



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 15, 2017 – 04:04 am GMT

PDB ID : 2JK0
Title : STRUCTURAL AND FUNCTIONAL INSIGHTS INTO ERWINIA CARO-
TOVORA L-ASPARAGINASE
Authors : Papageorgiou, A.C.; Posypanova, G.A.; Andersson, C.S.; Sokolov, N.N.; Kra-
sotkina, 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

<http://wwpdb.org/validation/2016/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity	:	4.02b-467
Mogul	:	1.7.2 (RC1), CSD as538be (2017)
Xtriage (Phenix)	:	1.9-1692
EDS	:	trunk28620
Percentile statistics	:	20161228.v01 (using entries in the PDB archive December 28th 2016)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	recalc28949

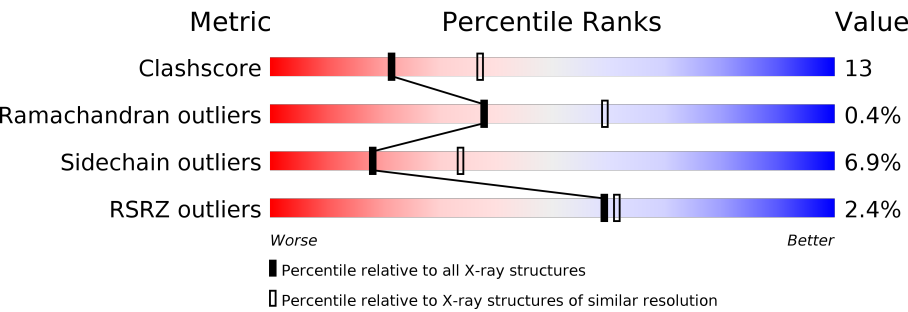
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.50 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	112137	4554 (2.50-2.50)
Ramachandran outliers	110173	4463 (2.50-2.50)
Sidechain outliers	110143	4465 (2.50-2.50)
RSRZ outliers	101464	3876 (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 on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	325	<div><div>3%</div><div><div></div><div>77%</div><div>21%</div><div>.</div></div></div>
1	B	325	<div><div>2%</div><div><div></div><div>77%</div><div>18%</div><div>..</div></div></div>
1	C	325	<div><div>2%</div><div><div></div><div>71%</div><div>22%</div><div>..</div></div></div>
1	D	325	<div><div>%</div><div><div></div><div>75%</div><div>21%</div><div>..</div></div></div>
1	E	325	<div><div>3%</div><div><div></div><div>70%</div><div>22%</div><div>..</div></div></div>
1	F	325	<div><div>3%</div><div><div></div><div>68%</div><div>26%</div><div>..</div></div></div>
1	G	325	<div><div>2%</div><div><div></div><div>73%</div><div>20%</div><div>. 5%</div></div></div>

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Mol	Chain	Length	Quality of chain
1	H	325	

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	ASP	E	1328	-	-	-	X
2	ASP	F	1328	-	-	-	X

2 Entry composition

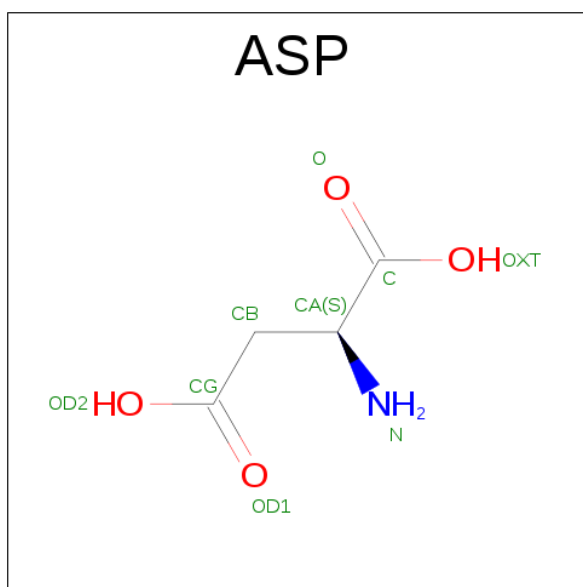
There are 3 unique types of molecules in this entry. The entry contains 19499 atoms, of which 0 are hydrogens and 0 are deuteriums.

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: C₄H₇NO₄).



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

- Molecule 3 is water.

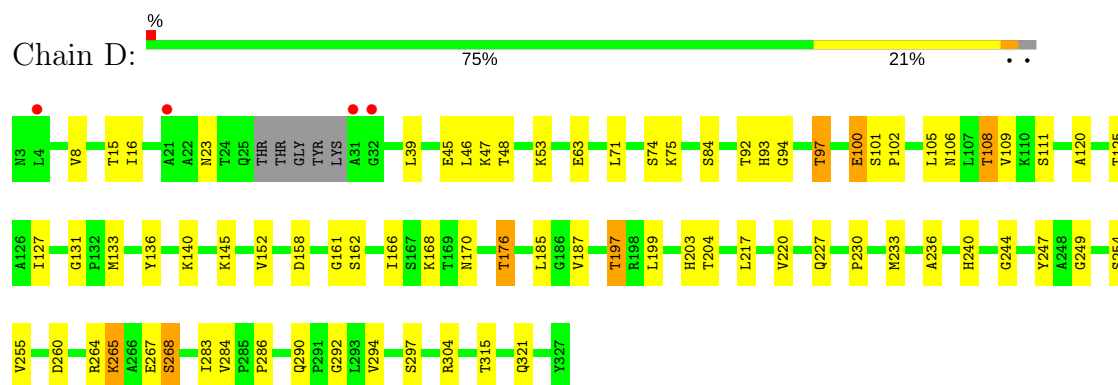
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	117	Total	O	0	0
			117	117		
3	B	86	Total	O	0	0
			86	86		
3	C	107	Total	O	0	0
			107	107		
3	D	108	Total	O	0	0
			108	108		

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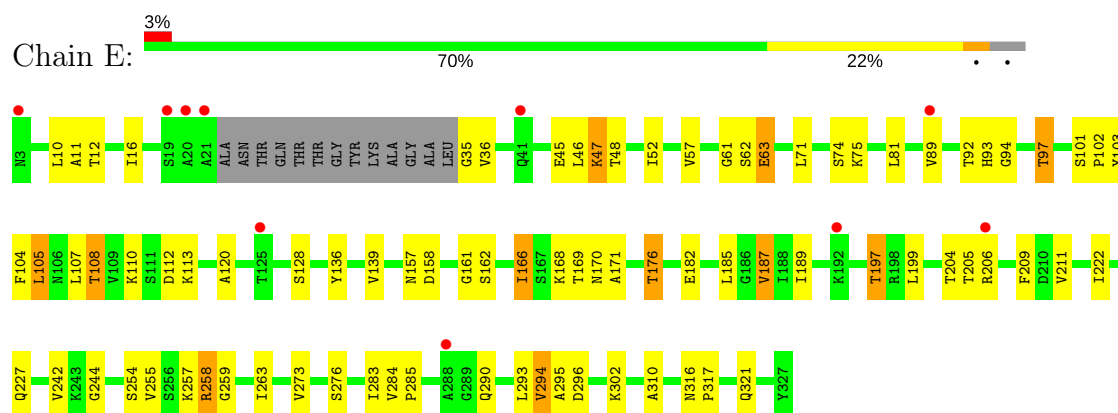
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	E	84	Total 84	O 84	0	0
3	F	68	Total 68	O 68	0	0
3	G	65	Total 65	O 65	0	0
3	H	73	Total 73	O 73	0	0

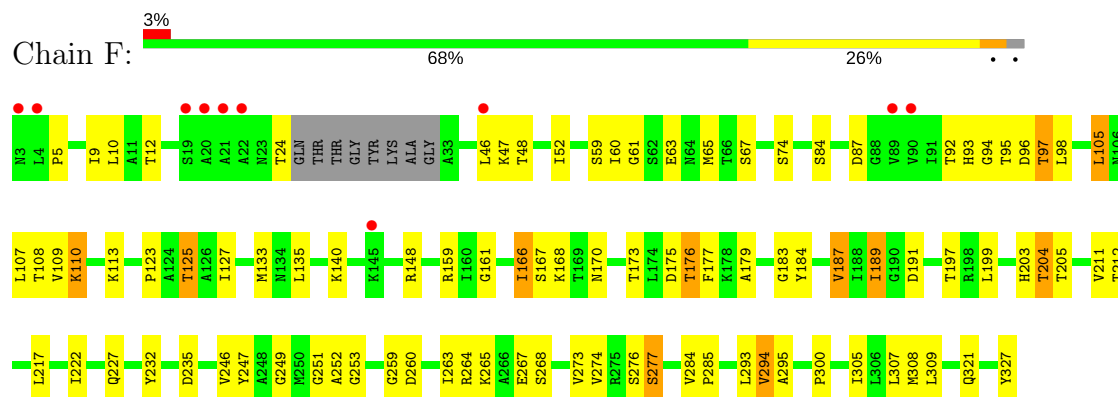
• Molecule 1: L-ASPARAGINASE



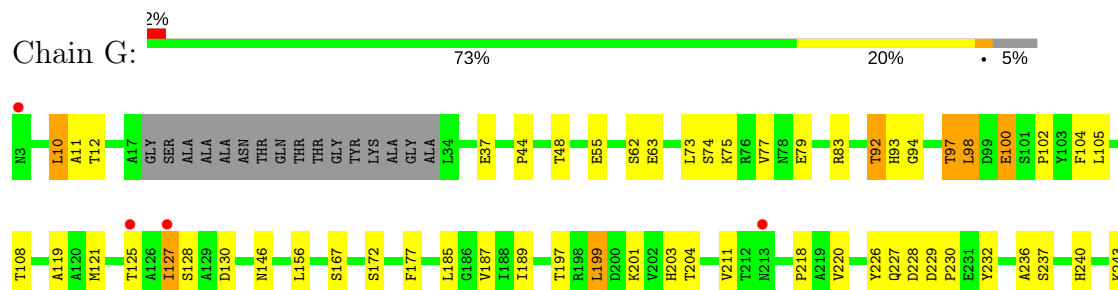
• Molecule 1: L-ASPARAGINASE



• Molecule 1: L-ASPARAGINASE

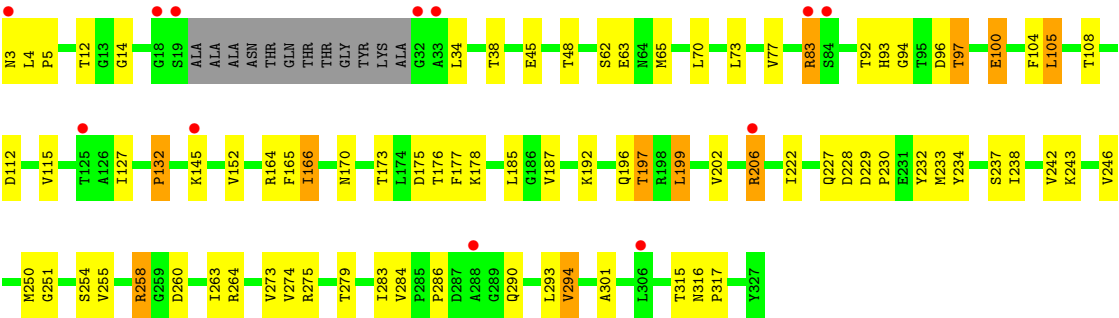


• Molecule 1: L-ASPARAGINASE





● Molecule 1: L-ASPARAGINASE



4 Data and refinement statistics

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
$\langle I/\sigma(I) \rangle$ ¹	1.69 (at 2.50Å)	Xtrriage
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.	DCC
Wilson B-factor (Å ²)	44.5	Xtrriage
Anisotropy	0.333	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 42.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
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

Xtrriage'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.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality [i](#)

5.1 Standard geometry [i](#)

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 [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	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:294:VAL:H	1:D:321:GLN:NE2	1.86	0.64
1:D:74:SER:OG	1:D:108:THR:CG2	2.45	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:O	1:B:97:THR:CG2	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:63:GLU:OE1	2:C:1328:ASP:N	2.36	0.59
1:C:47:LYS:HD3	3:C:2012:HOH:O	2.03	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:G:275:ARG:NH1	3:G:2055:HOH:O	2.36	0.58
1:E:227:GLN:NE2	1:G:97:THR:HG23	2.18	0.58
1:G:121:MET:CE	1:G:172:SER:HA	2.34	0.58
1:G:75:LYS:O	1:G:79:GLU:HB2	2.04	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:B:247:TYR:CZ	1:B:249:GLY:HA2	2.39	0.56
1:G:247:TYR:CZ	1:G:249:GLY:HA2	2.40	0.56
1:E:227:GLN:NE2	1:G:97:THR:CG2	2.65	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:D:92:THR:CG2	3:D:2003:HOH:O	2.53	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:251:GLY:O	1:F:277:SER:HB2	2.05	0.56
1:F:67:SER:HB2	1:F:217:LEU:HD12	1.88	0.56
1:F:97:THR:O	1:F:97:THR:HG23	2.06	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: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:F:168:LYS:HG2	1:H:279:THR:HG22	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:G:236:ALA:O	1:G:240:HIS:HD2	1.94	0.51
1:E:283:ILE:HD13	1:H:187:VAL:HG21	1.91	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:279:THR:HG21	1:C:170:ASN:C	2.31	0.51
1:A:62:SER:HB2	1:A:97:THR:HG22	1.91	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:285:PRO:O	1:F:294:VAL:HG21	2.11	0.50
1:F:97:THR:O	1:F:97:THR:CG2	2.59	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:HB2	1:C:258:ARG:HH11	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:185:LEU:HD23	1:D:197:THR:HG22	1.94	0.49
1:D:97:THR:CG2	1:D:97:THR:O	2.60	0.49
1:A:159:ARG:HH21	1:B:173:THR:CG2	2.19	0.49
1:A:18:GLY:HA2	1:A:30:LYS:O	2.13	0.49
1:C:169:THR:H	1:C:176:THR:HG22	1.77	0.49
1:D:220:VAL:HG12	1:D:304:ARG:HG3	1.94	0.49
1:D:71:LEU:O	1:D:75:LYS:HG3	2.13	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:192:LYS:HD3	3:A:2075:HOH:O	2.12	0.49
1:A:75:LYS:NZ	1:A:214:VAL:O	2.46	0.49
1:F:140:LYS:HE3	1:F:191:ASP:OD1	2.12	0.49
1:E:284:VAL:O	1:E:294:VAL:HG13	2.13	0.48
1:E:97:THR:HG23	1:G:227:GLN:HE21	1.78	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:O	1:H:164:ARG:HD2	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: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:F:95:THR:OG1	1:F:168:LYS:NZ	2.44	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:F:108:THR:OG1	1:F:211:VAL:HG22	2.15	0.46
1:F:222:ILE:HA	1:F:246:VAL:O	2.15	0.46
1:F:197:THR:HB	1:G:197:THR:OG1	2.15	0.46
1:E:222:ILE:HD12	1:G:226:TYR:CG	2.50	0.46
1:G:97:THR:O	1:G:97:THR:CG2	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:274:VAL:HG22	1:H:293:LEU:HB2	1.99	0.45
1:H:12:THR:CG2	1:H:65:MET:HE1	2.47	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:206:ARG:HD3	3:E:2019:HOH:O	2.16	0.45
1:E:61:GLY:HA3	1:E:63:GLU:OE1	2.17	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:N	1:F:175:ASP:OD1	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:HB2	1:E:258:ARG:HE	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:100:GLU:HG3	1:H:301:ALA:HB1	2.00	0.44
1:H:83:ARG:HA	3:H:2012:HOH:O	2.18	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:294:VAL:N	1:A:321:GLN:HE22	2.15	0.44
1:A:47:LYS:HG2	3:A:2013:HOH:O	2.17	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:HA	1:H:70:LEU:HD23	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: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:D:97:THR:O	1:D:97:THR:HG23	2.19	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:284:VAL:HG12	1:A:294:VAL:HG22	2.01	0.42
1:A:16:ILE:HG21	1:A:92:THR:HB	2.02	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:N	1:G:130:ASP:OD1	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: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:A:249:GLY:O	1:A:278:ARG:HG2	2.21	0.41
1:E:101:SER:HB2	1:E:102:PRO:HD3	2.03	0.41
1:E:81:LEU:HD22	1:E:113:LYS:HB2	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:158:ASP:O	1:D:187:VAL:HG13	2.22	0.40
1:D:47:LYS:HD2	3:D:2012:HOH:O	2.21	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%)	44	66
1	B	310/325 (95%)	294 (95%)	15 (5%)	1 (0%)	44	66
1	C	311/325 (96%)	299 (96%)	11 (4%)	1 (0%)	44	66
1	D	316/325 (97%)	303 (96%)	13 (4%)	0	100	100
1	E	308/325 (95%)	294 (96%)	12 (4%)	2 (1%)	28	48
1	F	313/325 (96%)	298 (95%)	13 (4%)	2 (1%)	28	48
1	G	305/325 (94%)	292 (96%)	13 (4%)	0	100	100
1	H	309/325 (95%)	290 (94%)	17 (6%)	2 (1%)	28	48
All	All	2495/2600 (96%)	2378 (95%)	108 (4%)	9 (0%)	38	59

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 ⓘ

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%)	17	32
1	B	251/260 (96%)	239 (95%)	12 (5%)	30	53
1	C	251/260 (96%)	228 (91%)	23 (9%)	11	20
1	D	253/260 (97%)	239 (94%)	14 (6%)	25	46
1	E	251/260 (96%)	238 (95%)	13 (5%)	27	49
1	F	253/260 (97%)	230 (91%)	23 (9%)	11	21
1	G	252/260 (97%)	236 (94%)	16 (6%)	21	38
1	H	251/260 (96%)	231 (92%)	20 (8%)	14	27
All	All	2015/2080 (97%)	1876 (93%)	139 (7%)	18	34

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

Some 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 [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

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	A	1328	-	1,8,8	0.18	0	1,10,10	0.60	0
2	ASP	B	1328	-	1,8,8	0.20	0	1,10,10	0.70	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	ASP	C	1328	-	1,8,8	0.25	0	1,10,10	0.75	0
2	ASP	D	1328	-	1,8,8	0.14	0	1,10,10	0.53	0
2	ASP	E	1328	-	1,8,8	0.17	0	1,10,10	0.30	0
2	ASP	F	1328	-	1,8,8	0.21	0	1,10,10	0.45	0
2	ASP	G	1328	-	1,8,8	0.12	0	1,10,10	0.31	0
2	ASP	H	1328	-	1,8,8	0.29	0	1,10,10	0.73	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	ASP	A	1328	-	-	0/2/8/8	0/0/0/0
2	ASP	B	1328	-	-	0/2/8/8	0/0/0/0
2	ASP	C	1328	-	-	0/2/8/8	0/0/0/0
2	ASP	D	1328	-	-	0/2/8/8	0/0/0/0
2	ASP	E	1328	-	-	0/2/8/8	0/0/0/0
2	ASP	F	1328	-	-	0/2/8/8	0/0/0/0
2	ASP	G	1328	-	-	0/2/8/8	0/0/0/0
2	ASP	H	1328	-	-	0/2/8/8	0/0/0/0

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.

5 monomers are involved in 6 short contacts:

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

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q < 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	325/325 (100%)	-0.29	9 (2%) 53 56	22, 30, 36, 40	0
1	B	314/325 (96%)	-0.35	6 (1%) 67 69	21, 29, 36, 38	0
1	C	315/325 (96%)	-0.25	5 (1%) 72 73	22, 30, 36, 40	0
1	D	320/325 (98%)	-0.33	4 (1%) 77 78	20, 28, 36, 40	0
1	E	312/325 (96%)	-0.11	10 (3%) 48 51	31, 38, 51, 59	0
1	F	317/325 (97%)	-0.02	10 (3%) 48 51	31, 39, 46, 49	0
1	G	309/325 (95%)	-0.17	5 (1%) 72 73	31, 38, 51, 56	0
1	H	313/325 (96%)	-0.01	12 (3%) 41 43	31, 39, 51, 56	0
All	All	2525/2600 (97%)	-0.19	61 (2%) 59 61	20, 34, 46, 59	0

All (61) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	F	22	ALA	6.5
1	F	21	ALA	6.5
1	F	20	ALA	5.6
1	C	21	ALA	5.5
1	B	21	ALA	5.5
1	E	20	ALA	5.4
1	D	21	ALA	5.3
1	H	33	ALA	5.1
1	B	20	ALA	5.0
1	C	20	ALA	4.6
1	E	19	SER	4.4
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	3.6

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Mol	Chain	Res	Type	RSRZ
1	E	3	ASN	3.4
1	F	89	VAL	3.4
1	B	22	ALA	3.4
1	G	3	ASN	3.3
1	E	206	ARG	3.3
1	A	24	THR	3.2
1	H	288	ALA	3.1
1	F	4	LEU	2.9
1	A	27	THR	2.9
1	B	19	SER	2.8
1	A	22	ALA	2.8
1	C	22	ALA	2.8
1	E	288	ALA	2.7
1	D	31	ALA	2.7
1	E	192	LYS	2.7
1	A	29	TYR	2.7
1	A	21	ALA	2.6
1	H	84	SER	2.6
1	G	213	ASN	2.6
1	B	18	GLY	2.5
1	H	125	THR	2.5
1	A	3	ASN	2.5
1	E	41	GLN	2.4
1	F	90	VAL	2.3
1	F	145	LYS	2.3
1	H	3	ASN	2.3
1	D	4	LEU	2.3
1	G	127	ILE	2.3
1	E	125	THR	2.2
1	H	206	ARG	2.2
1	C	213	ASN	2.2
1	F	3	ASN	2.2
1	C	125	THR	2.2
1	F	46	LEU	2.2
1	H	145	LYS	2.2
1	H	83	ARG	2.2
1	H	306	LEU	2.1
1	H	18	GLY	2.1
1	A	4	LEU	2.1
1	A	206	ARG	2.1
1	G	288	ALA	2.1
1	B	3	ASN	2.1

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Mol	Chain	Res	Type	RSRZ
1	F	19	SER	2.0
1	D	32	GLY	2.0
1	E	89	VAL	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 carbohydrates 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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q < 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å ²)	Q<0.9
2	ASP	F	1328	9/9	0.92	0.21	4.84	53,54,56,56	0
2	ASP	E	1328	9/9	0.87	0.24	3.11	60,62,62,63	0
2	ASP	D	1328	9/9	0.94	0.16	1.64	53,54,55,55	0
2	ASP	G	1328	9/9	0.93	0.18	1.34	48,49,50,50	0
2	ASP	H	1328	9/9	0.91	0.18	1.24	55,56,57,57	0
2	ASP	B	1328	9/9	0.95	0.13	0.15	35,38,38,39	0
2	ASP	C	1328	9/9	0.94	0.11	-0.94	45,45,48,49	0
2	ASP	A	1328	9/9	0.97	0.09	-1.29	34,36,36,36	0

6.5 Other polymers [i](#)

There are no such residues in this entry.