Full wwPDB X-ray Structure Validation Report (i)

Dec 10, 2023 – 07:54 am GMT

PDB ID	:	2JK0
Title	:	Structural and functional insights into Erwinia carotovora L- asparaginase
Authors	:	Papageorgiou, A.C.; Posypanova, G.A.; Andersson, C.S.; Sokolov, N.N.; Krasotkina, J.
Deposited on	:	2008-05-23
Resolution	:	2.50 Å(reported)

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

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the (i) 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 (i)) were used in the production of this report:

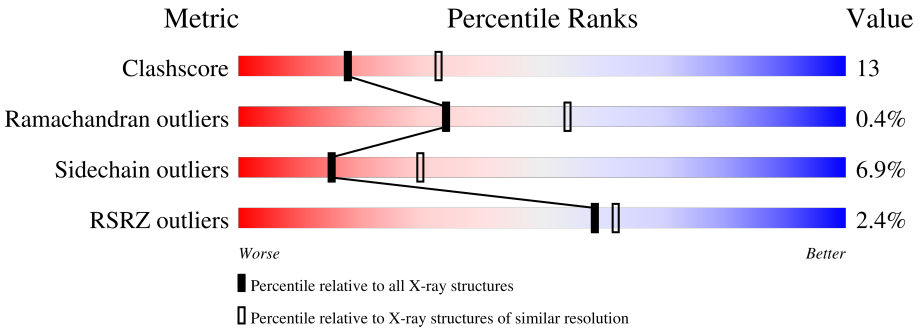
MolProbity	:	4.02b-467
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

1 Overall quality at a glance

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

The reported resolution of this entry is 2.50 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	141614	5346 (2.50-2.50)
Ramachandran outliers	138981	5231 (2.50-2.50)
Sidechain outliers	138945	5233 (2.50-2.50)
RSRZ outliers	127900	4559 (2.50-2.50)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5% The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	325	3% 77% 21%
1	B	325	2% 77% 18%
1	C	325	2% 71% 22%
1	D	325	% 75% 21%
1	E	325	3% 70% 22%
1	F	325	3% 68% 26%

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Mol	Chain	Length	Quality of chain
1	G	325	2% 73% 20% 5%
1	H	325	4% 71% 22%

2 Entry composition (i)

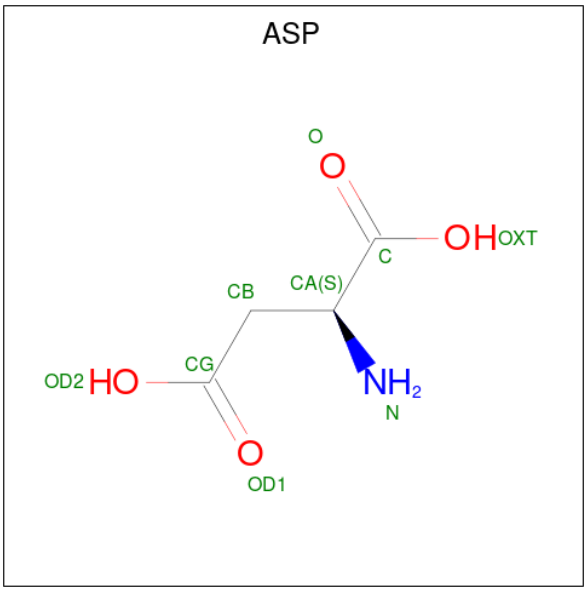
There are 3 unique types of molecules in this entry. The entry contains 19499 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 L-ASPARAGINASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	325	Total	C	N	O	S	0	0	0
			2386	1502	413	465	6			
1	B	314	Total	C	N	O	S	0	0	0
			2331	1472	401	452	6			
1	C	315	Total	C	N	O	S	0	0	0
			2335	1473	402	454	6			
1	D	320	Total	C	N	O	S	0	0	0
			2364	1489	408	461	6			
1	E	312	Total	C	N	O	S	0	0	0
			2320	1464	399	451	6			
1	F	317	Total	C	N	O	S	0	0	0
			2350	1481	405	458	6			
1	G	309	Total	C	N	O	S	0	0	0
			2309	1459	396	448	6			
1	H	313	Total	C	N	O	S	0	0	0
			2324	1466	400	452	6			

- Molecule 2 is ASPARTIC ACID (three-letter code: ASP) (formula: $C_4H_7NO_4$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total C N O 9 4 1 4	0	0
2	B	1	Total C N O 9 4 1 4	0	0
2	C	1	Total C N O 9 4 1 4	0	0
2	D	1	Total C N O 9 4 1 4	0	0
2	E	1	Total C N O 9 4 1 4	0	0
2	F	1	Total C N O 9 4 1 4	0	0
2	G	1	Total C N O 9 4 1 4	0	0
2	H	1	Total C N O 9 4 1 4	0	0

- Molecule 3 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	117	Total O 117 117	0	0
3	B	86	Total O 86 86	0	0
3	C	107	Total O 107 107	0	0
3	D	108	Total O 108 108	0	0

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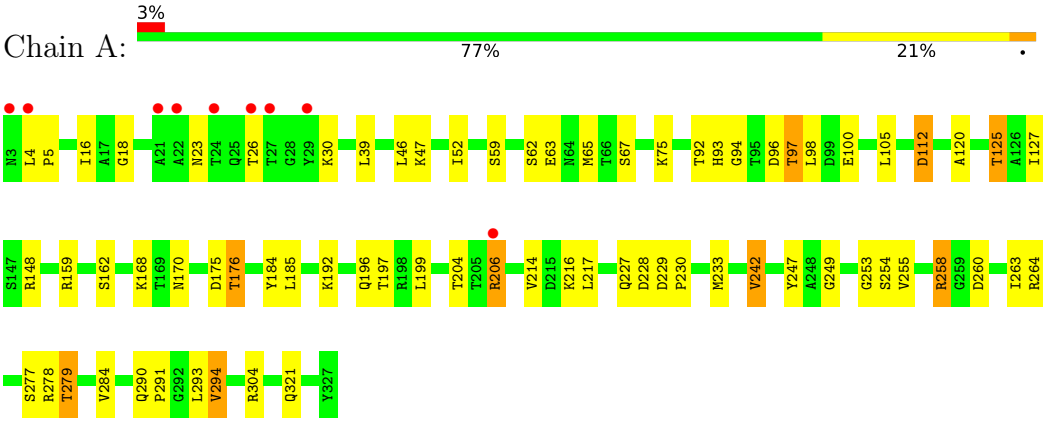
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	E	84	Total O 84 84	0	0
3	F	68	Total O 68 68	0	0
3	G	65	Total O 65 65	0	0
3	H	73	Total O 73 73	0	0

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 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.

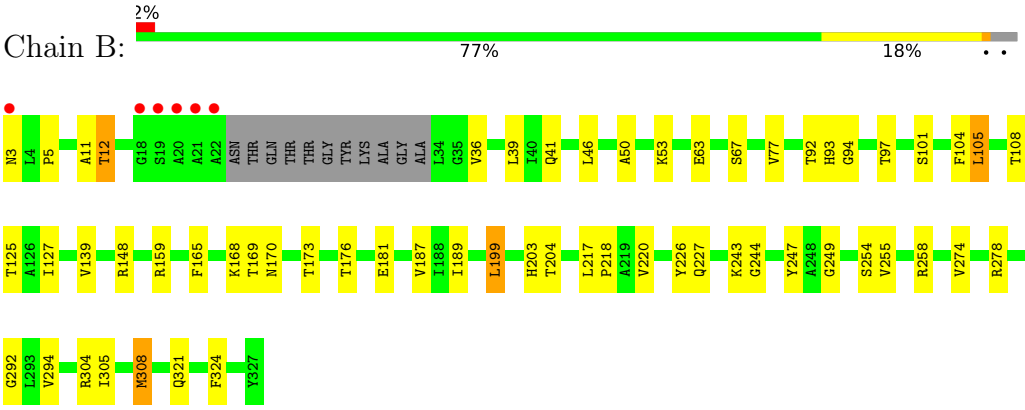
• Molecule 1: L-ASPARAGINASE

Chain A:



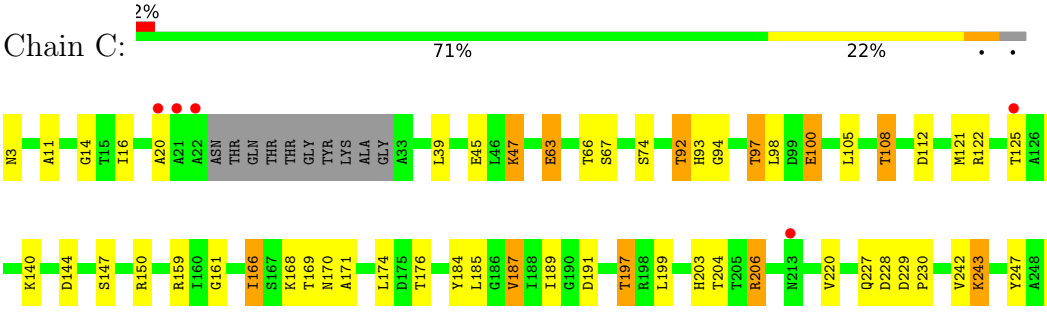
• Molecule 1: L-ASPARAGINASE

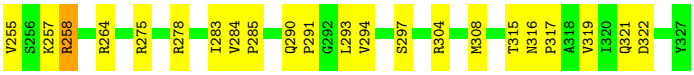
Chain B:



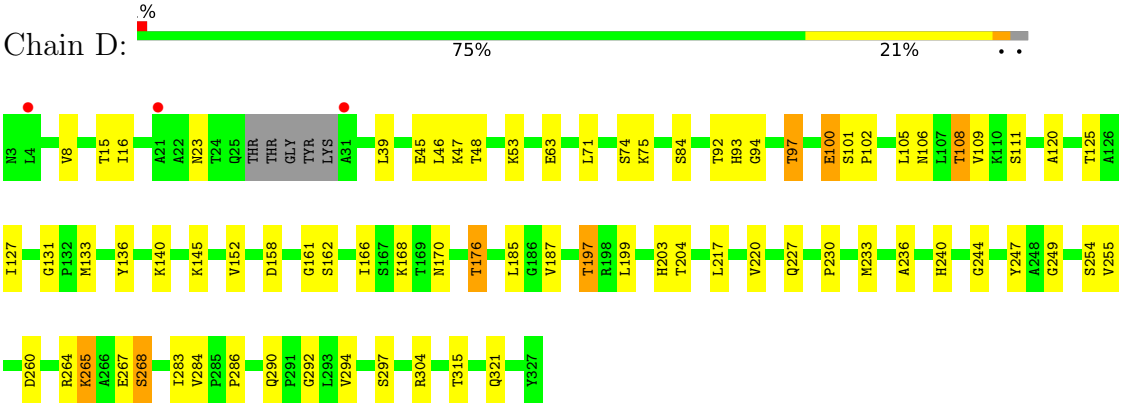
• Molecule 1: L-ASPARAGINASE

Chain C:

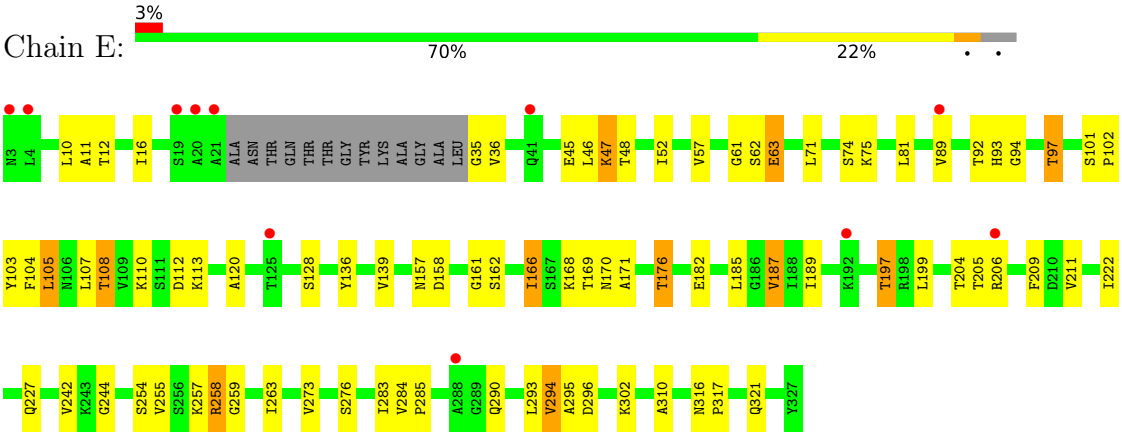




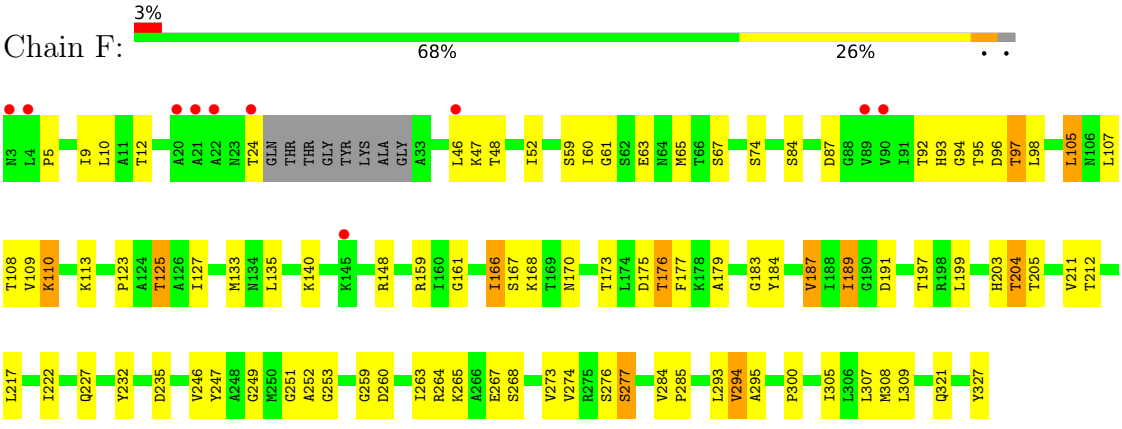
• Molecule 1: L-ASPARAGINASE



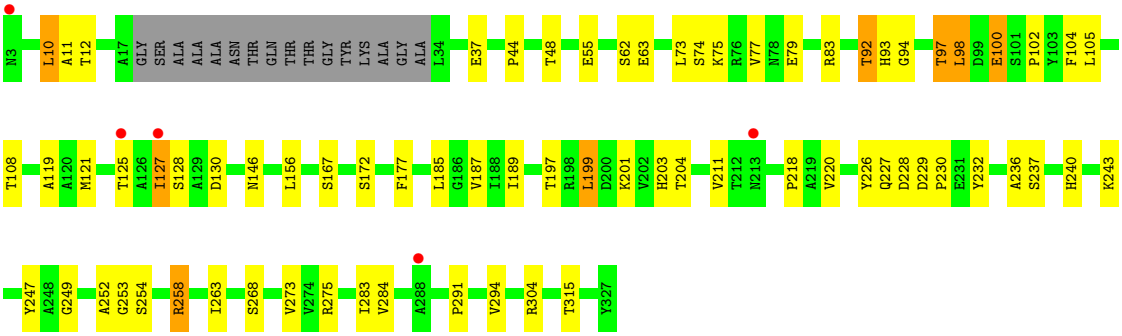
• Molecule 1: L-ASPARAGINASE



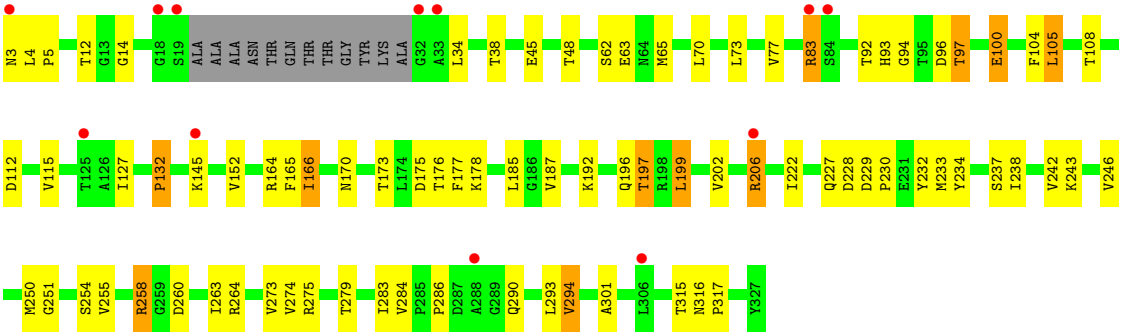
• Molecule 1: L-ASPARAGINASE



• Molecule 1: L-ASPARAGINASE



• Molecule 1: L-ASPARAGINASE



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	73.65Å 135.63Å 250.10Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	20.00 – 2.50 19.92 – 2.50	Depositor EDS
% Data completeness (in resolution range)	96.1 (20.00-2.50) 96.0 (19.92-2.50)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.69 (at 2.50Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.188 , 0.266 0.191 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å^2)	44.5	Xtriage
Anisotropy	0.333	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.30 , 42.4	EDS
L-test for twinning[2]	$< \|L\| > = 0.47$, $< L^2 > = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	19499	wwPDB-VP
Average B, all atoms (Å^2)	34.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 32.96 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 8.6345e-04. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

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	0.47	0/2421	0.67	0/3288
1	B	0.48	0/2365	0.65	0/3211
1	C	0.46	0/2369	0.64	0/3217
1	D	0.46	0/2398	0.64	0/3257
1	E	0.45	0/2354	0.62	0/3196
1	F	0.49	1/2384 (0.0%)	0.62	0/3238
1	G	0.44	0/2343	0.61	0/3181
1	H	0.45	0/2358	0.61	0/3201
All	All	0.46	1/18992 (0.0%)	0.64	0/25789

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	F	24	THR	C-O	11.38	1.45	1.23

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2386	0	2420	77	0
1	B	2331	0	2386	63	0
1	C	2335	0	2387	79	0
1	D	2364	0	2410	72	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	E	2320	0	2375	81	0
1	F	2350	0	2400	80	0
1	G	2309	0	2371	58	0
1	H	2324	0	2375	67	0
2	A	9	0	3	1	0
2	B	9	0	3	0	0
2	C	9	0	3	2	0
2	D	9	0	3	1	0
2	E	9	0	3	0	0
2	F	9	0	3	0	0
2	G	9	0	3	1	0
2	H	9	0	3	1	0
3	A	117	0	0	10	0
3	B	86	0	0	3	0
3	C	107	0	0	4	0
3	D	108	0	0	6	0
3	E	84	0	0	6	0
3	F	68	0	0	4	0
3	G	65	0	0	5	0
3	H	73	0	0	6	0
All	All	19499	0	19148	511	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 13.

All (511) 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:D:187:VAL:HB	3:D:2071:HOH:O	1.34	1.27
1:C:185:LEU:HA	1:C:197:THR:HG22	1.32	1.08
1:C:168:LYS:HG3	1:C:176:THR:HG21	1.30	1.06
1:E:263:ILE:HD12	1:E:273:VAL:HG11	1.41	0.99
1:B:97:THR:HG21	1:D:227:GLN:HE21	1.25	0.98
1:E:62:SER:HB2	1:E:97:THR:HG22	1.45	0.97
1:A:227:GLN:HE21	1:C:97:THR:CG2	1.78	0.96
1:H:170:ASN:HB3	1:H:176:THR:HG22	1.49	0.94
1:D:294:VAL:H	1:D:321:GLN:HE22	1.06	0.94
1:A:4:LEU:HB2	1:A:5:PRO:HD2	1.50	0.93
1:F:161:GLY:HA3	1:F:166:ILE:HG13	1.53	0.88
1:A:227:GLN:HE21	1:C:97:THR:HG23	1.39	0.87
1:B:97:THR:CG2	1:D:227:GLN:HE21	1.89	0.86

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:159:ARG:HH21	1:B:173:THR:HG21	1.38	0.86
1:A:255:VAL:HG22	1:A:290:GLN:HE21	1.40	0.86
1:E:227:GLN:HE21	1:G:97:THR:CG2	1.89	0.86
1:E:74:SER:OG	1:E:108:THR:CG2	2.25	0.85
1:E:12:THR:HB	1:E:92:THR:O	1.76	0.84
1:D:48:THR:HG21	3:D:2047:HOH:O	1.75	0.84
1:C:228:ASP:HA	1:C:258:ARG:HH22	1.42	0.82
1:A:254:SER:HB3	1:C:63:GLU:HG2	1.62	0.82
1:B:255:VAL:HG22	1:B:290:GLN:HE21	1.45	0.81
1:D:45:GLU:O	1:D:48:THR:HG22	1.80	0.81
1:A:159:ARG:CZ	3:A:2052:HOH:O	2.27	0.81
1:E:227:GLN:HE21	1:G:97:THR:HG21	1.47	0.80
1:C:170:ASN:H	1:C:176:THR:HG23	1.45	0.79
1:A:97:THR:CG2	1:C:227:GLN:HE21	1.96	0.78
1:B:168:LYS:HG3	1:B:176:THR:HG21	1.63	0.78
1:E:74:SER:OG	1:E:108:THR:HG21	1.82	0.78
1:C:255:VAL:HG22	1:C:290:GLN:HE21	1.49	0.78
1:C:228:ASP:HA	1:C:258:ARG:NH2	1.99	0.78
1:D:294:VAL:N	1:D:321:GLN:HE22	1.82	0.78
1:E:263:ILE:CD1	1:E:273:VAL:HG11	2.15	0.77
1:D:16:ILE:HG21	1:D:92:THR:HG23	1.68	0.76
1:E:255:VAL:HG22	1:E:290:GLN:HE21	1.50	0.76
1:B:97:THR:HG21	1:D:227:GLN:NE2	2.00	0.76
1:F:187:VAL:HG13	1:F:189:ILE:HD12	1.66	0.76
1:B:227:GLN:HE21	1:D:97:THR:CG2	1.98	0.75
1:B:104:PHE:O	1:B:108:THR:HG22	1.87	0.75
1:A:63:GLU:HG2	1:C:254:SER:HB3	1.69	0.75
1:E:254:SER:HA	1:E:290:GLN:HE22	1.52	0.74
1:B:227:GLN:HE21	1:D:97:THR:HG23	1.51	0.74
1:C:254:SER:HA	1:C:290:GLN:HE22	1.53	0.74
1:E:112:ASP:HB2	3:E:2033:HOH:O	1.88	0.74
1:C:161:GLY:HA3	1:C:166:ILE:HG13	1.69	0.73
1:E:10:LEU:HD13	1:E:89:VAL:HG13	1.68	0.73
1:F:227:GLN:HE21	1:H:97:THR:CG2	2.01	0.73
1:B:170:ASN:H	1:B:176:THR:CG2	2.01	0.73
1:F:168:LYS:HG3	1:F:176:THR:HG21	1.69	0.73
1:E:170:ASN:H	1:E:176:THR:CG2	2.02	0.72
1:C:168:LYS:CG	1:C:176:THR:HG21	2.16	0.72
1:A:170:ASN:H	1:A:176:THR:HG22	1.54	0.72
1:C:203:HIS:HD2	1:C:204:THR:OG1	1.73	0.72
1:H:45:GLU:O	1:H:48:THR:HG22	1.89	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:105:LEU:HA	1:C:108:THR:HG22	1.72	0.71
1:B:97:THR:CG2	1:D:227:GLN:NE2	2.54	0.71
1:A:227:GLN:NE2	1:C:97:THR:HG23	2.06	0.71
1:C:168:LYS:HG3	1:C:176:THR:CG2	2.18	0.70
1:D:16:ILE:CG2	1:D:92:THR:HG23	2.22	0.70
1:G:185:LEU:HA	1:G:197:THR:HG22	1.73	0.70
1:G:167:SER:HB3	3:G:2030:HOH:O	1.92	0.70
1:G:252:ALA:O	1:G:284:VAL:HG13	1.92	0.70
1:H:230:PRO:HB3	1:H:232:TYR:CZ	2.27	0.70
1:A:227:GLN:HE21	1:C:97:THR:HG21	1.56	0.70
1:D:161:GLY:HA3	1:D:166:ILE:HG13	1.72	0.69
1:E:168:LYS:HG3	1:E:176:THR:HG21	1.74	0.69
1:F:294:VAL:H	1:F:321:GLN:HE22	1.38	0.69
1:B:97:THR:O	1:B:97:THR:HG22	1.92	0.69
1:C:170:ASN:O	1:C:176:THR:HG23	1.93	0.69
1:F:170:ASN:O	1:F:176:THR:CG2	2.42	0.68
1:F:113:LYS:HG3	3:F:2017:HOH:O	1.92	0.68
1:E:11:ALA:HA	1:E:92:THR:HB	1.75	0.68
1:E:170:ASN:O	1:E:176:THR:CG2	2.42	0.68
1:B:170:ASN:H	1:B:176:THR:HG23	1.58	0.67
1:G:12:THR:HB	1:G:92:THR:O	1.95	0.67
1:E:162:SER:O	1:E:166:ILE:HB	1.93	0.67
1:F:123:PRO:HB2	1:F:125:THR:HG22	1.76	0.67
1:E:187:VAL:HG11	1:H:283:ILE:HD13	1.77	0.67
1:E:302:LYS:NZ	3:E:2078:HOH:O	2.25	0.67
1:H:185:LEU:HA	1:H:197:THR:HG22	1.78	0.66
1:A:170:ASN:O	1:A:176:THR:CG2	2.43	0.66
1:A:185:LEU:HD23	1:A:197:THR:HG22	1.76	0.66
1:D:170:ASN:O	1:D:176:THR:CG2	2.43	0.66
1:B:93:HIS:HD2	1:B:94:GLY:O	1.79	0.66
1:A:233:MET:HG3	3:A:2087:HOH:O	1.96	0.65
1:A:197:THR:HG21	3:A:2069:HOH:O	1.95	0.65
1:E:62:SER:CB	1:E:97:THR:HG22	2.23	0.65
1:D:283:ILE:HD13	1:D:297:SER:HB3	1.79	0.65
1:C:294:VAL:H	1:C:321:GLN:HE22	1.45	0.64
1:F:247:TYR:CZ	1:F:249:GLY:HA2	2.32	0.64
1:H:170:ASN:CB	1:H:176:THR:HG22	2.27	0.64
1:D:74:SER:OG	1:D:108:THR:CG2	2.45	0.64
1:D:294:VAL:H	1:D:321:GLN:NE2	1.86	0.64
1:A:228:ASP:HA	1:A:258:ARG:HH12	1.62	0.64
1:C:247:TYR:CE2	1:C:249:GLY:HA2	2.33	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:284:VAL:HG12	1:C:294:VAL:CG2	2.28	0.64
1:E:170:ASN:H	1:E:176:THR:HG22	1.62	0.64
1:F:97:THR:CG2	1:H:227:GLN:HE21	2.10	0.64
1:B:105:LEU:HA	1:B:108:THR:CG2	2.28	0.64
1:E:170:ASN:O	1:E:176:THR:HG23	1.97	0.64
1:B:170:ASN:O	1:B:176:THR:CG2	2.46	0.64
1:F:97:THR:HG23	1:H:227:GLN:HE21	1.62	0.64
1:H:104:PHE:O	1:H:108:THR:HG22	1.98	0.64
1:A:4:LEU:HB2	1:A:5:PRO:CD	2.28	0.63
1:F:187:VAL:HG13	1:F:189:ILE:CD1	2.27	0.63
1:A:97:THR:HG21	1:C:227:GLN:HE21	1.63	0.63
1:F:170:ASN:O	1:F:176:THR:HG23	1.98	0.63
1:A:185:LEU:HA	1:A:197:THR:HB	1.79	0.63
1:A:97:THR:HG23	1:C:227:GLN:HE21	1.62	0.63
1:C:249:GLY:O	1:C:278:ARG:HG2	1.99	0.63
1:F:63:GLU:HG2	1:H:254:SER:HB3	1.81	0.63
1:D:170:ASN:O	1:D:176:THR:HG23	1.99	0.63
1:G:93:HIS:HD2	1:G:94:GLY:O	1.81	0.63
1:F:170:ASN:H	1:F:176:THR:HG22	1.64	0.62
1:H:14:GLY:HA2	2:H:1328:ASP:OXT	1.98	0.62
1:E:128:SER:HB2	1:F:133:MET:HB2	1.80	0.62
1:G:220:VAL:HG12	1:G:304:ARG:HG3	1.81	0.62
1:A:159:ARG:HD2	1:A:184:TYR:CE1	2.34	0.62
1:C:132:PRO:HB3	1:D:127:ILE:HD11	1.81	0.62
1:C:170:ASN:H	1:C:176:THR:CG2	2.13	0.62
1:E:263:ILE:HD12	1:E:273:VAL:CG1	2.24	0.62
1:A:93:HIS:HD2	1:A:94:GLY:O	1.81	0.61
1:E:168:LYS:CG	1:E:176:THR:HG21	2.30	0.61
1:D:168:LYS:HG3	1:D:176:THR:HG21	1.81	0.61
1:E:227:GLN:CD	1:G:100:GLU:HG3	2.20	0.61
1:A:168:LYS:HG3	1:A:176:THR:HG21	1.82	0.61
1:B:97:THR:CG2	1:B:97:THR:O	2.49	0.61
1:E:171:ALA:HB1	1:G:252:ALA:HA	1.83	0.61
1:E:227:GLN:HE21	1:G:97:THR:HG23	1.65	0.61
1:F:170:ASN:H	1:F:176:THR:CG2	2.14	0.61
1:A:279:THR:HG21	1:C:171:ALA:N	2.16	0.60
1:B:67:SER:HB2	1:B:217:LEU:HD12	1.81	0.60
1:G:275:ARG:HD3	1:G:291:PRO:O	2.01	0.60
1:E:74:SER:OG	1:E:108:THR:HG23	2.00	0.60
1:C:304:ARG:O	1:C:308:MET:HB2	2.02	0.60
1:C:255:VAL:H	1:C:290:GLN:NE2	2.00	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:187:VAL:CG1	1:F:189:ILE:CD1	2.80	0.59
1:C:47:LYS:HD3	3:C:2012:HOH:O	2.03	0.59
1:C:63:GLU:OE1	2:C:1328:ASP:N	2.36	0.59
1:H:233:MET:HG3	3:H:2058:HOH:O	2.02	0.59
1:F:259:GLY:O	1:F:263:ILE:HG12	2.03	0.59
1:F:105:LEU:HA	1:F:108:THR:HG22	1.84	0.59
1:H:254:SER:HA	1:H:290:GLN:HE22	1.68	0.58
1:A:277:SER:OG	1:A:279:THR:HB	2.03	0.58
1:B:254:SER:HA	1:B:290:GLN:HE22	1.68	0.58
1:H:228:ASP:HA	1:H:258:ARG:HH12	1.68	0.58
1:D:8:VAL:HG22	1:D:53:LYS:HD2	1.86	0.58
1:H:286:PRO:HA	1:H:294:VAL:HG21	1.85	0.58
1:E:227:GLN:NE2	1:G:97:THR:HG23	2.18	0.58
1:G:275:ARG:NH1	3:G:2055:HOH:O	2.36	0.58
1:G:75:LYS:O	1:G:79:GLU:HB2	2.04	0.58
1:G:121:MET:CE	1:G:172:SER:HA	2.34	0.58
1:D:220:VAL:HA	1:D:244:GLY:O	2.03	0.57
1:C:128:SER:HB2	1:D:133:MET:HB2	1.85	0.57
1:D:265:LYS:O	1:D:268:SER:HB2	2.04	0.57
1:E:35:GLY:N	3:E:2004:HOH:O	2.37	0.57
1:B:5:PRO:O	1:B:50:ALA:HB1	2.04	0.57
1:C:93:HIS:HD2	1:C:94:GLY:O	1.88	0.57
1:A:67:SER:HB2	1:A:217:LEU:HD12	1.86	0.56
1:C:283:ILE:HD12	1:C:297:SER:HB3	1.87	0.56
1:A:279:THR:HG23	1:C:169:THR:C	2.26	0.56
1:B:187:VAL:HG13	1:B:189:ILE:HG12	1.87	0.56
1:B:247:TYR:CZ	1:B:249:GLY:HA2	2.39	0.56
1:D:92:THR:CG2	3:D:2003:HOH:O	2.53	0.56
1:E:227:GLN:NE2	1:G:97:THR:CG2	2.65	0.56
1:G:247:TYR:CZ	1:G:249:GLY:HA2	2.40	0.56
1:H:202:VAL:HG13	1:H:206:ARG:HB3	1.87	0.56
1:B:168:LYS:CG	1:B:176:THR:HG21	2.34	0.56
1:C:170:ASN:O	1:C:176:THR:CG2	2.54	0.56
1:F:67:SER:HB2	1:F:217:LEU:HD12	1.88	0.56
1:F:97:THR:HG23	1:F:97:THR:O	2.06	0.56
1:F:251:GLY:O	1:F:277:SER:HB2	2.05	0.56
1:D:93:HIS:HD2	1:D:94:GLY:O	1.89	0.56
1:E:197:THR:HG21	3:E:2047:HOH:O	2.05	0.56
1:H:284:VAL:O	1:H:294:VAL:HG13	2.06	0.56
1:H:260:ASP:OD1	1:H:264:ARG:NH1	2.39	0.56
1:G:11:ALA:HA	1:G:92:THR:HB	1.89	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:170:ASN:O	1:B:176:THR:HG21	2.06	0.55
1:C:319:VAL:O	1:C:322:ASP:HB2	2.06	0.55
1:D:106:ASN:HA	1:D:152:VAL:HG23	1.89	0.55
1:C:187:VAL:HG13	1:C:189:ILE:HG12	1.89	0.55
1:E:45:GLU:O	1:E:48:THR:HG22	2.06	0.55
1:E:97:THR:HG23	1:E:97:THR:O	2.07	0.55
1:B:170:ASN:O	1:B:176:THR:HG23	2.06	0.55
1:A:125:THR:HB	3:A:2007:HOH:O	2.07	0.55
1:C:203:HIS:CG	1:C:206:ARG:HH21	2.25	0.54
1:F:168:LYS:HG2	1:H:279:THR:HG22	1.89	0.54
1:F:305:ILE:HA	1:F:308:MET:HE3	1.89	0.54
1:G:218:PRO:HA	1:G:243:LYS:HE3	1.89	0.54
1:E:185:LEU:HD23	1:E:197:THR:HG22	1.89	0.54
1:B:305:ILE:HA	1:B:308:MET:HE3	1.90	0.54
1:G:203:HIS:HD2	1:G:204:THR:OG1	1.91	0.54
1:D:74:SER:OG	1:D:108:THR:HG23	2.07	0.54
1:F:285:PRO:HG3	3:H:2010:HOH:O	2.07	0.54
1:C:97:THR:O	1:C:100:GLU:HG2	2.07	0.54
1:A:97:THR:HG23	1:C:227:GLN:NE2	2.23	0.54
1:F:12:THR:HB	1:F:92:THR:O	2.07	0.54
1:F:168:LYS:HG3	1:F:176:THR:CG2	2.37	0.54
1:F:227:GLN:HE21	1:H:97:THR:HG23	1.70	0.54
1:D:74:SER:OG	1:D:108:THR:HG21	2.08	0.53
1:E:104:PHE:O	1:E:108:THR:HB	2.08	0.53
1:F:166:ILE:HD11	1:F:184:TYR:HE2	1.73	0.53
1:C:45:GLU:CD	1:D:23:ASN:HD21	2.11	0.53
1:F:187:VAL:CG1	1:F:189:ILE:HD12	2.35	0.53
1:F:294:VAL:N	1:F:321:GLN:HE22	2.06	0.53
1:D:92:THR:HG22	3:D:2003:HOH:O	2.07	0.53
1:H:166:ILE:CD1	1:H:177:PHE:HB3	2.38	0.53
1:D:236:ALA:O	1:D:240:HIS:HD2	1.92	0.53
1:B:220:VAL:HA	1:B:244:GLY:O	2.09	0.53
1:F:46:LEU:HB3	1:F:52:ILE:HD12	1.90	0.53
1:A:263:ILE:HG23	1:A:273:VAL:HG11	1.91	0.53
1:E:295:ALA:O	1:E:296:ASP:HB3	2.08	0.53
1:A:228:ASP:OD1	1:C:66:THR:HB	2.08	0.53
1:D:109:VAL:HG12	1:D:111:SER:H	1.74	0.53
1:B:77:VAL:HG21	1:B:105:LEU:HD11	1.91	0.53
1:B:254:SER:HB3	1:D:63:GLU:HG2	1.90	0.53
1:A:294:VAL:H	1:A:321:GLN:HE22	1.57	0.52
1:B:227:GLN:NE2	1:D:97:THR:HG23	2.21	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:105:LEU:HA	1:H:108:THR:HG22	1.90	0.52
1:G:104:PHE:HD2	1:G:105:LEU:HD23	1.73	0.52
1:H:166:ILE:HD12	1:H:177:PHE:HB3	1.92	0.52
1:B:93:HIS:CE1	1:B:101:SER:OG	2.63	0.52
1:E:71:LEU:O	1:E:75:LYS:HG3	2.09	0.52
1:E:97:THR:CG2	1:G:227:GLN:HE21	2.22	0.52
1:F:168:LYS:HG2	1:H:279:THR:CG2	2.40	0.52
1:A:175:ASP:OD1	1:B:159:ARG:NH2	2.42	0.52
1:A:26:THR:CB	3:B:2059:HOH:O	2.58	0.52
1:C:249:GLY:HA3	1:C:253:GLY:HA2	1.90	0.52
1:B:218:PRO:HB3	1:B:243:LYS:HD2	1.91	0.51
1:E:170:ASN:H	1:E:176:THR:HG23	1.74	0.51
1:E:283:ILE:HD13	1:H:187:VAL:HG21	1.91	0.51
1:G:236:ALA:O	1:G:240:HIS:HD2	1.94	0.51
1:H:62:SER:HB2	1:H:97:THR:HB	1.92	0.51
1:A:255:VAL:H	1:A:290:GLN:NE2	2.09	0.51
1:E:93:HIS:HD2	1:E:94:GLY:O	1.93	0.51
1:A:112:ASP:HB2	3:A:2031:HOH:O	2.11	0.51
1:A:62:SER:HB2	1:A:97:THR:HG22	1.91	0.51
1:A:279:THR:HG21	1:C:170:ASN:C	2.31	0.51
1:C:74:SER:OG	1:C:108:THR:HG23	2.10	0.51
1:F:276:SER:HA	1:F:295:ALA:HB3	1.93	0.51
1:A:159:ARG:NH2	1:B:173:THR:HG21	2.18	0.51
1:A:227:GLN:NE2	1:C:97:THR:CG2	2.61	0.51
1:E:187:VAL:CG1	1:E:189:ILE:HG12	2.41	0.51
1:F:167:SER:HB3	3:F:2023:HOH:O	2.10	0.51
1:H:255:VAL:HG22	1:H:290:GLN:HE21	1.75	0.51
1:C:275:ARG:HD3	1:C:291:PRO:O	2.12	0.50
1:C:293:LEU:HD21	1:C:317:PRO:HB3	1.93	0.50
1:F:93:HIS:HD2	1:F:94:GLY:O	1.93	0.50
1:B:304:ARG:HG2	1:B:308:MET:HE2	1.94	0.50
1:G:44:PRO:HD2	3:G:2008:HOH:O	2.11	0.50
1:C:247:TYR:CZ	1:C:249:GLY:HA2	2.45	0.50
1:H:12:THR:HG21	1:H:65:MET:CE	2.41	0.50
1:F:97:THR:CG2	1:F:97:THR:O	2.59	0.50
1:F:285:PRO:O	1:F:294:VAL:HG21	2.11	0.50
1:E:170:ASN:O	1:E:176:THR:HG21	2.11	0.50
1:A:170:ASN:H	1:A:176:THR:CG2	2.22	0.50
1:F:284:VAL:HG12	1:F:294:VAL:HG22	1.92	0.50
1:H:263:ILE:HG12	1:H:273:VAL:HG11	1.94	0.50
1:G:185:LEU:HD23	1:G:197:THR:HG23	1.94	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:278:ARG:NH2	1:C:100:GLU:OE2	2.42	0.49
1:A:192:LYS:HE2	3:A:2022:HOH:O	2.12	0.49
1:G:199:LEU:HD13	1:G:201:LYS:H	1.77	0.49
1:C:258:ARG:HH11	1:C:258:ARG:HB2	1.77	0.49
1:A:247:TYR:CZ	1:A:249:GLY:HA2	2.47	0.49
1:F:247:TYR:CE2	1:F:249:GLY:HA2	2.48	0.49
1:D:97:THR:CG2	1:D:97:THR:O	2.60	0.49
1:D:185:LEU:HD23	1:D:197:THR:HG22	1.94	0.49
1:A:18:GLY:HA2	1:A:30:LYS:O	2.13	0.49
1:A:159:ARG:HH21	1:B:173:THR:CG2	2.19	0.49
1:C:169:THR:H	1:C:176:THR:HG22	1.77	0.49
1:D:71:LEU:O	1:D:75:LYS:HG3	2.13	0.49
1:D:220:VAL:HG12	1:D:304:ARG:HG3	1.94	0.49
1:E:63:GLU:HG2	1:G:254:SER:HB3	1.95	0.49
1:F:97:THR:HG23	1:H:227:GLN:NE2	2.27	0.49
1:G:127:ILE:HD11	1:H:45:GLU:OE1	2.13	0.49
1:A:97:THR:HG23	1:A:97:THR:O	2.13	0.49
1:C:170:ASN:N	1:C:176:THR:HG23	2.20	0.49
1:E:10:LEU:HD23	1:E:57:VAL:HG21	1.95	0.49
1:A:75:LYS:NZ	1:A:214:VAL:O	2.46	0.49
1:A:192:LYS:HD3	3:A:2075:HOH:O	2.12	0.49
1:F:140:LYS:HE3	1:F:191:ASP:OD1	2.12	0.49
1:E:97:THR:HG23	1:G:227:GLN:HE21	1.78	0.48
1:E:284:VAL:O	1:E:294:VAL:HG13	2.13	0.48
1:A:260:ASP:O	1:A:264:ARG:HG3	2.13	0.48
1:B:249:GLY:O	1:B:278:ARG:HG2	2.13	0.48
1:B:3:ASN:HB3	3:B:2002:HOH:O	2.12	0.48
1:C:140:LYS:NZ	1:C:191:ASP:OD1	2.46	0.48
1:G:73:LEU:O	1:G:77:VAL:HG23	2.12	0.48
1:H:196:GLN:HG2	3:H:2048:HOH:O	2.12	0.48
1:F:267:GLU:HB2	3:F:2058:HOH:O	2.14	0.48
1:D:170:ASN:H	1:D:176:THR:HG22	1.79	0.48
1:H:170:ASN:O	1:H:176:THR:CG2	2.62	0.48
1:D:23:ASN:HB3	3:D:2042:HOH:O	2.12	0.48
1:H:164:ARG:HD2	1:H:164:ARG:O	2.13	0.48
1:A:170:ASN:O	1:A:176:THR:HG23	2.14	0.48
1:E:16:ILE:HA	1:E:120:ALA:HB3	1.96	0.48
1:A:23:ASN:HB2	1:A:127:ILE:HG23	1.95	0.47
1:B:181:GLU:OE1	1:C:159:ARG:NH1	2.47	0.47
1:E:293:LEU:HD22	1:E:321:GLN:HB2	1.94	0.47
1:F:109:VAL:HB	1:F:204:THR:HG22	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:284:VAL:O	1:A:294:VAL:HG13	2.14	0.47
1:C:74:SER:OG	1:C:108:THR:CG2	2.63	0.47
1:E:169:THR:N	1:E:176:THR:HG22	2.28	0.47
1:G:230:PRO:HB3	1:G:232:TYR:CZ	2.49	0.47
1:C:14:GLY:HA2	2:C:1328:ASP:OXT	2.14	0.47
1:H:173:THR:O	1:H:176:THR:HG23	2.14	0.47
1:C:121:MET:HB2	1:C:174:LEU:HD23	1.96	0.47
1:E:161:GLY:HA3	1:E:166:ILE:HG13	1.95	0.47
1:F:74:SER:OG	1:F:108:THR:CG2	2.63	0.47
1:G:62:SER:O	1:G:97:THR:HB	2.15	0.47
1:F:95:THR:OG1	1:F:168:LYS:NZ	2.44	0.47
1:F:96:ASP:O	1:H:250:MET:HB3	2.14	0.47
1:H:97:THR:CG2	1:H:97:THR:O	2.63	0.47
1:H:115:VAL:HB	1:H:152:VAL:HG22	1.97	0.47
1:B:169:THR:H	1:B:176:THR:HG22	1.80	0.47
1:C:11:ALA:HA	1:C:92:THR:HB	1.97	0.47
1:H:12:THR:CG2	1:H:65:MET:CE	2.93	0.47
1:A:170:ASN:O	1:A:176:THR:HG21	2.14	0.46
1:D:203:HIS:HD2	1:D:204:THR:OG1	1.97	0.46
1:A:206:ARG:HD3	3:A:2082:HOH:O	2.15	0.46
1:C:243:LYS:HD3	3:C:2072:HOH:O	2.15	0.46
1:F:284:VAL:HG12	1:F:294:VAL:CG2	2.45	0.46
1:E:222:ILE:HD12	1:G:226:TYR:CG	2.50	0.46
1:F:108:THR:OG1	1:F:211:VAL:HG22	2.15	0.46
1:F:197:THR:HB	1:G:197:THR:OG1	2.15	0.46
1:F:222:ILE:HA	1:F:246:VAL:O	2.15	0.46
1:G:97:THR:CG2	1:G:97:THR:O	2.63	0.46
1:C:144:ASP:O	1:C:147:SER:HB2	2.15	0.46
1:D:71:LEU:HD11	1:D:217:LEU:HG	1.97	0.46
1:E:168:LYS:HG3	1:E:176:THR:CG2	2.44	0.46
1:G:104:PHE:CD2	1:G:105:LEU:HD23	2.49	0.46
1:C:169:THR:N	1:C:176:THR:HG22	2.31	0.46
1:G:263:ILE:HG12	1:G:273:VAL:HG11	1.98	0.46
1:D:267:GLU:OE2	1:D:292:GLY:HA2	2.16	0.46
1:B:105:LEU:HA	1:B:108:THR:HG22	1.98	0.46
1:B:11:ALA:HB2	1:B:36:VAL:HB	1.98	0.46
1:C:203:HIS:CD2	1:C:206:ARG:HH21	2.34	0.46
1:E:255:VAL:HG22	1:E:290:GLN:NE2	2.24	0.46
1:E:276:SER:HA	1:E:295:ALA:HB3	1.98	0.45
1:F:9:ILE:HD13	1:F:135:LEU:HD11	1.99	0.45
1:F:263:ILE:HD12	1:F:273:VAL:HG11	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:230:PRO:HG2	1:D:233:MET:HG2	1.96	0.45
1:E:93:HIS:CD2	1:E:94:GLY:O	2.69	0.45
1:H:93:HIS:HD2	1:H:94:GLY:O	1.98	0.45
1:B:12:THR:HB	1:B:92:THR:O	2.16	0.45
1:B:278:ARG:NH2	1:D:100:GLU:OE2	2.39	0.45
1:G:108:THR:HG23	1:G:211:VAL:HG22	1.98	0.45
1:H:93:HIS:CD2	1:H:94:GLY:O	2.69	0.45
1:F:87:ASP:O	1:F:113:LYS:HG2	2.16	0.45
1:H:170:ASN:HB3	1:H:176:THR:CG2	2.35	0.45
1:H:170:ASN:O	1:H:176:THR:HG21	2.16	0.45
1:C:294:VAL:H	1:C:321:GLN:NE2	2.13	0.45
1:H:12:THR:CG2	1:H:65:MET:HE1	2.47	0.45
1:H:274:VAL:HG22	1:H:293:LEU:HB2	1.99	0.45
1:A:112:ASP:HB3	1:A:148:ARG:HD3	1.98	0.45
1:F:187:VAL:CG1	1:F:189:ILE:HD13	2.47	0.45
1:F:300:PRO:HD2	3:H:2057:HOH:O	2.17	0.45
1:H:185:LEU:HD23	1:H:197:THR:HG22	1.99	0.45
1:A:196:GLN:NE2	1:D:297:SER:OG	2.49	0.45
1:F:65:MET:HB3	1:F:97:THR:HG21	1.99	0.45
1:B:168:LYS:HG3	1:B:176:THR:CG2	2.40	0.45
1:B:169:THR:N	1:B:176:THR:HG22	2.32	0.45
1:D:105:LEU:O	1:D:109:VAL:HG23	2.17	0.45
1:E:47:LYS:HB2	3:E:2006:HOH:O	2.16	0.45
1:C:159:ARG:HB3	1:C:184:TYR:CD2	2.52	0.45
1:E:61:GLY:HA3	1:E:63:GLU:OE1	2.17	0.45
1:E:206:ARG:HD3	3:E:2019:HOH:O	2.16	0.45
1:H:175:ASP:O	1:H:178:LYS:HE2	2.16	0.44
1:A:62:SER:HB3	1:A:94:GLY:HA3	1.98	0.44
1:D:106:ASN:HA	1:D:152:VAL:CG2	2.47	0.44
1:D:220:VAL:CG1	1:D:304:ARG:HG3	2.47	0.44
1:G:98:LEU:O	1:G:102:PRO:CD	2.65	0.44
1:F:175:ASP:OD1	1:F:175:ASP:N	2.49	0.44
1:H:316:ASN:HA	1:H:317:PRO:HD3	1.87	0.44
1:C:122:ARG:NH1	1:C:174:LEU:HD11	2.32	0.44
1:E:258:ARG:HE	1:E:258:ARG:HB2	1.53	0.44
1:F:232:TYR:O	1:F:235:ASP:HB2	2.18	0.44
1:F:251:GLY:HA3	1:H:96:ASP:OD1	2.18	0.44
1:G:229:ASP:O	1:G:258:ARG:NH1	2.51	0.44
1:H:83:ARG:HA	3:H:2012:HOH:O	2.18	0.44
1:H:100:GLU:HG3	1:H:301:ALA:HB1	2.00	0.44
1:B:203:HIS:HD2	1:B:204:THR:OG1	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:255:VAL:HG22	1:D:290:GLN:HE21	1.82	0.44
1:H:230:PRO:HB3	1:H:232:TYR:CE2	2.53	0.44
1:C:16:ILE:HG21	1:C:92:THR:HG23	1.98	0.44
1:H:164:ARG:HG2	1:H:199:LEU:HD21	1.99	0.44
1:A:47:LYS:HG2	3:A:2013:HOH:O	2.17	0.44
1:A:294:VAL:N	1:A:321:GLN:HE22	2.15	0.44
1:B:289:GLY:HA3	3:B:2077:HOH:O	2.18	0.44
1:F:252:ALA:O	1:F:284:VAL:HG13	2.17	0.44
1:H:70:LEU:HD23	1:H:70:LEU:HA	1.86	0.44
1:A:293:LEU:HD22	1:A:321:GLN:HB2	2.00	0.44
1:B:165:PHE:CE1	1:B:199:LEU:HD23	2.52	0.44
1:D:120:ALA:HB2	1:D:131:GLY:HA2	1.99	0.44
1:F:61:GLY:HA3	1:F:63:GLU:OE1	2.18	0.44
1:G:10:LEU:HD12	1:G:55:GLU:HB3	2.00	0.44
1:B:93:HIS:CD2	1:B:94:GLY:O	2.66	0.44
1:E:316:ASN:HA	1:E:317:PRO:HD2	1.83	0.44
1:A:46:LEU:HD22	1:A:139:VAL:HG21	2.00	0.43
1:F:159:ARG:HH11	1:F:184:TYR:HE1	1.64	0.43
1:E:52:ILE:HD11	1:E:139:VAL:HG11	1.99	0.43
1:F:166:ILE:HD12	1:F:177:PHE:HB3	2.00	0.43
1:H:234:TYR:O	1:H:238:ILE:HG13	2.19	0.43
1:A:229:ASP:HA	1:A:230:PRO:HD3	1.86	0.43
1:B:254:SER:HB3	1:D:63:GLU:CG	2.48	0.43
1:G:74:SER:OG	1:G:108:THR:CG2	2.66	0.43
1:B:227:GLN:NE2	1:D:100:GLU:HG3	2.34	0.43
1:D:101:SER:HB2	1:D:102:PRO:HD3	1.99	0.43
1:F:203:HIS:HD2	1:F:204:THR:OG1	2.01	0.43
1:A:65:MET:HB3	1:A:97:THR:HG21	2.01	0.43
1:C:285:PRO:O	1:C:294:VAL:HG21	2.18	0.43
1:A:249:GLY:HA3	1:A:253:GLY:HA2	1.99	0.43
1:B:294:VAL:H	1:B:321:GLN:HE22	1.66	0.43
1:C:316:ASN:HA	1:C:317:PRO:HD3	1.82	0.43
1:D:93:HIS:CD2	1:D:94:GLY:O	2.70	0.43
1:E:284:VAL:HG12	1:E:294:VAL:HG22	2.01	0.43
1:D:247:TYR:CZ	1:D:249:GLY:HA2	2.53	0.43
1:A:254:SER:HA	1:A:290:GLN:HE22	1.84	0.43
1:E:110:LYS:O	1:E:205:THR:HG22	2.18	0.43
1:H:275:ARG:NH2	3:H:2063:HOH:O	2.32	0.43
1:A:264:ARG:NH1	1:A:291:PRO:HG3	2.34	0.43
1:C:264:ARG:NH2	3:C:2082:HOH:O	2.52	0.43
1:G:37:GLU:HB3	3:G:2006:HOH:O	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:12:THR:HG21	1:H:65:MET:HE1	1.99	0.43
1:E:161:GLY:HA3	1:E:166:ILE:CG1	2.49	0.43
1:F:74:SER:OG	1:F:108:THR:HG23	2.18	0.42
1:F:249:GLY:HA3	1:F:253:GLY:HA2	2.01	0.42
1:B:46:LEU:HD22	1:B:139:VAL:HG21	2.00	0.42
1:D:97:THR:HG23	1:D:97:THR:O	2.19	0.42
1:D:170:ASN:H	1:D:176:THR:CG2	2.32	0.42
1:D:254:SER:HA	1:D:290:GLN:HE22	1.83	0.42
1:B:170:ASN:H	1:B:176:THR:HG22	1.82	0.42
1:G:128:SER:OG	1:H:132:PRO:HB2	2.19	0.42
1:G:220:VAL:CG1	1:G:304:ARG:HG3	2.49	0.42
1:C:150:ARG:HD3	3:C:2038:HOH:O	2.19	0.42
1:G:119:ALA:HB3	1:G:156:LEU:HD21	2.02	0.42
1:B:112:ASP:HB2	1:B:148:ARG:HH12	1.84	0.42
1:B:274:VAL:HG11	1:B:324:PHE:CE2	2.54	0.42
1:C:97:THR:CG2	1:C:97:THR:O	2.67	0.42
1:E:242:VAL:CG1	1:E:244:GLY:O	2.68	0.42
1:H:164:ARG:HG3	1:H:165:PHE:CE2	2.55	0.42
1:H:229:ASP:HA	1:H:230:PRO:HD2	1.67	0.42
1:A:16:ILE:HG21	1:A:92:THR:HB	2.02	0.42
1:A:284:VAL:HG12	1:A:294:VAL:HG22	2.01	0.42
1:E:46:LEU:HD21	1:E:136:TYR:HA	2.01	0.42
1:A:242:VAL:O	1:A:271:ILE:HG12	2.19	0.42
1:D:15:THR:HB	2:D:1328:ASP:CG	2.40	0.42
1:D:286:PRO:HA	1:D:294:VAL:HG21	2.01	0.42
1:B:284:VAL:O	1:B:294:VAL:HG13	2.19	0.42
1:H:73:LEU:O	1:H:77:VAL:HG23	2.19	0.42
1:B:170:ASN:N	1:B:176:THR:HG23	2.27	0.42
1:D:284:VAL:O	1:D:294:VAL:HG13	2.20	0.42
1:F:96:ASP:OD1	1:H:251:GLY:HA3	2.20	0.42
1:G:203:HIS:CD2	1:G:204:THR:OG1	2.71	0.42
1:A:52:ILE:HD11	1:A:139:VAL:HG11	2.01	0.41
1:E:169:THR:H	1:E:176:THR:HG22	1.85	0.41
1:F:260:ASP:O	1:F:264:ARG:HG3	2.19	0.41
1:G:63:GLU:H	1:G:63:GLU:CD	2.22	0.41
1:G:94:GLY:HA3	2:G:1328:ASP:O	2.20	0.41
1:G:199:LEU:HD11	1:G:201:LYS:HB2	2.02	0.41
1:D:283:ILE:CD1	1:D:297:SER:HB3	2.48	0.41
1:G:130:ASP:OD1	1:G:130:ASP:N	2.49	0.41
1:G:187:VAL:CG1	1:G:189:ILE:HG12	2.49	0.41
1:B:187:VAL:CG1	1:B:189:ILE:HG12	2.50	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:229:ASP:HA	1:C:230:PRO:HD2	1.94	0.41
1:C:128:SER:HB2	1:D:133:MET:CB	2.49	0.41
1:C:220:VAL:HG12	1:C:304:ARG:HG3	2.02	0.41
1:D:162:SER:HB2	1:D:185:LEU:HD11	2.03	0.41
1:E:259:GLY:O	1:E:263:ILE:HG12	2.20	0.41
1:F:265:LYS:O	1:F:268:SER:OG	2.36	0.41
1:A:304:ARG:NH2	3:A:2106:HOH:O	2.54	0.41
1:B:255:VAL:H	1:B:290:GLN:NE2	2.19	0.41
1:B:284:VAL:O	1:B:294:VAL:CG1	2.68	0.41
1:F:107:LEU:HD22	1:F:327:TYR:CD2	2.55	0.41
1:A:16:ILE:HA	1:A:120:ALA:HB3	2.01	0.41
1:A:228:ASP:CA	1:A:258:ARG:HH12	2.33	0.41
1:F:107:LEU:HD22	1:F:327:TYR:HD2	1.86	0.41
1:G:268:SER:HB2	3:G:2053:HOH:O	2.19	0.41
1:C:203:HIS:H	1:C:206:ARG:NH2	2.18	0.41
1:D:100:GLU:H	1:D:100:GLU:HG2	1.57	0.41
1:E:157:ASN:O	1:E:158:ASP:HB2	2.20	0.41
1:F:173:THR:O	1:F:176:THR:OG1	2.39	0.41
1:F:274:VAL:HG23	1:F:307:LEU:HD22	2.02	0.41
1:H:222:ILE:HA	1:H:246:VAL:O	2.21	0.41
1:A:249:GLY:O	1:A:278:ARG:HG2	2.21	0.41
1:D:260:ASP:OD1	1:D:264:ARG:NH1	2.54	0.41
1:E:75:LYS:HE2	1:E:211:VAL:O	2.21	0.41
1:E:81:LEU:HD22	1:E:113:LYS:HB2	2.03	0.41
1:E:101:SER:HB2	1:E:102:PRO:HD3	2.03	0.41
1:E:182:GLU:OE2	1:H:196:GLN:NE2	2.54	0.41
1:E:209:PHE:HE2	1:E:310:ALA:HA	1.85	0.41
1:F:166:ILE:HD11	1:F:184:TYR:CE2	2.54	0.41
1:F:273:VAL:O	1:F:293:LEU:N	2.49	0.41
1:G:97:THR:HG23	1:G:97:THR:O	2.21	0.41
1:A:96:ASP:OD2	2:A:1328:ASP:N	2.53	0.40
1:E:285:PRO:O	1:E:294:VAL:HG21	2.21	0.40
1:G:228:ASP:C	1:G:258:ARG:HH12	2.24	0.40
1:H:237:SER:O	1:H:242:VAL:HB	2.21	0.40
1:G:98:LEU:HD12	1:G:177:PHE:CZ	2.56	0.40
1:D:47:LYS:HD2	3:D:2012:HOH:O	2.21	0.40
1:D:158:ASP:O	1:D:187:VAL:HG13	2.22	0.40
1:F:110:LYS:HG2	3:F:2048:HOH:O	2.21	0.40
1:F:263:ILE:HG23	1:F:273:VAL:HG11	2.04	0.40
1:G:249:GLY:HA3	1:G:253:GLY:HA2	2.03	0.40
1:H:4:LEU:HA	1:H:5:PRO:HD3	1.93	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:121:MET:HG3	1:B:173:THR:O	2.21	0.40
1:D:46:LEU:HD21	1:D:136:TYR:HA	2.04	0.40
1:E:103:TYR:CE2	1:E:107:LEU:HD11	2.56	0.40
1:F:179:ALA:O	1:F:183:GLY:N	2.49	0.40
1:E:104:PHE:HD2	1:E:105:LEU:HD23	1.87	0.40
1:E:294:VAL:H	1:E:321:GLN:HE22	1.68	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	323/325 (99%)	308 (95%)	14 (4%)	1 (0%)	41	61
1	B	310/325 (95%)	294 (95%)	15 (5%)	1 (0%)	41	61
1	C	311/325 (96%)	299 (96%)	11 (4%)	1 (0%)	41	61
1	D	316/325 (97%)	303 (96%)	13 (4%)	0	100	100
1	E	308/325 (95%)	294 (96%)	12 (4%)	2 (1%)	25	43
1	F	313/325 (96%)	298 (95%)	13 (4%)	2 (1%)	25	43
1	G	305/325 (94%)	292 (96%)	13 (4%)	0	100	100
1	H	309/325 (95%)	290 (94%)	17 (6%)	2 (1%)	25	43
All	All	2495/2600 (96%)	2378 (95%)	108 (4%)	9 (0%)	34	54

All (9) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	F	5	PRO
1	F	204	THR
1	H	34	LEU
1	A	204	THR

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Mol	Chain	Res	Type
1	C	20	ALA
1	E	36	VAL
1	E	204	THR
1	H	132	PRO
1	B	292	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	253/260 (97%)	235 (93%)	18 (7%)	14 28
1	B	251/260 (96%)	239 (95%)	12 (5%)	25 48
1	C	251/260 (96%)	228 (91%)	23 (9%)	9 18
1	D	253/260 (97%)	239 (94%)	14 (6%)	21 41
1	E	251/260 (96%)	238 (95%)	13 (5%)	23 44
1	F	253/260 (97%)	230 (91%)	23 (9%)	9 18
1	G	252/260 (97%)	236 (94%)	16 (6%)	18 34
1	H	251/260 (96%)	231 (92%)	20 (8%)	12 23
All	All	2015/2080 (97%)	1876 (93%)	139 (7%)	15 30

All (139) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	39	LEU
1	A	59	SER
1	A	97	THR
1	A	98	LEU
1	A	100	GLU
1	A	105	LEU
1	A	112	ASP
1	A	125	THR
1	A	146	ASN
1	A	162	SER

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Mol	Chain	Res	Type
1	A	176	THR
1	A	199	LEU
1	A	206	ARG
1	A	216	LYS
1	A	242	VAL
1	A	258	ARG
1	A	279	THR
1	A	294	VAL
1	B	12	THR
1	B	39	LEU
1	B	41	GLN
1	B	53	LYS
1	B	63	GLU
1	B	105	LEU
1	B	125	THR
1	B	127	ILE
1	B	199	LEU
1	B	226	TYR
1	B	258	ARG
1	B	308	MET
1	C	3	ASN
1	C	39	LEU
1	C	47	LYS
1	C	63	GLU
1	C	67	SER
1	C	92	THR
1	C	97	THR
1	C	98	LEU
1	C	100	GLU
1	C	108	THR
1	C	112	ASP
1	C	125	THR
1	C	127	ILE
1	C	166	ILE
1	C	187	VAL
1	C	197	THR
1	C	199	LEU
1	C	206	ARG
1	C	242	VAL
1	C	243	LYS
1	C	257	LYS
1	C	258	ARG

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Mol	Chain	Res	Type
1	C	315	THR
1	D	39	LEU
1	D	84	SER
1	D	97	THR
1	D	100	GLU
1	D	108	THR
1	D	125	THR
1	D	140	LYS
1	D	145	LYS
1	D	176	THR
1	D	197	THR
1	D	199	LEU
1	D	265	LYS
1	D	268	SER
1	D	315	THR
1	E	47	LYS
1	E	63	GLU
1	E	97	THR
1	E	105	LEU
1	E	108	THR
1	E	166	ILE
1	E	176	THR
1	E	187	VAL
1	E	197	THR
1	E	199	LEU
1	E	257	LYS
1	E	258	ARG
1	E	294	VAL
1	F	10	LEU
1	F	47	LYS
1	F	48	THR
1	F	59	SER
1	F	60	ILE
1	F	84	SER
1	F	97	THR
1	F	98	LEU
1	F	105	LEU
1	F	110	LYS
1	F	125	THR
1	F	127	ILE
1	F	148	ARG
1	F	166	ILE

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Mol	Chain	Res	Type
1	F	176	THR
1	F	187	VAL
1	F	189	ILE
1	F	199	LEU
1	F	205	THR
1	F	212	THR
1	F	277	SER
1	F	294	VAL
1	F	309	LEU
1	G	10	LEU
1	G	48	THR
1	G	83	ARG
1	G	92	THR
1	G	97	THR
1	G	98	LEU
1	G	100	GLU
1	G	125	THR
1	G	127	ILE
1	G	146	ASN
1	G	199	LEU
1	G	237	SER
1	G	258	ARG
1	G	283	ILE
1	G	294	VAL
1	G	315	THR
1	H	3	ASN
1	H	38	THR
1	H	63	GLU
1	H	83	ARG
1	H	92	THR
1	H	97	THR
1	H	100	GLU
1	H	105	LEU
1	H	112	ASP
1	H	127	ILE
1	H	145	LYS
1	H	166	ILE
1	H	192	LYS
1	H	197	THR
1	H	199	LEU
1	H	206	ARG
1	H	243	LYS

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Mol	Chain	Res	Type
1	H	258	ARG
1	H	294	VAL
1	H	315	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (47) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	93	HIS
1	A	196	GLN
1	A	203	HIS
1	A	227	GLN
1	A	290	GLN
1	A	321	GLN
1	B	93	HIS
1	B	196	GLN
1	B	203	HIS
1	B	227	GLN
1	B	290	GLN
1	B	321	GLN
1	C	93	HIS
1	C	196	GLN
1	C	203	HIS
1	C	227	GLN
1	C	290	GLN
1	C	321	GLN
1	D	3	ASN
1	D	93	HIS
1	D	196	GLN
1	D	203	HIS
1	D	227	GLN
1	D	240	HIS
1	D	290	GLN
1	D	321	GLN
1	E	93	HIS
1	E	146	ASN
1	E	203	HIS
1	E	227	GLN
1	E	290	GLN
1	E	321	GLN
1	F	93	HIS
1	F	146	ASN
1	F	196	GLN

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Mol	Chain	Res	Type
1	F	203	HIS
1	F	227	GLN
1	F	321	GLN
1	G	93	HIS
1	G	203	HIS
1	G	227	GLN
1	G	240	HIS
1	H	93	HIS
1	H	146	ASN
1	H	203	HIS
1	H	227	GLN
1	H	290	GLN

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

8 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
2	ASP	B	1328	-	6,8,8	1.20	0	8,10,10	1.44	2 (25%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
2	ASP	C	1328	-	6,8,8	1.15	1 (16%)	8,10,10	1.60	2 (25%)
2	ASP	E	1328	-	6,8,8	1.28	1 (16%)	8,10,10	1.63	2 (25%)
2	ASP	H	1328	-	6,8,8	1.12	1 (16%)	8,10,10	1.52	2 (25%)
2	ASP	A	1328	-	6,8,8	1.24	1 (16%)	8,10,10	1.50	2 (25%)
2	ASP	F	1328	-	6,8,8	1.20	1 (16%)	8,10,10	1.78	2 (25%)
2	ASP	D	1328	-	6,8,8	1.28	1 (16%)	8,10,10	1.52	2 (25%)
2	ASP	G	1328	-	6,8,8	1.18	0	8,10,10	1.60	2 (25%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	ASP	B	1328	-	-	4/8/8/8	-
2	ASP	C	1328	-	-	4/8/8/8	-
2	ASP	E	1328	-	-	2/8/8/8	-
2	ASP	H	1328	-	-	4/8/8/8	-
2	ASP	A	1328	-	-	4/8/8/8	-
2	ASP	F	1328	-	-	3/8/8/8	-
2	ASP	D	1328	-	-	2/8/8/8	-
2	ASP	G	1328	-	-	2/8/8/8	-

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	1328	ASP	OXT-C	-2.27	1.23	1.30
2	D	1328	ASP	OXT-C	-2.26	1.23	1.30
2	E	1328	ASP	OXT-C	-2.20	1.23	1.30
2	A	1328	ASP	OXT-C	-2.17	1.23	1.30
2	F	1328	ASP	OXT-C	-2.15	1.23	1.30
2	H	1328	ASP	OXT-C	-2.02	1.23	1.30

All (16) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	F	1328	ASP	OXT-C-O	-3.12	117.01	124.09
2	C	1328	ASP	OXT-C-O	-2.94	117.40	124.09

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	F	1328	ASP	OXT-C-CA	2.85	123.10	113.38
2	G	1328	ASP	OXT-C-O	-2.76	117.81	124.09
2	E	1328	ASP	OXT-C-O	-2.74	117.87	124.09
2	G	1328	ASP	OXT-C-CA	2.71	122.61	113.38
2	D	1328	ASP	OXT-C-O	-2.71	117.94	124.09
2	B	1328	ASP	OXT-C-O	-2.70	117.95	124.09
2	E	1328	ASP	OXT-C-CA	2.67	122.48	113.38
2	A	1328	ASP	OXT-C-O	-2.58	118.23	124.09
2	H	1328	ASP	OXT-C-O	-2.52	118.37	124.09
2	B	1328	ASP	OXT-C-CA	2.31	121.27	113.38
2	C	1328	ASP	OXT-C-CA	2.28	121.15	113.38
2	D	1328	ASP	OXT-C-CA	2.24	121.01	113.38
2	A	1328	ASP	OXT-C-CA	2.18	120.81	113.38
2	H	1328	ASP	OD1-CG-CB	-2.06	116.20	122.80

There are no chirality outliers.

All (25) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	1328	ASP	O-C-CA-N
2	B	1328	ASP	O-C-CA-N
2	C	1328	ASP	O-C-CA-N
2	D	1328	ASP	O-C-CA-N
2	E	1328	ASP	O-C-CA-N
2	F	1328	ASP	O-C-CA-N
2	G	1328	ASP	O-C-CA-N
2	H	1328	ASP	O-C-CA-N
2	A	1328	ASP	OXT-C-CA-N
2	E	1328	ASP	OXT-C-CA-N
2	H	1328	ASP	OXT-C-CA-N
2	F	1328	ASP	OXT-C-CA-N
2	G	1328	ASP	OXT-C-CA-N
2	B	1328	ASP	OXT-C-CA-N
2	C	1328	ASP	OXT-C-CA-N
2	D	1328	ASP	OXT-C-CA-N
2	B	1328	ASP	OXT-C-CA-CB
2	B	1328	ASP	O-C-CA-CB
2	C	1328	ASP	O-C-CA-CB
2	C	1328	ASP	OXT-C-CA-CB
2	H	1328	ASP	O-C-CA-CB
2	H	1328	ASP	OXT-C-CA-CB
2	A	1328	ASP	O-C-CA-CB

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Mol	Chain	Res	Type	Atoms
2	A	1328	ASP	OXT-C-CA-CB
2	F	1328	ASP	N-CA-CB-CG

There are no ring outliers.

5 monomers are involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	C	1328	ASP	2	0
2	H	1328	ASP	1	0
2	A	1328	ASP	1	0
2	D	1328	ASP	1	0
2	G	1328	ASP	1	0

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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, 95^{th} 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	325/325 (100%)	-0.29	9 (2%)	53	56	22, 30, 36, 40	0
1	B	314/325 (96%)	-0.35	6 (1%)	66	69	21, 29, 36, 38	0
1	C	315/325 (96%)	-0.24	5 (1%)	72	74	22, 30, 36, 40	0
1	D	320/325 (98%)	-0.33	3 (0%)	84	86	20, 28, 36, 40	0
1	E	312/325 (96%)	-0.11	11 (3%)	44	47	31, 38, 51, 59	0
1	F	317/325 (97%)	-0.01	10 (3%)	47	51	31, 39, 46, 49	0
1	G	309/325 (95%)	-0.17	5 (1%)	72	74	31, 38, 51, 56	0
1	H	313/325 (96%)	-0.01	12 (3%)	40	43	31, 39, 51, 56	0
All	All	2525/2600 (97%)	-0.19	61 (2%)	59	62	20, 34, 46, 59	0

All (61) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	F	22	ALA	6.4
1	F	21	ALA	6.4
1	F	20	ALA	5.6
1	C	21	ALA	5.5
1	B	21	ALA	5.4
1	E	20	ALA	5.4
1	D	21	ALA	5.3
1	B	20	ALA	5.0
1	H	33	ALA	5.0
1	C	20	ALA	4.5
1	E	19	SER	4.5
1	E	21	ALA	4.0
1	H	32	GLY	3.8
1	A	26	THR	3.7
1	G	125	THR	3.6
1	H	19	SER	3.5

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Mol	Chain	Res	Type	RSRZ
1	G	3	ASN	3.5
1	E	3	ASN	3.4
1	F	89	VAL	3.4
1	B	22	ALA	3.3
1	E	206	ARG	3.2
1	A	24	THR	3.2
1	H	288	ALA	3.0
1	F	4	LEU	2.9
1	B	19	SER	2.9
1	A	27	THR	2.8
1	A	22	ALA	2.8
1	D	31	ALA	2.8
1	E	192	LYS	2.8
1	E	288	ALA	2.7
1	C	22	ALA	2.7
1	H	84	SER	2.7
1	A	21	ALA	2.6
1	G	213	ASN	2.6
1	A	29	TYR	2.6
1	B	18	GLY	2.5
1	H	125	THR	2.5
1	A	3	ASN	2.4
1	E	41	GLN	2.4
1	F	90	VAL	2.4
1	D	4	LEU	2.4
1	F	145	LYS	2.3
1	H	3	ASN	2.3
1	G	127	ILE	2.3
1	H	83	ARG	2.2
1	E	125	THR	2.2
1	C	213	ASN	2.2
1	F	3	ASN	2.2
1	C	125	THR	2.2
1	H	206	ARG	2.2
1	F	46	LEU	2.2
1	H	145	LYS	2.2
1	H	306	LEU	2.1
1	H	18	GLY	2.1
1	F	24	THR	2.1
1	A	4	LEU	2.1
1	A	206	ARG	2.1
1	G	288	ALA	2.0

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Mol	Chain	Res	Type	RSRZ
1	E	89	VAL	2.0
1	B	3	ASN	2.0
1	E	4	LEU	2.0

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

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

6.3 Carbohydrates (i)

There are no monosaccharides in this entry.

6.4 Ligands (i)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	ASP	E	1328	9/9	0.86	0.24	60,62,62,63	0
2	ASP	H	1328	9/9	0.91	0.18	55,56,57,57	0
2	ASP	F	1328	9/9	0.92	0.21	53,54,56,56	0
2	ASP	G	1328	9/9	0.93	0.18	48,49,50,50	0
2	ASP	C	1328	9/9	0.94	0.11	45,45,48,49	0
2	ASP	D	1328	9/9	0.94	0.17	53,54,55,55	0
2	ASP	B	1328	9/9	0.95	0.13	35,38,38,39	0
2	ASP	A	1328	9/9	0.97	0.09	34,36,36,36	0

6.5 Other polymers (i)

There are no such residues in this entry.