0.56
1:A:219:LYS:O	1:A:222:GLU:HG3	2.05	0.56
1:B:87:ASN:ND2	1:B:89:SER:H	2.03	0.56
1:E:54:ASP:CB	3:E:611:HOH:O	2.40	0.56
1:A:225:ARG:HG3	1:A:275:GLU:HG3	1.88	0.56
1:E:31:ILE:HG23	3:E:677:HOH:O	2.06	0.56
1:E:33:ARG:HG2	3:E:677:HOH:O	2.05	0.56
1:B:113:THR:HG23	1:B:117:ARG:HD2	1.88	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:225:ARG:HG3	1:B:275:GLU:CG	2.36	0.55
1:C:244:GLU:HG3	1:C:245:ILE:N	2.22	0.55
1:E:278:VAL:HG11	1:E:305:VAL:HG11	1.88	0.55
1:B:42:LYS:HE3	3:B:661:HOH:O	2.05	0.55
1:C:225:ARG:HG3	1:C:275:GLU:HG3	1.89	0.55
1:E:211:THR:CG2	1:E:212:GLY:N	2.69	0.55
1:F:13:GLU:O	1:F:14:LEU:O	2.24	0.55
1:B:42:LYS:CE	3:B:661:HOH:O	2.55	0.55
3:B:655:HOH:O	1:C:264:THR:HG22	2.05	0.55
1:D:310:ASN:OD1	1:D:312:GLU:HB2	2.07	0.55
1:D:278:VAL:CG1	1:D:305:VAL:HG11	2.37	0.55
1:E:33:ARG:HH22	1:E:78:ASP:CG	2.10	0.55
1:D:225:ARG:NH1	1:D:275:GLU:OE2	2.40	0.55
1:B:225:ARG:HG3	1:B:275:GLU:HG3	1.89	0.55
1:D:33:ARG:HH22	1:D:78:ASP:CG	2.10	0.55
1:A:264:THR:CG2	1:C:252:GLU:OE1	2.38	0.55
1:A:225:ARG:NH1	1:A:275:GLU:OE2	2.39	0.55
1:F:225:ARG:HG3	1:F:275:GLU:HG2	1.88	0.54
1:A:211:THR:CG2	1:A:212:GLY:H	2.21	0.54
1:C:211:THR:CG2	1:C:212:GLY:N	2.71	0.54
1:D:265:ILE:HG13	1:F:265:ILE:HG21	1.90	0.54
1:F:210:LEU:HD22	1:F:216:LEU:HD21	1.89	0.54
1:A:87:ASN:ND2	1:A:89:SER:H	2.02	0.54
1:B:161:PRO:HB2	3:B:674:HOH:O	2.07	0.54
3:B:655:HOH:O	1:C:264:THR:CG2	2.56	0.54
1:D:256:LEU:H	1:E:258:ASN:ND2	2.06	0.54
1:C:132:ILE:HD12	1:C:151:LEU:HD21	1.89	0.54
1:E:194:VAL:CG1	1:F:297:LYS:HZ1	2.20	0.54
1:A:211:THR:CG2	1:A:212:GLY:N	2.70	0.53
1:A:280:ILE:CB	3:A:695:HOH:O	2.42	0.53
1:B:13:GLU:O	1:B:14:LEU:O	2.25	0.53
1:B:244:GLU:HG3	1:B:245:ILE:N	2.22	0.53
1:E:258:ASN:HD22	1:E:259:GLU:N	2.04	0.53
1:B:38:LYS:CE	3:B:600:HOH:O	2.53	0.53
1:E:210:LEU:HD22	1:E:216:LEU:HD21	1.90	0.53
1:E:225:ARG:NE	3:E:682:HOH:O	2.39	0.53
1:B:170:VAL:H	1:B:204:ASN:ND2	2.07	0.53
1:B:289:HIS:C	1:B:291:ILE:N	2.60	0.53
1:F:225:ARG:NH1	1:F:275:GLU:OE2	2.42	0.53
1:A:21:THR:OG1	1:A:70:ARG:HD3	2.08	0.53
1:B:194:VAL:HG13	1:C:297:LYS:HZ2	1.73	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:225:ARG:HG3	1:E:275:GLU:HG2	1.91	0.53
1:D:124:LYS:NZ	3:D:699:HOH:O	2.42	0.53
1:C:170:VAL:H	1:C:204:ASN:ND2	2.07	0.53
1:F:124:LYS:CE	3:F:642:HOH:O	2.56	0.53
1:A:35:TYR:CE1	3:A:690:HOH:O	2.54	0.53
1:C:220:ALA:N	1:C:306:GLU:O	2.31	0.53
1:A:242:ILE:HG12	3:C:682:HOH:O	2.09	0.52
1:B:211:THR:CG2	1:B:212:GLY:H	2.22	0.52
1:B:127:GLN:HE21	1:C:260:ASN:ND2	2.06	0.52
1:F:163:VAL:HG13	1:F:223:THR:O	2.08	0.52
1:B:219:LYS:O	1:B:222:GLU:HG3	2.08	0.52
1:C:87:ASN:ND2	1:C:89:SER:H	2.02	0.52
1:E:194:VAL:CG1	1:F:297:LYS:NZ	2.73	0.52
1:F:33:ARG:HH22	1:F:78:ASP:CG	2.12	0.52
1:B:225:ARG:NH2	3:B:592:HOH:O	2.30	0.52
1:D:258:ASN:ND2	1:D:259:GLU:H	2.07	0.52
1:A:13:GLU:N	3:A:552:HOH:O	2.42	0.52
1:B:211:THR:CG2	1:B:212:GLY:N	2.70	0.52
1:F:258:ASN:ND2	1:F:259:GLU:H	2.06	0.52
1:A:244:GLU:HG3	1:A:245:ILE:N	2.24	0.52
1:D:289:HIS:C	1:D:291:ILE:N	2.62	0.52
1:E:280:ILE:HG21	1:E:313:ILE:HG21	1.91	0.52
1:C:211:THR:CG2	1:C:212:GLY:H	2.23	0.52
1:A:170:VAL:H	1:A:204:ASN:ND2	2.07	0.52
1:C:19:ALA:HB2	1:C:39:VAL:HG12	1.91	0.52
1:C:219:LYS:O	1:C:222:GLU:HG3	2.09	0.52
1:D:194:VAL:O	1:E:297:LYS:NZ	2.43	0.52
1:A:196:GLU:HG2	1:A:234:ASN:HB3	1.92	0.52
1:A:21:THR:HB	1:A:70:ARG:HB3	1.91	0.51
1:B:170:VAL:H	1:B:204:ASN:HD21	1.58	0.51
1:E:170:VAL:H	1:E:204:ASN:ND2	2.08	0.51
1:A:291:ILE:HG21	1:C:141:GLY:HA2	1.92	0.51
1:B:179:LYS:HE2	3:B:608:HOH:O	2.10	0.51
1:E:289:HIS:C	1:E:291:ILE:N	2.59	0.51
1:F:289:HIS:C	1:F:291:ILE:N	2.63	0.51
1:B:33:ARG:HH22	1:B:78:ASP:CG	2.13	0.51
1:A:168:TYR:C	1:A:169:ILE:HD12	2.30	0.51
1:D:170:VAL:H	1:D:204:ASN:ND2	2.08	0.51
1:D:161:PRO:O	1:D:225:ARG:NH2	2.44	0.51
1:A:313:ILE:O	1:C:123:PHE:HA	2.11	0.51
1:E:163:VAL:HG13	1:E:223:THR:O	2.10	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:258:ASN:HD22	1:F:259:GLU:N	2.05	0.51
1:A:54:ASP:CB	3:A:699:HOH:O	2.58	0.51
1:B:127:GLN:HE21	1:C:260:ASN:HD22	1.59	0.51
1:C:33:ARG:HH22	1:C:78:ASP:CG	2.14	0.51
1:D:127:GLN:HE21	1:E:260:ASN:ND2	2.06	0.51
1:F:292:PHE:O	1:F:296:ASN:HB2	2.11	0.51
1:E:258:ASN:ND2	1:E:259:GLU:H	2.05	0.51
1:E:261:VAL:HG11	1:E:264:THR:HG23	1.93	0.51
1:A:289:HIS:C	1:A:291:ILE:N	2.63	0.51
1:C:225:ARG:NH1	1:C:275:GLU:OE2	2.43	0.51
1:E:225:ARG:NH1	1:E:275:GLU:OE2	2.43	0.51
1:A:247:ASP:OD1	1:C:127:GLN:NE2	2.44	0.51
1:A:256:LEU:H	1:B:258:ASN:HD21	1.59	0.50
1:B:225:ARG:NH1	1:B:275:GLU:OE2	2.44	0.50
1:B:168:TYR:C	1:B:169:ILE:HD12	2.31	0.50
1:C:112:PHE:O	1:C:117:ARG:NH1	2.44	0.50
1:E:255:LYS:NZ	3:E:678:HOH:O	2.35	0.50
1:C:289:HIS:C	1:C:291:ILE:N	2.62	0.50
1:E:21:THR:OG1	1:E:70:ARG:HD3	2.11	0.50
1:A:19:ALA:HB2	1:A:39:VAL:HG12	1.93	0.50
1:A:279:ASP:OD2	1:C:102:THR:HG21	2.12	0.50
1:D:225:ARG:HG3	1:D:275:GLU:HG2	1.93	0.50
1:D:278:VAL:HG11	1:D:305:VAL:HG11	1.94	0.50
1:E:215:ALA:CB	1:E:304:LYS:HD2	2.41	0.50
1:A:124:LYS:NZ	3:A:698:HOH:O	2.21	0.50
1:F:173:ASP:OD1	1:F:233:PRO:HD2	2.12	0.50
1:D:33:ARG:NH2	1:D:78:ASP:OD2	2.45	0.50
3:E:592:HOH:O	1:F:261:VAL:HG21	2.12	0.49
1:D:297:LYS:CE	3:D:693:HOH:O	2.49	0.49
1:C:292:PHE:O	1:C:296:ASN:HB2	2.12	0.49
1:F:170:VAL:H	1:F:204:ASN:ND2	2.11	0.49
1:C:33:ARG:HG2	3:C:677:HOH:O	2.11	0.49
1:D:173:ASP:OD1	1:D:233:PRO:HD2	2.13	0.49
1:A:283:ASN:OD1	1:A:304:LYS:HG2	2.12	0.49
1:D:163:VAL:HG13	1:D:223:THR:O	2.13	0.49
1:E:33:ARG:NH2	1:E:78:ASP:OD2	2.46	0.49
1:E:161:PRO:O	1:E:225:ARG:NH2	2.45	0.49
1:A:170:VAL:H	1:A:204:ASN:HD21	1.61	0.49
1:C:168:TYR:C	1:C:169:ILE:HD12	2.33	0.49
1:D:247:ASP:OD1	1:F:127:GLN:NE2	2.45	0.49
1:A:33:ARG:HH22	1:A:78:ASP:CG	2.15	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:161:PRO:O	1:F:225:ARG:NH2	2.41	0.49
1:D:261:VAL:HG11	1:D:264:THR:HG23	1.94	0.49
1:E:194:VAL:HG13	1:F:297:LYS:NZ	2.28	0.49
1:B:283:ASN:OD1	1:B:304:LYS:HG2	2.12	0.48
1:C:170:VAL:H	1:C:204:ASN:HD21	1.61	0.48
1:D:215:ALA:CB	1:D:304:LYS:HD2	2.42	0.48
1:D:258:ASN:ND2	1:F:256:LEU:H	2.11	0.48
1:F:261:VAL:HG11	1:F:264:THR:HG23	1.94	0.48
1:F:285:THR:HB	3:F:643:HOH:O	2.13	0.48
1:B:75:ARG:NE	3:B:662:HOH:O	2.46	0.48
1:F:19:ALA:HB2	1:F:39:VAL:HG13	1.94	0.48
1:A:33:ARG:HD3	3:A:670:HOH:O	2.13	0.48
1:A:112:PHE:O	1:A:117:ARG:NH1	2.46	0.48
1:A:211:THR:HG23	1:A:302:GLN:CD	2.33	0.48
1:A:256:LEU:H	1:B:258:ASN:ND2	2.11	0.48
1:E:20:VAL:HA	3:E:604:HOH:O	2.13	0.48
1:C:283:ASN:OD1	1:C:304:LYS:HG2	2.13	0.48
1:C:196:GLU:HG2	1:C:234:ASN:HB3	1.96	0.48
1:B:278:VAL:HG11	1:B:305:VAL:CG2	2.29	0.48
1:B:75:ARG:CZ	3:B:662:HOH:O	2.61	0.48
1:B:165:LYS:HD2	3:B:677:HOH:O	2.14	0.48
1:A:286:LEU:N	1:A:286:LEU:HD23	2.29	0.47
1:E:308:ALA:CB	3:E:610:HOH:O	2.59	0.47
1:F:24:ALA:N	3:F:593:HOH:O	2.47	0.47
1:A:157:LYS:HE2	3:A:591:HOH:O	2.13	0.47
1:B:112:PHE:O	1:B:117:ARG:NH1	2.47	0.47
3:B:683:HOH:O	1:C:242:ILE:HG12	2.13	0.47
1:C:109:ALA:HB3	3:C:624:HOH:O	2.14	0.47
1:D:242:ILE:HG12	3:F:657:HOH:O	2.13	0.47
1:F:225:ARG:HG3	1:F:275:GLU:CG	2.44	0.47
1:A:132:ILE:HD12	1:A:151:LEU:HD21	1.96	0.47
1:A:256:LEU:HG	1:C:256:LEU:HD21	1.95	0.47
1:B:44:GLU:HA	1:B:85:SER:O	2.15	0.47
1:C:51:LYS:HE3	3:C:551:HOH:O	2.14	0.47
1:E:256:LEU:HB2	1:F:258:ASN:ND2	2.30	0.47
1:B:292:PHE:O	1:B:296:ASN:HB2	2.14	0.47
1:C:211:THR:HG23	1:C:302:GLN:CD	2.35	0.47
1:B:32:ASP:CB	3:B:590:HOH:O	2.63	0.47
1:D:211:THR:CG2	1:D:212:GLY:H	2.28	0.47
1:D:292:PHE:CZ	1:F:193:ALA:HB1	2.50	0.47
1:E:13:GLU:CG	1:E:13:GLU:O	2.63	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:310:ASN:OD1	1:E:312:GLU:HB2	2.15	0.47
1:C:286:LEU:N	1:C:286:LEU:HD23	2.30	0.46
1:A:132:ILE:HD12	1:A:151:LEU:CD2	2.45	0.46
1:D:34:ASP:HB2	3:D:708:HOH:O	2.15	0.46
1:F:215:ALA:CB	1:F:304:LYS:HD2	2.44	0.46
1:D:314:MET:HG3	1:F:121:PHE:HE1	1.79	0.46
1:D:13:GLU:CA	3:D:530:HOH:O	2.43	0.46
1:E:289:HIS:C	1:E:291:ILE:H	2.17	0.46
1:A:71:MET:HB2	1:A:168:TYR:CE2	2.51	0.46
1:B:286:LEU:HD23	1:B:286:LEU:N	2.31	0.46
1:C:152:ILE:O	1:C:152:ILE:HG23	2.15	0.46
1:E:292:PHE:O	1:E:296:ASN:HB2	2.16	0.46
1:B:211:THR:HG23	1:B:302:GLN:CD	2.36	0.46
1:B:196:GLU:HG2	1:B:234:ASN:HB3	1.98	0.46
1:C:71:MET:HB2	1:C:168:TYR:CE2	2.51	0.46
1:F:286:LEU:N	1:F:286:LEU:HD23	2.31	0.46
1:E:127:GLN:HE21	1:F:260:ASN:HD22	1.64	0.45
1:C:61:TRP:O	1:C:148:MET:HG2	2.16	0.45
1:C:117:ARG:HG2	1:C:118:THR:H	1.79	0.45
1:D:286:LEU:HD23	1:D:286:LEU:N	2.31	0.45
1:E:278:VAL:HG12	1:E:305:VAL:HG11	1.98	0.45
1:F:211:THR:CG2	1:F:212:GLY:H	2.28	0.45
1:F:278:VAL:HG11	1:F:305:VAL:HG11	1.98	0.45
1:A:44:GLU:HA	1:A:85:SER:O	2.17	0.45
1:D:225:ARG:HG3	1:D:275:GLU:CG	2.47	0.45
1:A:265:ILE:HG13	1:C:265:ILE:HG21	1.97	0.45
1:D:51:LYS:HE3	1:D:55:GLY:H	1.81	0.45
1:D:70:ARG:NH2	3:D:551:HOH:O	2.49	0.45
1:F:13:GLU:N	3:F:511:HOH:O	2.49	0.45
1:F:33:ARG:NH2	1:F:78:ASP:OD2	2.49	0.45
1:B:76:GLU:OE1	1:B:157:LYS:HG2	2.16	0.45
1:B:117:ARG:HG2	1:B:118:THR:H	1.80	0.45
1:F:70:ARG:CZ	3:F:656:HOH:O	2.65	0.45
1:A:252:GLU:OE1	1:B:264:THR:CG2	2.51	0.45
1:D:258:ASN:HD22	1:D:259:GLU:N	2.09	0.45
3:D:661:HOH:O	1:E:314:MET:HG2	2.16	0.45
1:A:186:GLN:HA	1:A:187:PRO:HD3	1.85	0.45
1:A:292:PHE:O	1:A:296:ASN:HB2	2.17	0.44
1:D:264:THR:HG23	1:F:252:GLU:OE1	2.15	0.44
1:F:242:ILE:HD12	1:F:285:THR:OG1	2.16	0.44
1:D:71:MET:HB2	1:D:168:TYR:CE2	2.52	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:278:VAL:HG12	1:F:305:VAL:HG11	1.99	0.44
1:A:297:LYS:NZ	1:C:194:VAL:O	2.50	0.44
1:C:175:TYR:N	1:C:175:TYR:CD1	2.86	0.44
1:F:23:HIS:HE1	3:F:639:HOH:O	1.97	0.44
1:B:215:ALA:HB3	1:B:304:LYS:HD2	1.99	0.44
1:C:163:VAL:HG13	1:C:223:THR:O	2.17	0.44
1:D:95:ASN:HB3	1:D:112:PHE:HA	1.99	0.44
1:B:64:ASP:HA	3:B:660:HOH:O	2.17	0.44
1:C:44:GLU:HA	1:C:85:SER:O	2.17	0.44
1:E:95:ASN:HB3	1:E:112:PHE:HA	2.00	0.44
1:E:225:ARG:HG3	1:E:275:GLU:CG	2.47	0.44
1:C:73:ARG:NE	1:C:155:GLU:OE2	2.48	0.44
1:C:95:ASN:HB3	1:C:112:PHE:HA	1.99	0.44
1:F:75:ARG:NH1	3:F:515:HOH:O	2.49	0.44
1:A:251:VAL:HG22	3:A:577:HOH:O	2.18	0.44
1:B:34:ASP:CA	3:B:662:HOH:O	2.36	0.44
1:B:95:ASN:HB3	1:B:112:PHE:HA	2.00	0.44
1:C:310:ASN:OD1	1:C:312:GLU:HB2	2.18	0.44
1:A:54:ASP:HB2	3:A:706:HOH:O	2.17	0.44
3:A:696:HOH:O	1:C:134:HIS:CD2	2.70	0.44
1:A:76:GLU:OE1	1:A:157:LYS:HG2	2.18	0.43
1:B:132:ILE:HD12	1:B:151:LEU:HD21	1.99	0.43
1:E:286:LEU:N	1:E:286:LEU:HD23	2.32	0.43
1:B:132:ILE:HD12	1:B:151:LEU:CD2	2.47	0.43
1:B:258:ASN:ND2	1:B:259:GLU:N	2.61	0.43
1:D:279:ASP:C	3:D:690:HOH:O	2.56	0.43
1:A:196:GLU:HG2	1:A:234:ASN:CB	2.48	0.43
1:B:175:TYR:CD1	1:B:175:TYR:N	2.86	0.43
1:D:21:THR:HB	1:D:70:ARG:HB3	2.01	0.43
1:E:127:GLN:HE21	1:F:260:ASN:ND2	2.17	0.43
1:C:24:ALA:N	3:C:589:HOH:O	2.52	0.43
1:D:14:LEU:HA	1:D:15:PRO:HD3	1.90	0.43
1:D:162:LYS:HE2	3:D:599:HOH:O	2.18	0.43
1:D:292:PHE:O	1:D:296:ASN:HB2	2.17	0.43
1:E:211:THR:CG2	1:E:212:GLY:H	2.30	0.43
1:F:289:HIS:C	1:F:291:ILE:H	2.22	0.43
1:A:117:ARG:HG2	1:A:118:THR:H	1.80	0.43
1:E:225:ARG:HD2	1:E:227:TYR:CZ	2.54	0.43
1:D:309:GLU:HG3	3:D:597:HOH:O	2.18	0.43
1:F:226:MET:CE	1:F:276:PHE:HE2	2.31	0.43
1:D:225:ARG:HD2	1:D:227:TYR:CZ	2.53	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:51:LYS:HE3	1:E:55:GLY:H	1.83	0.43
1:F:95:ASN:HB3	1:F:112:PHE:HA	2.00	0.43
1:F:310:ASN:OD1	1:F:312:GLU:HB2	2.19	0.43
1:E:13:GLU:N	3:E:614:HOH:O	2.52	0.42
1:E:242:ILE:HD12	1:E:285:THR:OG1	2.19	0.42
1:F:244:GLU:HG3	1:F:245:ILE:N	2.34	0.42
1:B:19:ALA:HB2	1:B:39:VAL:HG12	2.01	0.42
1:C:132:ILE:HD12	1:C:151:LEU:HD23	2.01	0.42
1:C:215:ALA:HB3	1:C:304:LYS:HD2	2.00	0.42
1:E:71:MET:HB2	1:E:168:TYR:CE2	2.54	0.42
1:E:186:GLN:HG3	3:E:507:HOH:O	2.18	0.42
1:A:310:ASN:OD1	1:A:312:GLU:HB2	2.20	0.42
1:E:13:GLU:O	1:E:13:GLU:HG3	2.19	0.42
1:A:280:ILE:HA	1:A:281:PRO:HD3	1.89	0.42
1:B:194:VAL:CG1	1:C:297:LYS:HZ2	2.32	0.42
1:D:264:THR:HG22	1:F:252:GLU:CD	2.33	0.42
1:A:64:ASP:OD1	3:A:537:HOH:O	2.21	0.42
1:A:171:GLN:HG2	3:A:687:HOH:O	2.19	0.42
1:C:186:GLN:HA	1:C:187:PRO:HD3	1.87	0.42
1:E:291:ILE:HA	1:E:291:ILE:HD13	1.86	0.42
1:A:175:TYR:CD1	1:A:175:TYR:N	2.87	0.42
1:E:87:ASN:HA	1:E:88:PRO:HD3	1.94	0.42
1:C:196:GLU:HG2	1:C:234:ASN:CB	2.50	0.42
1:B:33:ARG:NH2	1:B:78:ASP:OD2	2.52	0.42
1:A:215:ALA:HB3	1:A:304:LYS:HD2	2.02	0.42
1:D:117:ARG:HG2	1:D:118:THR:H	1.84	0.42
1:F:186:GLN:HA	1:F:187:PRO:HD3	1.87	0.42
1:B:71:MET:HB2	1:B:168:TYR:CE2	2.55	0.42
1:B:280:ILE:HA	1:B:281:PRO:HD3	1.90	0.42
1:C:213:ASP:CG	3:C:666:HOH:O	2.58	0.42
1:D:194:VAL:CG1	1:E:297:LYS:HZ1	2.33	0.42
1:F:51:LYS:HE3	1:F:55:GLY:H	1.83	0.42
1:F:225:ARG:HD2	1:F:227:TYR:CZ	2.55	0.41
1:F:226:MET:HE1	1:F:276:PHE:HE2	1.85	0.41
1:B:162:LYS:HE2	1:B:162:LYS:HA	2.00	0.41
1:B:163:VAL:HG23	3:B:674:HOH:O	2.20	0.41
1:D:13:GLU:O	1:D:13:GLU:CD	2.59	0.41
1:D:244:GLU:HG3	1:D:245:ILE:N	2.35	0.41
1:D:297:LYS:NZ	1:F:194:VAL:HG12	2.35	0.41
1:B:14:LEU:N	3:B:542:HOH:O	2.54	0.41
1:A:279:ASP:OD2	1:A:279:ASP:N	2.41	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:244:GLU:HG3	1:E:245:ILE:N	2.35	0.41
1:A:89:SER:HA	3:A:566:HOH:O	2.20	0.41
1:A:95:ASN:HB3	1:A:112:PHE:HA	2.02	0.41
1:D:163:VAL:CG1	1:D:164:ASP:N	2.83	0.41
1:A:73:ARG:NE	1:A:155:GLU:OE2	2.50	0.41
1:A:163:VAL:HG13	1:A:223:THR:O	2.21	0.41
1:B:97:ASP:OD2	1:B:97:ASP:C	2.59	0.41
1:B:152:ILE:HG23	1:B:152:ILE:O	2.21	0.41
1:F:13:GLU:O	1:F:13:GLU:CG	2.68	0.41
1:F:71:MET:HB2	1:F:168:TYR:CE2	2.56	0.41
1:C:51:LYS:CD	3:C:668:HOH:O	2.68	0.41
1:C:237:SER:O	1:C:265:ILE:HA	2.21	0.41
1:C:289:HIS:C	1:C:291:ILE:H	2.24	0.41
1:C:113:THR:HA	1:C:117:ARG:NH1	2.36	0.41
1:C:280:ILE:HA	1:C:281:PRO:HD3	1.88	0.41
1:E:152:ILE:O	1:E:152:ILE:HG23	2.20	0.41
1:D:151:LEU:HD12	1:D:168:TYR:CE1	2.57	0.41
1:F:117:ARG:HG2	1:F:118:THR:H	1.82	0.41
1:A:87:ASN:ND2	1:A:88:PRO:HD2	2.36	0.40
1:A:162:LYS:HE2	1:A:162:LYS:HA	2.01	0.40
1:B:163:VAL:HG13	1:B:223:THR:O	2.21	0.40
1:C:279:ASP:OD2	1:C:279:ASP:N	2.42	0.40
1:B:72:ILE:HD11	3:B:628:HOH:O	2.21	0.40
1:D:87:ASN:HA	1:D:88:PRO:HD3	1.92	0.40
1:F:14:LEU:HA	1:F:15:PRO:HD3	1.89	0.40
1:A:157:LYS:CE	3:A:591:HOH:O	2.69	0.40
1:C:242:ILE:HB	1:C:285:THR:HG23	2.03	0.40
1:D:43:MET:CE	1:D:98:PHE:HZ	2.35	0.40
1:E:173:ASP:OD1	1:E:233:PRO:HD2	2.21	0.40
1:E:36:PRO:HA	3:E:515:HOH:O	2.20	0.40
1:A:33:ARG:NH2	1:A:78:ASP:OD2	2.54	0.40
1:A:113:THR:HA	1:A:117:ARG:NH1	2.36	0.40
1:A:124:LYS:HD2	3:A:698:HOH:O	2.22	0.40
1:B:87:ASN:HA	1:B:88:PRO:HD3	1.94	0.40
1:F:152:ILE:O	1:F:152:ILE:HG23	2.22	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	300/327 (92%)	289 (96%)	7 (2%)	4 (1%)	12	17
1	B	300/327 (92%)	289 (96%)	7 (2%)	4 (1%)	12	17
1	C	300/327 (92%)	289 (96%)	7 (2%)	4 (1%)	12	17
1	D	300/327 (92%)	288 (96%)	9 (3%)	3 (1%)	15	23
1	E	300/327 (92%)	286 (95%)	11 (4%)	3 (1%)	15	23
1	F	300/327 (92%)	286 (95%)	10 (3%)	4 (1%)	12	17
All	All	1800/1962 (92%)	1727 (96%)	51 (3%)	22 (1%)	13	19

All (22) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	25	PRO
1	B	14	LEU
1	B	25	PRO
1	C	25	PRO
1	D	25	PRO
1	E	14	LEU
1	F	14	LEU
1	F	25	PRO
1	A	291	ILE
1	B	291	ILE
1	C	291	ILE
1	D	291	ILE
1	E	291	ILE
1	F	291	ILE
1	A	14	LEU
1	C	309	GLU
1	D	104	GLN
1	B	104	GLN
1	E	104	GLN
1	F	104	GLN

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Mol	Chain	Res	Type
1	A	205	GLY
1	C	205	GLY

5.3.2 Protein sidechains (i)

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	239/259 (92%)	227 (95%)	12 (5%)	24	40
1	B	239/259 (92%)	227 (95%)	12 (5%)	24	40
1	C	239/259 (92%)	227 (95%)	12 (5%)	24	40
1	D	239/259 (92%)	226 (95%)	13 (5%)	22	36
1	E	239/259 (92%)	225 (94%)	14 (6%)	19	32
1	F	239/259 (92%)	225 (94%)	14 (6%)	19	32
All	All	1434/1554 (92%)	1357 (95%)	77 (5%)	22	36

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

Mol	Chain	Res	Type
1	A	33	ARG
1	A	46	VAL
1	A	121	PHE
1	A	132	ILE
1	A	173	ASP
1	A	179	LYS
1	A	258	ASN
1	A	279	ASP
1	A	280	ILE
1	A	285	THR
1	A	286	LEU
1	A	291	ILE
1	B	33	ARG
1	B	46	VAL
1	B	121	PHE
1	B	132	ILE

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Mol	Chain	Res	Type
1	B	173	ASP
1	B	179	LYS
1	B	258	ASN
1	B	279	ASP
1	B	280	ILE
1	B	285	THR
1	B	286	LEU
1	B	291	ILE
1	C	33	ARG
1	C	46	VAL
1	C	121	PHE
1	C	132	ILE
1	C	173	ASP
1	C	179	LYS
1	C	258	ASN
1	C	279	ASP
1	C	280	ILE
1	C	285	THR
1	C	286	LEU
1	C	291	ILE
1	D	33	ARG
1	D	46	VAL
1	D	121	PHE
1	D	132	ILE
1	D	158	GLU
1	D	173	ASP
1	D	258	ASN
1	D	264	THR
1	D	279	ASP
1	D	280	ILE
1	D	285	THR
1	D	286	LEU
1	D	291	ILE
1	E	33	ARG
1	E	46	VAL
1	E	121	PHE
1	E	132	ILE
1	E	158	GLU
1	E	173	ASP
1	E	258	ASN
1	E	264	THR
1	E	279	ASP

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Mol	Chain	Res	Type
1	E	280	ILE
1	E	285	THR
1	E	286	LEU
1	E	290	SER
1	E	291	ILE
1	F	33	ARG
1	F	46	VAL
1	F	121	PHE
1	F	132	ILE
1	F	158	GLU
1	F	173	ASP
1	F	258	ASN
1	F	264	THR
1	F	279	ASP
1	F	280	ILE
1	F	285	THR
1	F	286	LEU
1	F	290	SER
1	F	291	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (31) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	23	HIS
1	A	87	ASN
1	A	204	ASN
1	A	258	ASN
1	A	260	ASN
1	A	296	ASN
1	B	87	ASN
1	B	204	ASN
1	B	258	ASN
1	B	260	ASN
1	B	296	ASN
1	C	23	HIS
1	C	87	ASN
1	C	204	ASN
1	C	258	ASN
1	C	260	ASN
1	C	296	ASN
1	D	87	ASN
1	D	204	ASN

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Mol	Chain	Res	Type
1	D	258	ASN
1	D	260	ASN
1	E	87	ASN
1	E	204	ASN
1	E	258	ASN
1	E	260	ASN
1	F	23	HIS
1	F	87	ASN
1	F	127	GLN
1	F	204	ASN
1	F	258	ASN
1	F	260	ASN

5.3.3 RNA

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates

There are no monosaccharides in this entry.

5.6 Ligand geometry

Of 12 ligands modelled in this entry, 12 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers (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.