Full wwPDB X-ray Structure Validation Report (i)

Jan 29, 2024 – 08:05 PM EST

PDB ID	:	1FB1
Title	:	CRYSTAL STRUCTURE OF HUMAN GTP CYCLOHYDROLASE I
Authors	:	Auerbach, G.; Herrmann, A.; Bracher, A.; Bader, G.; Gutlich, M.; Fischer, M.; Neukamm, M.; Nar, H.; Garrido-Franco, M.; Richardson, J.; Huber, R.; Bacher, A.
Deposited on	:	2000-07-14
Resolution	:	3.10 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:

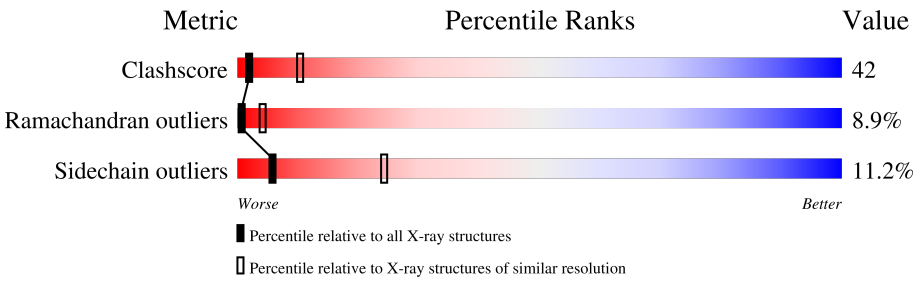
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

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 3.10 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	1184 (3.10-3.10)
Ramachandran outliers	138981	1141 (3.10-3.10)
Sidechain outliers	138945	1141 (3.10-3.10)

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	196	43% 46% 9% •
1	B	196	37% 49% 13% •
1	C	196	38% 48% 13% •
1	D	196	41% 47% 11%
1	E	196	35% 52% 13% •

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	IPA	B	303	-	-	X	-

2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 7750 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.

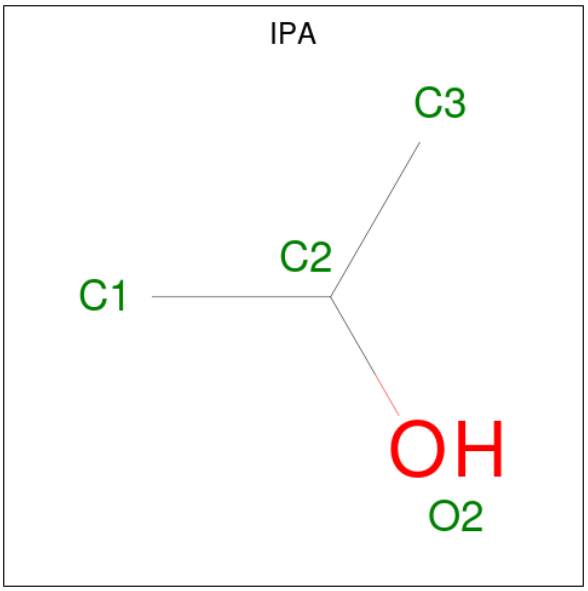
- Molecule 1 is a protein called GTP CYCLOHYDROLASE I.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	196	1545	972	272	290	11	120	0	0
1	B	196	1545	972	272	290	11	119	0	0
1	C	196	1545	972	272	290	11	182	0	0
1	D	196	1545	972	272	290	11	143	0	0
1	E	196	1545	972	272	290	11	119	0	0

- Molecule 2 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Zn		
2	A	1	1	1	0	0
2	B	1	1	1	0	0
2	C	1	1	1	0	0
2	D	1	1	1	0	0
2	E	1	1	1	0	0

- Molecule 3 is ISOPROPYL ALCOHOL (three-letter code: IPA) (formula: C_3H_8O).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	C	O		
3	A	1	4	3	1	0	0
			Total	C	O		
3	B	1	4	3	1	0	0
			Total	C	O		
3	B	1	4	3	1	0	0
			Total	C	O		
3	D	1	4	3	1	0	0
			Total	C	O		
3	D	1	4	3	1	0	0

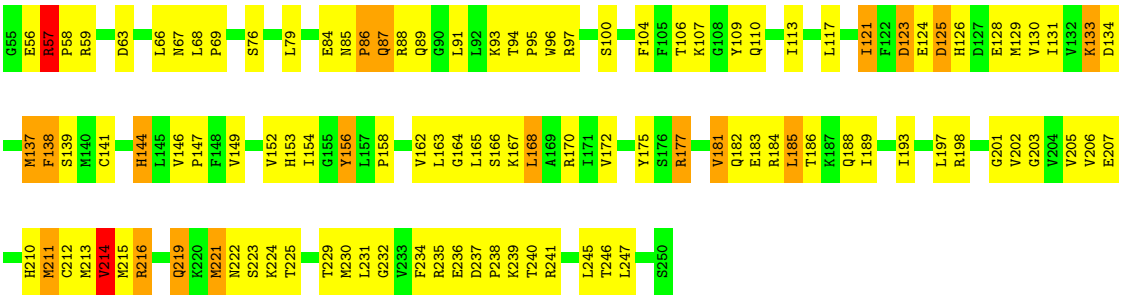
3 Residue-property plots (i)

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.

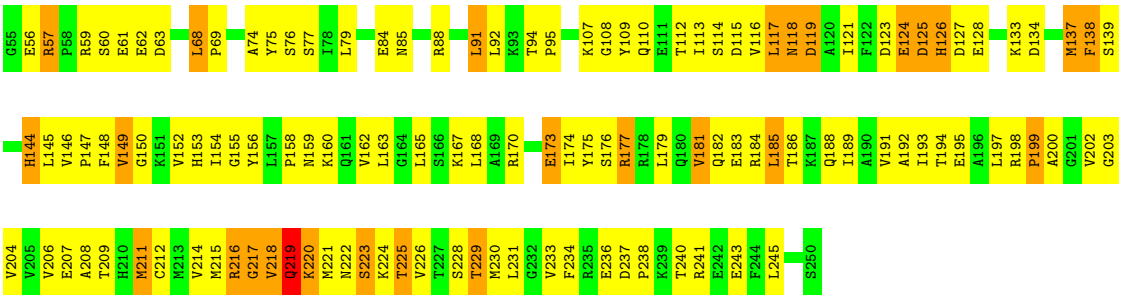
• Molecule 1: GTP CYCLOHYDROLASE I

Chain A: 43% 46% 9%



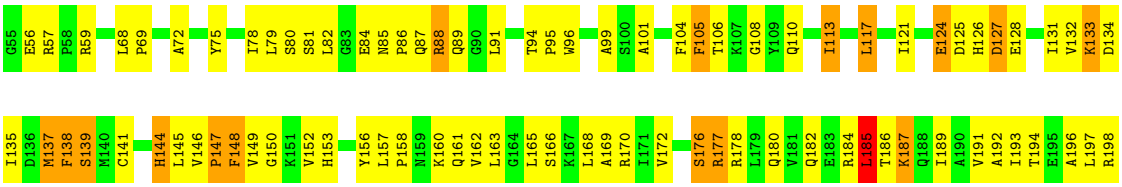
• Molecule 1: GTP CYCLOHYDROLASE I

Chain B: 37% 49% 13%



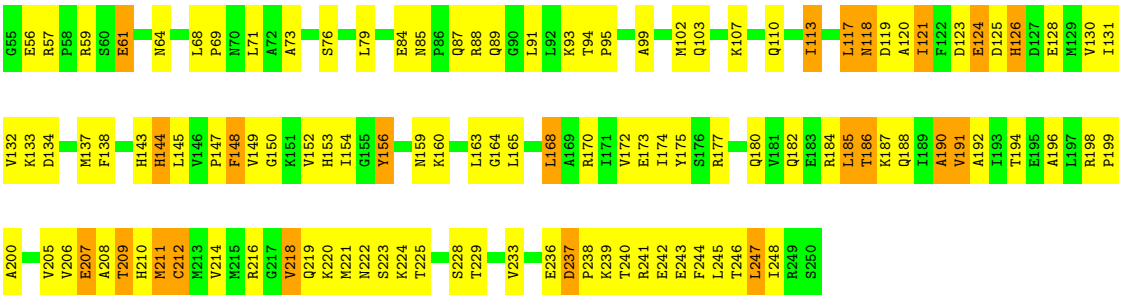
• Molecule 1: GTP CYCLOHYDROLASE I

Chain C: 38% 48% 13%



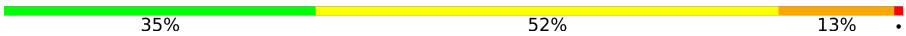
• Molecule 1: GTP CYCLOHYDROLASE I

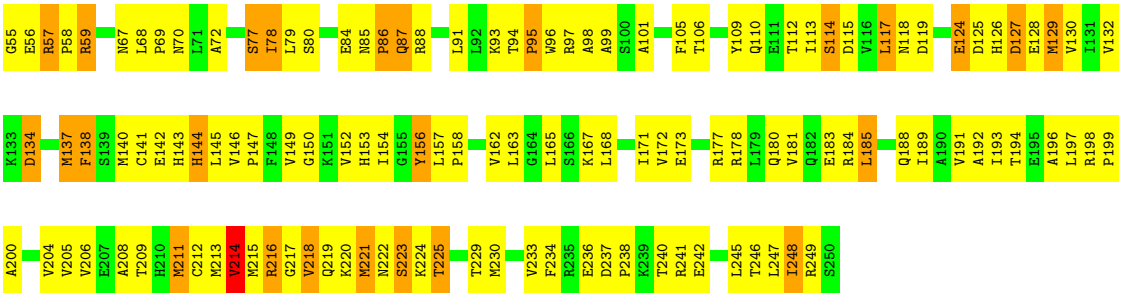
Chain D:



• Molecule 1: GTP CYCLOHYDROLASE I

Chain E:





4 Data and refinement statistics (i)

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

Property	Value	Source
Space group	P 65 2 2	Depositor
Cell constants a, b, c, α, β, γ	115.11Å 115.11Å 387.31Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	14.97 – 3.10	Depositor
% Data completeness (in resolution range)	84.2 (14.97-3.10)	Depositor
R_{merge}	0.17	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	CNS 1.0	Depositor
R, R_{free}	0.204 , 0.293	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	7750	wwPDB-VP
Average B, all atoms (Å^2)	93.0	wwPDB-VP

5 Model quality (i)

5.1 Standard geometry (i)

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

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	0.56	0/1570	0.78	1/2119 (0.0%)
1	B	0.52	0/1570	0.78	0/2119
1	C	0.46	0/1570	0.71	0/2119
1	D	0.48	0/1570	0.77	1/2119 (0.0%)
1	E	0.52	0/1570	0.76	0/2119
All	All	0.51	0/7850	0.76	2/10595 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	181	VAL	N-CA-C	-6.36	93.84	111.00
1	D	148	PHE	N-CA-C	-5.39	96.45	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	1545	0	1565	104	0
1	B	1545	0	1565	142	0
1	C	1545	0	1565	138	0
1	D	1545	0	1565	103	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	E	1545	0	1565	111	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
2	C	1	0	0	0	0
2	D	1	0	0	0	0
2	E	1	0	0	0	0
3	A	4	0	7	1	0
3	B	8	0	15	5	0
3	D	8	0	16	3	0
All	All	7750	0	7863	586	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 42.

All (586) 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:A:211:MET:HA	1:A:214:VAL:HG12	1.33	1.11
1:B:230:MET:HG3	1:B:241:ARG:HD3	1.38	1.05
1:B:113:ILE:H	1:B:113:ILE:HD12	1.20	1.03
1:C:235:ARG:HH11	1:C:235:ARG:HB2	1.24	0.99
1:C:235:ARG:HH11	1:C:235:ARG:CB	1.78	0.96
1:D:61:GLU:HA	1:D:64:ASN:HB2	1.44	0.95
1:A:230:MET:HG3	1:A:241:ARG:HD3	1.51	0.91
1:C:75:TYR:HA	1:C:78:ILE:HG22	1.52	0.91
1:C:165:LEU:HA	1:C:168:LEU:HD12	1.51	0.91
1:B:91:LEU:HD12	1:B:91:LEU:H	1.33	0.91
1:A:165:LEU:HD23	1:E:225:THR:HG21	1.54	0.90
1:A:79:LEU:HD13	1:A:91:LEU:HD23	1.53	0.90
1:B:221:MET:HG2	1:B:222:ASN:H	1.36	0.89
1:B:134:ASP:H	1:B:153:HIS:HD2	1.18	0.89
1:D:212:CYS:O	1:D:216:ARG:HG2	1.73	0.89
1:B:116:VAL:HG11	1:B:170:ARG:HG2	1.56	0.86
1:B:214:VAL:HG23	1:B:221:MET:HA	1.56	0.86
1:B:146:VAL:CG1	1:B:211:MET:HB3	2.04	0.86
1:C:134:ASP:H	1:C:153:HIS:CD2	1.94	0.86
1:D:113:ILE:O	1:D:117:LEU:HD13	1.76	0.85
1:B:84:GLU:HG2	1:B:91:LEU:HD21	1.55	0.85
1:B:85:ASN:HD22	1:B:88:ARG:HG3	1.41	0.84
1:D:211:MET:HA	1:D:214:VAL:HG12	1.60	0.84
1:B:138:PHE:HA	1:B:149:VAL:HG13	1.58	0.83

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:163:LEU:HD11	1:B:167:LYS:HB2	1.58	0.83
1:B:84:GLU:HG3	1:B:85:ASN:H	1.44	0.82
1:B:118:ASN:O	1:B:119:ASP:HB2	1.78	0.81
1:B:79:LEU:HD22	1:B:91:LEU:HD23	1.63	0.81
1:B:84:GLU:HG2	1:B:91:LEU:CD2	2.10	0.81
1:B:134:ASP:H	1:B:153:HIS:CD2	1.98	0.81
1:C:84:GLU:HG2	1:C:91:LEU:HD21	1.60	0.81
1:A:134:ASP:H	1:A:153:HIS:CD2	1.99	0.81
1:B:146:VAL:HG12	1:B:211:MET:HB3	1.62	0.81
1:D:152:VAL:HG22	1:D:206:VAL:HG22	1.63	0.80
1:D:154:ILE:HG21	1:D:168:LEU:CD2	2.12	0.80
1:A:166:SER:H	3:A:306:IPA:H12	1.47	0.79
1:A:222:ASN:O	1:A:224:LYS:N	2.14	0.79
3:B:303:IPA:H12	1:C:166:SER:H	1.46	0.79
1:B:216:ARG:HD3	1:B:217:GLY:N	1.99	0.78
1:A:84:GLU:HG2	1:A:91:LEU:HD21	1.65	0.78
1:E:158:PRO:HB3	1:E:162:VAL:HG22	1.65	0.78
1:A:235:ARG:HG3	1:A:235:ARG:HH11	1.47	0.78
1:C:79:LEU:HD13	1:C:91:LEU:HD23	1.65	0.77
1:E:218:VAL:O	1:E:220:LYS:HG3	1.84	0.77
1:E:79:LEU:HD13	1:E:91:LEU:HD23	1.65	0.77
1:B:234:PHE:O	1:B:241:ARG:HB2	1.85	0.77
1:E:154:ILE:HG23	1:E:204:VAL:HG22	1.65	0.77
1:B:112:THR:O	1:B:115:ASP:HB3	1.85	0.76
1:D:222:ASN:O	1:D:224:LYS:N	2.19	0.75
1:D:154:ILE:HD13	1:D:168:LEU:HD23	1.68	0.75
1:A:230:MET:O	1:A:231:LEU:HD23	1.87	0.75
1:C:214:VAL:O	1:C:219:GLN:HA	1.87	0.75
1:C:138:PHE:HB3	1:C:149:VAL:HG12	1.67	0.75
1:C:158:PRO:HB3	1:C:162:VAL:HG22	1.68	0.75
1:B:200:ALA:O	1:B:233:VAL:HG23	1.87	0.74
1:B:163:LEU:HB3	1:B:197:LEU:HD11	1.68	0.74
1:B:222:ASN:O	1:B:224:LYS:N	2.20	0.74
1:D:121:ILE:HD12	1:D:121:ILE:H	1.52	0.74
1:D:175:TYR:CE1	1:D:188:GLN:HB3	2.23	0.74
1:C:84:GLU:HG2	1:C:91:LEU:CD2	2.18	0.74
1:C:191:VAL:HG12	1:C:192:ALA:N	2.03	0.73
1:A:84:GLU:HG2	1:A:91:LEU:CD2	2.18	0.73
1:D:211:MET:CE	1:D:214:VAL:HG11	2.19	0.73
1:E:185:LEU:O	1:E:185:LEU:HD22	1.89	0.72
1:C:235:ARG:HB2	1:C:235:ARG:NH1	2.01	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:214:VAL:HG22	1:E:221:MET:HA	1.71	0.72
1:A:225:THR:HG21	1:B:165:LEU:HD23	1.72	0.72
1:D:211:MET:HE2	1:D:214:VAL:HG11	1.72	0.72
1:C:124:GLU:O	1:C:126:HIS:N	2.22	0.71
1:C:132:VAL:HG21	1:C:168:LEU:HD13	1.71	0.71
1:A:59:ARG:O	1:A:110:GLN:HB3	1.90	0.71
1:B:113:ILE:H	1:B:113:ILE:CD1	1.98	0.71
1:A:130:VAL:HB	1:A:156:TYR:CE2	2.25	0.71
3:B:303:IPA:C1	1:C:166:SER:H	2.03	0.71
1:C:134:ASP:H	1:C:153:HIS:HD2	1.38	0.70
1:A:211:MET:HA	1:A:214:VAL:CG1	2.18	0.70
1:B:91:LEU:HA	1:B:94:THR:OG1	1.92	0.70
1:B:74:ALA:O	1:B:77:SER:HB3	1.92	0.70
1:B:85:ASN:ND2	1:B:88:ARG:HG3	2.06	0.70
1:C:165:LEU:HD12	1:C:165:LEU:H	1.55	0.70
1:B:156:TYR:CE1	1:B:158:PRO:HG3	2.28	0.69
1:C:72:ALA:HA	1:C:95:PRO:O	1.92	0.69
1:D:209:THR:HG23	1:D:224:LYS:HG2	1.75	0.69
1:D:175:TYR:CD1	1:D:188:GLN:HB3	2.28	0.69
1:D:154:ILE:HG21	1:D:168:LEU:HD22	1.73	0.68
1:B:170:ARG:HG2	1:B:170:ARG:HH11	1.58	0.68
1:D:91:LEU:HD12	1:D:91:LEU:H	1.57	0.68
1:B:218:VAL:HG23	1:B:219:GLN:H	1.59	0.68
1:E:193:ILE:HG23	1:E:197:LEU:HD12	1.75	0.68
1:B:211:MET:HA	1:B:214:VAL:HG12	1.76	0.68
1:E:163:LEU:HD11	1:E:167:LYS:CB	2.24	0.68
1:B:84:GLU:HG3	1:B:85:ASN:N	2.08	0.68
1:B:134:ASP:N	1:B:153:HIS:HD2	1.90	0.67
1:E:93:LYS:O	1:E:97:ARG:HG3	1.94	0.67
1:C:241:ARG:O	1:C:244:PHE:HB3	1.95	0.67
1:E:241:ARG:HG2	1:E:241:ARG:HH11	1.59	0.67
1:E:167:LYS:O	1:E:171:ILE:HG13	1.95	0.67
1:C:80:SER:C	1:C:82:LEU:H	1.97	0.67
1:C:185:LEU:CD2	1:C:189:ILE:HD11	2.25	0.66
1:D:147:PRO:O	1:D:211:MET:HB2	1.96	0.66
1:D:170:ARG:O	1:D:174:ILE:HG13	1.95	0.66
1:A:185:LEU:O	1:A:189:ILE:HG13	1.96	0.66
1:C:95:PRO:O	1:C:99:ALA:HB2	1.96	0.66
1:C:113:ILE:O	1:C:117:LEU:HD13	1.96	0.66
1:D:242:GLU:O	1:D:246:THR:HG23	1.96	0.66
1:C:75:TYR:HA	1:C:78:ILE:CG2	2.24	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:108:GLY:H	1:B:177:ARG:HB3	1.61	0.65
1:D:102:MET:HA	1:D:102:MET:HE2	1.78	0.65
1:D:241:ARG:O	1:D:244:PHE:HB3	1.95	0.65
1:E:242:GLU:O	1:E:246:THR:HG23	1.96	0.65
1:D:107:LYS:O	1:D:110:GLN:HG2	1.96	0.65
1:B:237:ASP:OD2	1:B:240:THR:HG23	1.96	0.65
1:C:185:LEU:HD22	1:C:189:ILE:HD11	1.79	0.65
1:C:238:PRO:HB3	1:C:241:ARG:NH2	2.12	0.65
1:D:236:GLU:O	1:D:238:PRO:HD3	1.97	0.65
1:B:88:ARG:NH1	1:B:91:LEU:HD11	2.12	0.65
1:C:101:ALA:O	1:C:105:PHE:HD1	1.79	0.65
1:D:91:LEU:HA	1:D:94:THR:OG1	1.97	0.65
1:D:134:ASP:H	1:D:153:HIS:CD2	2.14	0.65
1:E:84:GLU:HG3	1:E:85:ASN:H	1.61	0.65
1:A:181:VAL:HG23	1:A:184:ARG:NH2	2.12	0.64
1:B:116:VAL:HG21	1:B:174:ILE:HD11	1.78	0.64
1:B:221:MET:HG2	1:B:222:ASN:N	2.09	0.64
1:B:152:VAL:HG22	1:B:206:VAL:HG22	1.78	0.64
1:D:222:ASN:O	1:D:224:LYS:HG3	1.97	0.64
1:C:185:LEU:O	1:C:189:ILE:HG13	1.97	0.64
1:C:148:PHE:HB2	1:C:210:HIS:HA	1.80	0.64
1:E:124:GLU:O	1:E:126:HIS:N	2.30	0.64
1:E:230:MET:HG3	1:E:241:ARG:HD3	1.79	0.64
1:C:78:ILE:O	1:C:82:LEU:HB2	1.98	0.64
1:A:163:LEU:HD11	1:A:167:LYS:HB2	1.80	0.63
1:A:186:THR:HG22	1:A:229:THR:HG22	1.80	0.63
1:C:211:MET:CE	1:C:214:VAL:HG11	2.28	0.63
1:A:58:PRO:HB3	1:A:110:GLN:HA	1.79	0.63
1:A:79:LEU:HD22	1:A:91:LEU:CD2	2.28	0.63
1:B:137:MET:HE3	1:B:139:SER:HB2	1.80	0.63
1:E:230:MET:HG3	1:E:241:ARG:CD	2.29	0.63
1:A:94:THR:N	1:A:95:PRO:HD2	2.14	0.62
1:E:142:GLU:HG3	1:E:143:HIS:HD2	1.64	0.62
1:A:186:THR:HG22	1:A:229:THR:CG2	2.29	0.62
1:C:218:VAL:HG23	1:C:220:LYS:HG3	1.81	0.62
1:A:107:LYS:O	1:A:110:GLN:HG2	1.98	0.62
1:B:91:LEU:HD12	1:B:91:LEU:N	2.11	0.62
1:D:123:ASP:O	1:D:125:ASP:N	2.31	0.62
1:E:112:THR:HB	1:E:115:ASP:OD1	1.98	0.62
1:C:235:ARG:HH11	1:C:235:ARG:CG	2.13	0.62
1:E:229:THR:HG23	1:E:229:THR:O	1.99	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:221:MET:CG	1:B:222:ASN:H	2.11	0.62
1:C:72:ALA:O	1:C:95:PRO:HB2	1.99	0.62
1:E:209:THR:HG22	1:E:224:LYS:HG2	1.81	0.62
1:E:236:GLU:O	1:E:238:PRO:HD3	2.00	0.61
1:A:133:LYS:HB2	1:A:153:HIS:HD2	1.65	0.61
1:C:101:ALA:O	1:C:104:PHE:HB3	2.00	0.61
1:C:117:LEU:HD21	1:C:196:ALA:CB	2.30	0.61
1:E:150:GLY:HA3	1:E:208:ALA:HA	1.82	0.61
1:A:96:TRP:O	1:A:100:SER:HB2	2.00	0.61
1:D:200:ALA:O	1:D:233:VAL:HG23	2.00	0.61
1:C:186:THR:HG22	1:C:229:THR:HG22	1.82	0.61
1:B:177:ARG:HG3	1:B:177:ARG:HH11	1.66	0.61
1:B:220:LYS:HD2	1:C:169:ALA:HB1	1.81	0.60
1:A:207:GLU:HB2	1:A:224:LYS:HE2	1.82	0.60
1:B:207:GLU:HB2	1:B:224:LYS:HE2	1.84	0.60
1:E:59:ARG:O	1:E:110:GLN:HB3	2.01	0.60
1:E:172:VAL:HG22	1:E:189:ILE:HD13	1.82	0.60
1:C:172:VAL:O	1:C:176:SER:HB3	2.01	0.60
1:B:212:CYS:O	1:B:216:ARG:HG3	2.02	0.60
1:A:211:MET:CE	1:A:214:VAL:HG11	2.32	0.59
1:C:79:LEU:HD22	1:C:91:LEU:CD2	2.32	0.59
1:E:114:SER:O	1:E:117:LEU:HB2	2.01	0.59
1:C:170:ARG:HG2	1:C:170:ARG:HH11	1.66	0.59
1:D:182:GLN:OE1	1:D:208:ALA:HB3	2.01	0.59
1:A:146:VAL:HG12	1:A:147:PRO:HD2	1.84	0.59
1:E:218:VAL:O	1:E:220:LYS:N	2.34	0.59
1:B:156:TYR:OH	1:B:162:VAL:HG13	2.03	0.59
1:C:147:PRO:O	1:C:148:PHE:HB3	2.02	0.59
1:B:116:VAL:CG1	1:B:170:ARG:HG2	2.32	0.59
1:B:229:THR:HG23	1:B:229:THR:O	2.02	0.59
1:C:117:LEU:HD21	1:C:196:ALA:HB1	1.84	0.59
1:B:123:ASP:O	1:B:125:ASP:N	2.35	0.59
1:A:93:LYS:O	1:A:97:ARG:HG3	2.03	0.58
1:D:154:ILE:HD13	1:D:168:LEU:CD2	2.32	0.58
1:B:234:PHE:O	1:B:241:ARG:NE	2.37	0.58
1:E:214:VAL:CG2	1:E:221:MET:HA	2.33	0.58
1:B:126:HIS:CD2	1:B:128:GLU:HB2	2.39	0.58
1:D:118:ASN:O	1:D:120:ALA:N	2.37	0.58
1:E:68:LEU:N	1:E:69:PRO:HD2	2.18	0.58
1:B:163:LEU:CB	1:B:197:LEU:HD11	2.33	0.58
1:B:163:LEU:HD23	1:B:168:LEU:HG	1.84	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:130:VAL:HB	1:E:156:TYR:CE2	2.39	0.58
1:B:221:MET:CG	1:B:222:ASN:N	2.66	0.57
1:C:191:VAL:CG1	1:C:192:ALA:N	2.66	0.57
1:D:94:THR:N	1:D:95:PRO:HD2	2.19	0.57
1:E:144:HIS:HB2	1:E:146:VAL:HG23	1.86	0.57
1:A:79:LEU:O	1:A:84:GLU:HB3	2.04	0.57
1:A:79:LEU:HD22	1:A:91:LEU:HD21	1.86	0.57
1:A:177:ARG:HG3	1:A:177:ARG:HH11	1.68	0.57
1:B:146:VAL:HG11	1:B:211:MET:HB3	1.84	0.57
1:C:79:LEU:HD13	1:C:86:PRO:HB3	1.86	0.57
1:C:139:SER:HB3	1:C:148:PHE:CE2	2.40	0.57
1:E:58:PRO:HB3	1:E:110:GLN:HA	1.87	0.57
1:C:160:LYS:C	1:C:161:GLN:HG3	2.24	0.57
1:D:233:VAL:HG12	1:D:237:ASP:HB3	1.87	0.57
1:E:137:MET:HG2	1:E:138:PHE:N	2.19	0.57
1:B:88:ARG:O	1:B:92:LEU:HB2	2.05	0.57
1:B:158:PRO:HB3	1:B:162:VAL:HG22	1.87	0.56
1:D:91:LEU:HD12	1:D:91:LEU:N	2.20	0.56
1:B:113:ILE:HD12	1:B:113:ILE:N	2.06	0.56
1:B:116:VAL:HG11	1:B:170:ARG:CG	2.32	0.56
1:B:163:LEU:HB2	1:B:197:LEU:HD21	1.87	0.56
1:C:186:THR:HG22	1:C:229:THR:CG2	2.35	0.56
1:D:237:ASP:O	1:D:240:THR:HB	2.04	0.56
1:E:132:VAL:HG21	1:E:168:LEU:HD13	1.86	0.56
1:C:235:ARG:HG2	1:C:236:GLU:HG3	1.86	0.56
1:D:159:ASN:HB2	1:D:199:PRO:HA	1.88	0.56
1:A:163:LEU:HG	1:A:164:GLY:O	2.06	0.56
1:E:245:LEU:O	1:E:249:ARG:HD2	2.06	0.56
1:C:163:LEU:CB	1:C:197:LEU:HD11	2.36	0.56
1:E:183:GLU:OE2	1:E:183:GLU:N	2.35	0.55
1:C:202:VAL:HG12	1:C:203:GLY:N	2.21	0.55
1:A:213:MET:O	1:A:215:MET:N	2.39	0.55
1:C:203:GLY:HA3	1:C:234:PHE:CD2	2.42	0.55
1:D:93:LYS:C	1:D:95:PRO:HD2	2.27	0.55
1:A:221:MET:SD	1:A:222:ASN:N	2.76	0.55
1:A:146:VAL:HG12	1:A:147:PRO:CD	2.36	0.55
1:A:163:LEU:HD23	1:A:168:LEU:HG	1.88	0.55
1:A:186:THR:CG2	1:A:229:THR:HG22	2.37	0.55
1:B:113:ILE:O	1:B:117:LEU:HD13	2.07	0.55
1:A:156:TYR:OH	1:A:162:VAL:HG13	2.06	0.54
1:D:79:LEU:HD13	1:D:91:LEU:HD23	1.89	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:95:PRO:O	1:E:99:ALA:HB2	2.07	0.54
1:A:181:VAL:HG12	1:A:183:GLU:OE2	2.07	0.54
1:D:218:VAL:O	1:D:220:LYS:HD2	2.07	0.54
1:B:84:GLU:CD	1:B:88:ARG:HH11	2.10	0.54
1:D:180:GLN:OE1	1:D:184:ARG:HD2	2.07	0.54
1:A:184:ARG:O	1:A:188:GLN:HG3	2.07	0.54
1:B:79:LEU:HD13	1:B:91:LEU:HB3	1.89	0.54
1:C:163:LEU:HB2	1:C:197:LEU:HD11	1.90	0.54
1:B:221:MET:C	1:B:223:SER:H	2.10	0.54
1:C:222:ASN:O	1:C:224:LYS:N	2.41	0.54
1:C:144:HIS:HB2	1:C:146:VAL:HG23	1.88	0.54
1:E:72:ALA:HA	1:E:95:PRO:O	2.08	0.54
1:D:186:THR:HG22	1:D:229:THR:HG22	1.90	0.54
1:E:84:GLU:HG2	1:E:91:LEU:CD2	2.38	0.54
1:C:84:GLU:HG3	1:C:85:ASN:N	2.22	0.54
1:D:229:THR:O	1:D:229:THR:HG23	2.08	0.54
1:A:144:HIS:O	1:A:146:VAL:HG23	2.07	0.53
1:B:107:LYS:O	1:B:110:GLN:HG2	2.08	0.53
1:C:79:LEU:CD1	1:C:91:LEU:HD23	2.37	0.53
1:C:202:VAL:CG1	1:C:203:GLY:N	2.71	0.53
1:E:109:TYR:CE2	1:E:178:ARG:HB3	2.43	0.53
1:A:79:LEU:CD1	1:A:91:LEU:HD23	2.35	0.53
1:C:212:CYS:O	1:C:216:ARG:HG3	2.08	0.53
1:E:113:ILE:O	1:E:117:LEU:HD13	2.09	0.53
1:B:214:VAL:HG23	1:B:221:MET:CA	2.34	0.53
1:A:237:ASP:OD1	1:A:237:ASP:C	2.47	0.53
1:B:163:LEU:CD2	1:B:168:LEU:HG	2.39	0.53
1:D:149:VAL:HG12	1:D:150:GLY:N	2.22	0.53
1:A:84:GLU:O	1:A:86:PRO:HD3	2.08	0.53
1:B:154:ILE:HG23	1:B:204:VAL:HG22	1.89	0.53
1:B:218:VAL:HG23	1:B:219:GLN:N	2.22	0.53
1:C:160:LYS:O	1:C:161:GLN:HG3	2.09	0.53
1:A:235:ARG:HG3	1:A:235:ARG:NH1	2.17	0.53
1:D:143:HIS:ND1	3:D:305:IPA:H31	2.24	0.53
1:B:127:ASP:O	1:B:128:GLU:HG2	2.09	0.53
1:D:117:LEU:O	1:D:118:ASN:CB	2.57	0.53
1:E:105:PHE:H	1:E:105:PHE:HD1	1.57	0.53
1:E:147:PRO:O	1:E:211:MET:HB2	2.07	0.53
1:B:238:PRO:HA	1:B:241:ARG:NH2	2.23	0.52
1:B:186:THR:HG22	1:B:229:THR:CG2	2.40	0.52
1:D:191:VAL:O	1:D:192:ALA:C	2.47	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:58:PRO:O	1:E:59:ARG:C	2.48	0.52
1:C:108:GLY:O	1:C:178:ARG:NH2	2.38	0.52
1:B:91:LEU:H	1:B:91:LEU:CD1	2.10	0.52
1:E:163:LEU:HB2	1:E:197:LEU:HD21	1.92	0.52
1:A:58:PRO:HB3	1:A:109:TYR:O	2.10	0.52
1:E:79:LEU:HD22	1:E:91:LEU:HD21	1.91	0.52
1:B:88:ARG:CZ	1:B:91:LEU:HD11	2.38	0.52
1:A:79:LEU:HD22	1:A:91:LEU:HD23	1.92	0.52
1:C:211:MET:HE3	1:C:214:VAL:HG11	1.92	0.52
1:D:132:VAL:HG21	1:D:168:LEU:HD13	1.92	0.52
1:D:187:LYS:HA	1:D:229:THR:HG21	1.93	0.51
1:E:163:LEU:HB2	1:E:197:LEU:HD11	1.92	0.51
1:B:198:ARG:N	1:B:199:PRO:HD3	2.25	0.51
1:E:142:GLU:HG3	1:E:143:HIS:CD2	2.45	0.51
1:E:248:ILE:C	1:E:249:ARG:HG3	2.30	0.51
1:E:118:ASN:O	1:E:119:ASP:HB2	2.11	0.51
1:E:200:ALA:O	1:E:233:VAL:HG23	2.10	0.51
1:D:225:THR:HG21	1:E:165:LEU:HD23	1.92	0.51
1:E:129:MET:HA	1:E:156:TYR:O	2.10	0.51
1:C:79:LEU:HB3	1:C:86:PRO:HB3	1.91	0.51
1:B:181:VAL:O	1:B:182:GLN:C	2.49	0.51
1:B:185:LEU:CD2	1:B:189:ILE:HD11	2.41	0.51
1:C:79:LEU:HD22	1:C:91:LEU:HD23	1.93	0.51
1:C:230:MET:O	1:C:235:ARG:NH1	2.44	0.50
1:D:198:ARG:N	1:D:199:PRO:CD	2.74	0.50
1:B:177:ARG:HG3	1:B:177:ARG:NH1	2.25	0.50
1:A:107:LYS:C	1:A:109:TYR:H	2.15	0.50
1:B:218:VAL:HG23	1:B:220:LYS:H	1.77	0.50
1:D:239:LYS:O	1:D:243:GLU:HB3	2.11	0.50
1:B:218:VAL:CG2	1:B:219:GLN:H	2.20	0.50
1:C:141:CYS:O	1:C:145:LEU:N	2.39	0.50
1:C:186:THR:CG2	1:C:229:THR:HG22	2.41	0.50
1:D:85:ASN:OD1	1:D:87:GLN:HB2	2.11	0.50
1:E:241:ARG:HG2	1:E:241:ARG:NH1	2.24	0.50
1:B:84:GLU:HG2	1:B:91:LEU:HD22	1.92	0.50
1:A:181:VAL:CG2	1:A:184:ARG:NH2	2.74	0.50
1:C:146:VAL:HB	1:C:212:CYS:SG	2.51	0.50
1:A:211:MET:HE3	1:A:214:VAL:HG11	1.93	0.50
1:D:211:MET:HE3	1:D:214:VAL:HG11	1.91	0.50
1:E:94:THR:O	1:E:96:TRP:N	2.45	0.50
1:B:216:ARG:O	1:B:218:VAL:N	2.45	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:144:HIS:O	1:A:146:VAL:CG2	2.60	0.49
1:E:146:VAL:HG12	1:E:211:MET:HB3	1.95	0.49
1:B:170:ARG:HG2	1:B:170:ARG:NH1	2.24	0.49
1:C:94:THR:N	1:C:95:PRO:HD2	2.27	0.49
1:C:225:THR:HA	1:D:131:ILE:O	2.11	0.49
1:E:84:GLU:HG2	1:E:91:LEU:HD21	1.94	0.49
1:C:80:SER:C	1:C:82:LEU:N	2.65	0.49
1:C:184:ARG:O	1:C:186:THR:N	2.45	0.49
1:D:180:GLN:HE22	1:D:185:LEU:HA	1.78	0.49
1:E:163:LEU:HD11	1:E:167:LYS:HB2	1.92	0.49
1:A:123:ASP:O	1:A:125:ASP:N	2.46	0.49
1:A:163:LEU:HD11	1:A:167:LYS:CB	2.42	0.49
1:A:245:LEU:C	1:A:247:LEU:H	2.16	0.49
1:C:79:LEU:HD22	1:C:91:LEU:HD21	1.93	0.49
1:C:157:LEU:HB2	1:C:200:ALA:HB3	1.94	0.49
1:A:107:LYS:C	1:A:109:TYR:N	2.64	0.49
1:C:185:LEU:HD22	1:C:189:ILE:CD1	2.42	0.48
1:C:79:LEU:CD1	1:C:86:PRO:HB3	2.43	0.48
1:D:121:ILE:H	1:D:121:ILE:CD1	2.23	0.48
1:A:104:PHE:C	1:A:106:THR:H	2.15	0.48
1:D:84:GLU:HG3	1:D:85:ASN:H	1.78	0.48
1:B:60:SER:O	1:B:62:GLU:N	2.47	0.48
1:C:235:ARG:NH1	1:C:235:ARG:CG	2.74	0.48
1:B:163:LEU:HD23	1:B:168:LEU:CD2	2.43	0.48
1:E:229:THR:O	1:E:229:THR:CG2	2.61	0.48
1:A:66:LEU:O	1:A:69:PRO:HD2	2.14	0.48
1:A:158:PRO:HB3	1:A:162:VAL:HG22	1.96	0.48
1:E:79:LEU:HD13	1:E:91:LEU:CD2	2.41	0.48
1:C:149:VAL:O	1:C:208:ALA:HB1	2.14	0.48
1:D:124:GLU:HA	1:D:160:LYS:C	2.33	0.48
1:B:191:VAL:HG12	1:B:192:ALA:N	2.26	0.48
1:C:191:VAL:O	1:C:192:ALA:C	2.52	0.48
1:E:184:ARG:O	1:E:188:GLN:HG3	2.13	0.48
1:A:211:MET:CA	1:A:214:VAL:HG12	2.23	0.48
1:B:59:ARG:O	1:B:110:GLN:HB3	2.14	0.48
1:B:241:ARG:HG2	1:B:241:ARG:HH11	1.79	0.48
1:D:102:MET:HA	1:D:102:MET:CE	2.43	0.48
1:E:67:ASN:O	1:E:68:LEU:C	2.52	0.48
1:E:105:PHE:N	1:E:105:PHE:CD1	2.81	0.48
1:C:211:MET:HE2	1:C:214:VAL:HG11	1.94	0.48
1:B:134:ASP:N	1:B:153:HIS:CD2	2.72	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:190:ALA:HB2	1:D:229:THR:HG23	1.96	0.47
1:C:87:GLN:O	1:C:88:ARG:O	2.33	0.47
1:D:133:LYS:HB2	1:D:153:HIS:HD2	1.79	0.47
1:D:233:VAL:O	1:D:237:ASP:N	2.47	0.47
1:E:224:LYS:HB3	1:E:224:LYS:HE2	1.54	0.47
1:C:152:VAL:HG22	1:C:206:VAL:HG22	1.95	0.47
1:D:228:SER:O	1:E:128:GLU:HB3	2.14	0.47
1:C:233:VAL:O	1:C:237:ASP:N	2.42	0.47
1:E:238:PRO:HA	1:E:241:ARG:HB3	1.96	0.47
1:C:79:LEU:HD23	1:C:79:LEU:HA	1.77	0.47
1:E:213:MET:O	1:E:215:MET:N	2.48	0.47
1:A:68:LEU:N	1:A:69:PRO:HD2	2.29	0.47
1:A:237:ASP:OD1	1:A:239:LYS:N	2.46	0.47
1:C:132:VAL:HG12	1:C:135:ILE:HD11	1.97	0.47
1:C:185:LEU:CD2	1:C:185:LEU:O	2.63	0.47
1:E:157:LEU:HB2	1:E:200:ALA:HB3	1.96	0.47
1:A:212:CYS:O	1:A:216:ARG:HG3	2.14	0.47
1:C:211:MET:HA	1:C:214:VAL:HG12	1.97	0.47
1:E:180:GLN:OE1	1:E:184:ARG:HD2	2.15	0.47
1:A:230:MET:HE3	1:A:241:ARG:HG2	1.95	0.47
1:C:191:VAL:HG12	1:C:192:ALA:H	1.76	0.47
1:B:124:GLU:N	1:B:160:LYS:O	2.47	0.46
1:B:173:GLU:HA	1:B:176:SER:HG	1.80	0.46
1:D:79:LEU:HD13	1:D:91:LEU:CD2	2.44	0.46
1:E:77:SER:O	1:E:80:SER:N	2.46	0.46
1:C:221:MET:C	1:C:223:SER:H	2.19	0.46
1:E:67:ASN:O	1:E:70:ASN:N	2.48	0.46
1:A:211:MET:HE2	1:A:214:VAL:HG11	1.98	0.46
1:D:84:GLU:CD	1:D:88:ARG:NH1	2.68	0.46
1:A:156:TYR:HA	1:A:201:GLY:O	2.15	0.46
1:B:185:LEU:HD23	1:B:185:LEU:O	2.15	0.46
1:C:88:ARG:HD3	1:C:91:LEU:HD13	1.96	0.46
1:C:180:GLN:HE22	1:C:185:LEU:HA	1.81	0.46
1:B:159:ASN:HB2	1:B:199:PRO:HA	1.96	0.46
1:B:191:VAL:O	1:B:195:GLU:HG3	2.15	0.46
1:C:80:SER:O	1:C:82:LEU:N	2.49	0.46
1:C:150:GLY:HA3	1:C:208:ALA:HB2	1.98	0.46
1:C:233:VAL:CG1	1:C:237:ASP:HB3	2.46	0.46
1:C:233:VAL:HG12	1:C:237:ASP:HB3	1.96	0.46
1:E:163:LEU:HD11	1:E:167:LYS:HB3	1.98	0.46
1:A:214:VAL:HG23	1:A:221:MET:HA	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:116:VAL:O	1:B:117:LEU:O	2.33	0.46
1:D:79:LEU:CD1	1:D:91:LEU:HD23	2.46	0.46
1:C:104:PHE:HE2	1:C:177:ARG:NH2	2.13	0.46
1:C:200:ALA:O	1:C:233:VAL:HG23	2.16	0.46
1:E:129:MET:HE1	1:E:234:PHE:CZ	2.50	0.46
1:E:191:VAL:HG12	1:E:192:ALA:N	2.30	0.46
1:B:230:MET:HB3	1:B:234:PHE:CB	2.45	0.46
1:A:84:GLU:HG3	1:A:85:ASN:N	2.31	0.45
1:A:85:ASN:O	1:A:87:GLN:N	2.49	0.45
1:A:203:GLY:HA3	1:A:234:PHE:CD2	2.52	0.45
1:B:186:THR:HG22	1:B:229:THR:HG22	1.98	0.45
1:B:124:GLU:CA	1:B:160:LYS:O	2.63	0.45
1:C:101:ALA:O	1:C:105:PHE:CD1	2.64	0.45
1:A:229:THR:HG23	1:A:229:THR:O	2.16	0.45
1:C:96:TRP:O	1:C:99:ALA:HB3	2.16	0.45
1:D:156:TYR:H	1:D:156:TYR:HD2	1.64	0.45
1:D:163:LEU:HG	1:D:164:GLY:N	2.30	0.45
1:D:170:ARG:C	1:D:172:VAL:N	2.70	0.45
1:D:173:GLU:O	1:D:177:ARG:HB2	2.16	0.45
1:E:127:ASP:HA	1:E:158:PRO:O	2.16	0.45
1:B:211:MET:O	1:B:215:MET:HB2	2.16	0.45
1:C:194:THR:HA	1:C:199:PRO:CD	2.47	0.45
1:B:206:VAL:O	1:B:226:VAL:HA	2.16	0.45
1:D:190:ALA:HB2	1:D:229:THR:CG2	2.46	0.45
1:E:180:GLN:HA	1:E:184:ARG:NH1	2.32	0.45
1:B:182:GLN:O	1:B:183:GLU:C	2.56	0.45
3:B:303:IPA:H11	1:C:165:LEU:HB2	1.99	0.45
1:E:117:LEU:HD21	1:E:196:ALA:CB	2.47	0.45
1:C:184:ARG:C	1:C:186:THR:N	2.70	0.44
1:D:153:HIS:HE1	1:D:207:GLU:OE2	2.00	0.44
1:D:165:LEU:HB2	3:D:304:IPA:H13	1.98	0.44
1:C:126:HIS:O	1:C:128:GLU:N	2.50	0.44
1:D:191:VAL:O	1:D:194:THR:N	2.50	0.44
1:B:60:SER:C	1:B:62:GLU:H	2.20	0.44
1:B:68:LEU:N	1:B:69:PRO:HD2	2.33	0.44
1:C:78:ILE:O	1:C:78:ILE:HG12	2.18	0.44
1:C:96:TRP:HA	1:C:99:ALA:CB	2.47	0.44
1:D:152:VAL:HG12	1:D:153:HIS:N	2.32	0.44
1:B:165:LEU:HD12	1:B:165:LEU:H	1.81	0.44
1:E:197:LEU:O	1:E:198:ARG:C	2.55	0.44
1:B:149:VAL:HG12	1:B:150:GLY:N	2.33	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:225:THR:HG21	1:C:165:LEU:CD2	2.48	0.44
1:B:230:MET:O	1:B:231:LEU:HD23	2.17	0.44
1:C:185:LEU:O	1:C:185:LEU:HD23	2.18	0.44
1:D:126:HIS:CD2	1:D:128:GLU:HB2	2.53	0.44
1:B:191:VAL:C	1:B:193:ILE:N	2.71	0.44
1:E:101:ALA:O	1:E:105:PHE:HD1	1.99	0.44
1:B:207:GLU:HA	1:B:225:THR:O	2.18	0.44
1:A:153:HIS:C	1:A:154:ILE:HG13	2.37	0.44
1:B:181:VAL:HG12	1:B:183:GLU:OE2	2.17	0.44
1:E:84:GLU:HG3	1:E:85:ASN:N	2.30	0.44
1:E:98:ALA:O	1:E:99:ALA:C	2.56	0.44
1:A:128:GLU:OE1	1:E:229:THR:HA	2.18	0.44
1:C:186:THR:O	1:C:187:LYS:C	2.56	0.44
1:B:113:ILE:HG12	1:B:175:TYR:OH	2.18	0.43
1:C:131:ILE:HG21	1:C:248:ILE:HG22	2.00	0.43
1:D:79:LEU:HD22	1:D:91:LEU:HD23	2.00	0.43
1:D:117:LEU:HD21	1:D:196:ALA:HB2	2.00	0.43
1:A:131:ILE:O	1:E:225:THR:HA	2.18	0.43
1:A:152:VAL:HG22	1:A:206:VAL:HG22	2.01	0.43
1:A:197:LEU:O	1:A:198:ARG:C	2.55	0.43
1:D:79:LEU:HD23	1:D:79:LEU:HA	1.75	0.43
1:D:209:THR:CG2	1:D:224:LYS:HG2	2.46	0.43
1:E:84:GLU:CG	1:E:91:LEU:HD22	2.48	0.43
1:E:129:MET:CE	1:E:234:PHE:CZ	3.01	0.43
1:E:156:TYR:N	1:E:156:TYR:CD2	2.86	0.43
1:E:247:LEU:HA	1:E:247:LEU:HD12	1.71	0.43
1:B:68:LEU:HB3	1:B:69:PRO:CD	2.48	0.43
1:D:143:HIS:ND1	3:D:305:IPA:C3	2.82	0.43
1:E:221:MET:C	1:E:223:SER:H	2.22	0.43
1:B:127:ASP:C	1:B:128:GLU:HG2	2.39	0.43
1:B:198:ARG:N	1:B:199:PRO:CD	2.81	0.43
1:C:72:ALA:HB1	1:C:96:TRP:CE2	2.53	0.43
1:C:182:GLN:HG2	1:C:227:THR:OG1	2.19	0.43
1:C:245:LEU:HD13	1:D:247:LEU:CD1	2.48	0.43
1:E:59:ARG:NH1	1:E:106:THR:O	2.48	0.43
1:D:88:ARG:CZ	1:D:91:LEU:HD11	2.49	0.43
1:A:182:GLN:NE2	1:A:206:VAL:O	2.52	0.43
1:B:173:GLU:HA	1:B:176:SER:OG	2.18	0.43
1:E:142:GLU:CD	1:E:181:VAL:HG23	2.39	0.43
1:E:185:LEU:HD22	1:E:185:LEU:C	2.39	0.43
1:D:84:GLU:HG3	1:D:85:ASN:N	2.33	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:99:ALA:O	1:D:103:GLN:HG3	2.17	0.43
1:E:247:LEU:C	1:E:249:ARG:H	2.22	0.43
1:E:212:CYS:O	1:E:216:ARG:HG2	2.19	0.43
1:A:177:ARG:HG3	1:A:177:ARG:NH1	2.33	0.43
1:A:222:ASN:O	1:A:224:LYS:HB2	2.19	0.43
1:B:118:ASN:O	1:B:119:ASP:CB	2.59	0.43
1:C:182:GLN:NE2	1:C:225:THR:O	2.45	0.43
1:A:231:LEU:HA	1:A:235:ARG:HD2	2.00	0.42
1:A:104:PHE:C	1:A:106:THR:N	2.72	0.42
1:A:141:CYS:HB3	1:A:146:VAL:O	2.19	0.42
1:C:172:VAL:HG13	1:C:189:ILE:HD13	2.00	0.42
1:C:191:VAL:O	1:C:194:THR:N	2.50	0.42
1:E:58:PRO:CB	1:E:110:GLN:HA	2.48	0.42
1:A:104:PHE:HE2	1:A:177:ARG:NH2	2.16	0.42
1:A:137:MET:HE3	1:A:139:SER:N	2.34	0.42
1:B:202:VAL:CG1	1:B:203:GLY:N	2.83	0.42
1:C:68:LEU:HD12	1:C:99:ALA:HB1	2.01	0.42
1:C:133:LYS:CB	1:C:153:HIS:HD2	2.32	0.42
1:D:144:HIS:O	1:D:145:LEU:HB2	2.20	0.42
1:E:233:VAL:O	1:E:237:ASP:N	2.53	0.42
1:A:193:ILE:HG22	1:A:202:VAL:HG21	2.00	0.42
1:A:232:GLY:O	1:A:235:ARG:N	2.53	0.42
1:B:107:LYS:C	1:B:109:TYR:N	2.72	0.42
1:B:145:LEU:CD2	1:B:179:LEU:HD22	2.49	0.42
1:C:165:LEU:H	1:C:165:LEU:CD1	2.28	0.42
1:C:211:MET:HA	1:C:214:VAL:CG1	2.49	0.42
1:B:230:MET:HB3	1:B:234:PHE:HB3	2.02	0.42
1:D:233:VAL:CG1	1:D:237:ASP:HB3	2.49	0.42
1:E:152:VAL:HG13	1:E:206:VAL:HG22	2.00	0.42
1:C:163:LEU:HB3	1:C:197:LEU:HD11	2.02	0.42
1:D:68:LEU:O	1:D:71:LEU:N	2.52	0.42
1:D:134:ASP:H	1:D:153:HIS:HD2	1.63	0.42
1:E:150:GLY:HA3	1:E:208:ALA:CA	2.50	0.42
1:A:210:HIS:CD2	1:A:210:HIS:N	2.87	0.42
1:A:238:PRO:HB3	1:A:241:ARG:HH22	1.85	0.42
1:B:146:VAL:HG13	1:B:147:PRO:HD2	2.02	0.42
1:B:202:VAL:HG12	1:B:203:GLY:N	2.35	0.42
1:A:134:ASP:H	1:A:153:HIS:HD2	1.57	0.42
1:C:133:LYS:H	1:C:133:LYS:HG3	1.63	0.42
1:C:214:VAL:CG1	1:C:215:MET:N	2.83	0.42
1:D:190:ALA:O	1:D:191:VAL:C	2.59	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:77:SER:O	1:E:78:ILE:C	2.58	0.42
1:B:116:VAL:CG2	1:B:174:ILE:HD11	2.49	0.42
1:C:180:GLN:NE2	1:C:185:LEU:HA	2.34	0.42
1:C:240:THR:HG22	1:C:241:ARG:N	2.33	0.42
1:D:152:VAL:HG22	1:D:206:VAL:CG2	2.40	0.42
1:E:173:GLU:O	1:E:173:GLU:HG3	2.20	0.42
1:D:236:GLU:O	1:D:238:PRO:CD	2.67	0.41
1:E:140:MET:HE3	1:E:145:LEU:HA	2.01	0.41
1:A:121:ILE:HD12	1:A:121:ILE:H	1.84	0.41
1:D:117:LEU:O	1:D:118:ASN:HB3	2.20	0.41
1:D:180:GLN:NE2	1:D:185:LEU:HA	2.34	0.41
1:A:57:ARG:HA	1:A:58:PRO:HD3	1.75	0.41
1:B:84:GLU:CG	1:B:85:ASN:H	2.24	0.41
1:C:197:LEU:O	1:C:198:ARG:C	2.57	0.41
1:E:55:GLY:O	1:E:56:GLU:HB2	2.20	0.41
1:A:237:ASP:HA	1:A:238:PRO:HD2	1.93	0.41
1:B:75:TYR:O	1:B:76:SER:C	2.57	0.41
1:B:184:ARG:HG2	1:B:188:GLN:OE1	2.20	0.41
1:A:63:ASP:O	1:A:67:ASN:ND2	2.53	0.41
1:A:165:LEU:HD12	1:A:165:LEU:N	2.35	0.41
1:B:186:THR:HG22	1:B:229:THR:HG21	2.03	0.41
1:D:130:VAL:HB	1:D:156:TYR:CE2	2.55	0.41
1:E:86:PRO:HA	1:E:91:LEU:HB3	2.03	0.41
1:B:94:THR:N	1:B:95:PRO:HD2	2.35	0.41
1:B:113:ILE:CD1	1:B:113:ILE:N	2.75	0.41
1:C:104:PHE:C	1:C:106:THR:H	2.24	0.41
1:E:222:ASN:O	1:E:224:LYS:N	2.54	0.41
1:A:94:THR:N	1:A:95:PRO:CD	2.83	0.41
1:A:138:PHE:HA	1:A:149:VAL:HG13	2.02	0.41
1:A:168:LEU:O	1:A:172:VAL:HG23	2.21	0.41
1:B:221:MET:C	1:B:223:SER:N	2.73	0.41
1:C:105:PHE:HD1	1:C:105:PHE:H	1.68	0.41
1:D:73:ALA:O	1:D:76:SER:HB3	2.20	0.41
1:E:134:ASP:H	1:E:153:HIS:CD2	2.38	0.41
1:A:85:ASN:OD1	1:A:87:GLN:HB2	2.21	0.41
1:B:137:MET:O	1:B:149:VAL:CG1	2.69	0.41
1:D:94:THR:N	1:D:95:PRO:CD	2.82	0.41
1:E:191:VAL:O	1:E:194:THR:N	2.53	0.41
1:A:167:LYS:O	1:A:170:ARG:HB3	2.20	0.41
1:B:116:VAL:O	1:B:116:VAL:HG12	2.20	0.41
1:C:137:MET:CE	1:C:139:SER:HB2	2.50	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:156:TYR:CE1	1:C:158:PRO:HG3	2.56	0.41
1:D:68:LEU:HB3	1:D:69:PRO:CD	2.51	0.41
1:E:141:CYS:O	1:E:145:LEU:HA	2.21	0.41
1:E:158:PRO:HB3	1:E:162:VAL:CG2	2.42	0.41
1:A:84:GLU:HG2	1:A:91:LEU:HD22	1.96	0.41
1:A:88:ARG:HD3	1:A:91:LEU:HD13	2.02	0.41
1:B:225:THR:HG21	1:C:165:LEU:HD23	2.03	0.40
1:D:84:GLU:OE2	1:D:88:ARG:NH1	2.49	0.40
1:D:148:PHE:HB2	1:D:210:HIS:HA	2.02	0.40
1:A:113:ILE:HG21	1:A:175:TYR:OH	2.21	0.40
1:B:84:GLU:CG	1:B:91:LEU:HD22	2.51	0.40
1:B:191:VAL:O	1:B:193:ILE:N	2.54	0.40
1:C:68:LEU:N	1:C:69:PRO:CD	2.85	0.40
1:C:138:PHE:CD1	1:C:138:PHE:N	2.87	0.40
1:C:191:VAL:O	1:C:193:ILE:N	2.54	0.40
1:E:68:LEU:N	1:E:69:PRO:CD	2.85	0.40
1:E:245:LEU:HA	1:E:248:ILE:HG12	2.02	0.40
1:B:154:ILE:HG22	1:B:155:GLY:N	2.36	0.40
1:B:165:LEU:HD12	1:B:165:LEU:N	2.36	0.40
3:B:303:IPA:H13	1:C:166:SER:OG	2.22	0.40
1:C:235:ARG:HG2	1:C:236:GLU:N	2.36	0.40
1:C:245:LEU:HD13	1:D:247:LEU:HD11	2.03	0.40
1:D:245:LEU:HA	1:D:248:ILE:HG12	2.03	0.40
1:E:79:LEU:HD22	1:E:91:LEU:CD2	2.51	0.40
1:E:87:GLN:C	1:E:88:ARG:O	2.58	0.40
1:A:107:LYS:O	1:A:109:TYR:N	2.54	0.40
1:B:144:HIS:NE2	3:B:303:IPA:H32	2.37	0.40
1:B:149:VAL:O	1:B:208:ALA:HB1	2.21	0.40
1:D:150:GLY:HA3	1:D:207:GLU:O	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	194/196 (99%)	154 (79%)	26 (13%)	14 (7%)	1 6
1	B	194/196 (99%)	147 (76%)	29 (15%)	18 (9%)	0 3
1	C	194/196 (99%)	149 (77%)	27 (14%)	18 (9%)	0 3
1	D	194/196 (99%)	151 (78%)	27 (14%)	16 (8%)	1 5
1	E	194/196 (99%)	145 (75%)	29 (15%)	20 (10%)	0 3
All	All	970/980 (99%)	746 (77%)	138 (14%)	86 (9%)	1 4

All (86) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	56	GLU
1	A	117	LEU
1	A	125	ASP
1	A	214	VAL
1	A	223	SER
1	B	57	ARG
1	B	117	LEU
1	B	119	ASP
1	B	125	ASP
1	B	223	SER
1	B	236	GLU
1	C	57	ARG
1	C	88	ARG
1	C	117	LEU
1	C	125	ASP
1	C	127	ASP
1	C	223	SER
1	D	57	ARG
1	D	117	LEU
1	D	118	ASN
1	D	119	ASP
1	D	121	ILE
1	D	218	VAL
1	D	223	SER
1	E	78	ILE
1	E	125	ASP
1	E	214	VAL
1	E	219	GLN
1	A	124	GLU
1	A	126	HIS
1	A	129	MET

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Mol	Chain	Res	Type
1	B	56	GLU
1	B	61	GLU
1	B	118	ASN
1	B	219	GLN
1	B	220	LYS
1	B	245	LEU
1	C	148	PHE
1	C	185	LEU
1	D	61	GLU
1	D	126	HIS
1	D	191	VAL
1	D	219	GLN
1	E	117	LEU
1	E	129	MET
1	B	121	ILE
1	B	124	GLU
1	B	229	THR
1	C	56	GLU
1	C	81	SER
1	C	124	GLU
1	D	56	GLU
1	D	124	GLU
1	D	186	THR
1	E	77	SER
1	E	223	SER
1	A	236	GLU
1	B	126	HIS
1	C	110	GLN
1	C	147	PRO
1	C	218	VAL
1	D	190	ALA
1	E	134	ASP
1	E	218	VAL
1	A	219	GLN
1	A	246	THR
1	B	218	VAL
1	C	121	ILE
1	C	187	LYS
1	E	124	GLU
1	E	216	ARG
1	A	86	PRO
1	C	105	PHE

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Mol	Chain	Res	Type
1	E	57	ARG
1	E	59	ARG
1	E	86	PRO
1	E	114	SER
1	E	127	ASP
1	E	248	ILE
1	C	113	ILE
1	D	237	ASP
1	E	95	PRO
1	E	217	GLY
1	B	217	GLY
1	A	57	ARG
1	A	121	ILE

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	172/172 (100%)	152 (88%)	20 (12%)	5 22
1	B	172/172 (100%)	148 (86%)	24 (14%)	3 15
1	C	172/172 (100%)	152 (88%)	20 (12%)	5 22
1	D	172/172 (100%)	156 (91%)	16 (9%)	9 32
1	E	172/172 (100%)	156 (91%)	16 (9%)	9 32
All	All	860/860 (100%)	764 (89%)	96 (11%)	6 24

All (96) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	57	ARG
1	A	76	SER
1	A	87	GLN
1	A	89	GLN
1	A	123	ASP
1	A	133	LYS

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Mol	Chain	Res	Type
1	A	137	MET
1	A	138	PHE
1	A	144	HIS
1	A	156	TYR
1	A	168	LEU
1	A	177	ARG
1	A	185	LEU
1	A	205	VAL
1	A	211	MET
1	A	214	VAL
1	A	216	ARG
1	A	219	GLN
1	A	221	MET
1	A	240	THR
1	B	57	ARG
1	B	63	ASP
1	B	68	LEU
1	B	91	LEU
1	B	114	SER
1	B	133	LYS
1	B	137	MET
1	B	138	PHE
1	B	144	HIS
1	B	148	PHE
1	B	149	VAL
1	B	173	GLU
1	B	177	ARG
1	B	181	VAL
1	B	185	LEU
1	B	194	THR
1	B	199	PRO
1	B	209	THR
1	B	211	MET
1	B	216	ARG
1	B	219	GLN
1	B	225	THR
1	B	228	SER
1	B	243	GLU
1	C	59	ARG
1	C	89	GLN
1	C	127	ASP
1	C	133	LYS

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Mol	Chain	Res	Type
1	C	137	MET
1	C	138	PHE
1	C	139	SER
1	C	144	HIS
1	C	176	SER
1	C	177	ARG
1	C	185	LEU
1	C	205	VAL
1	C	211	MET
1	C	213	MET
1	C	216	ARG
1	C	219	GLN
1	C	221	MET
1	C	225	THR
1	C	227	THR
1	C	235	ARG
1	D	59	ARG
1	D	89	GLN
1	D	113	ILE
1	D	137	MET
1	D	138	PHE
1	D	144	HIS
1	D	156	TYR
1	D	168	LEU
1	D	185	LEU
1	D	205	VAL
1	D	207	GLU
1	D	209	THR
1	D	211	MET
1	D	212	CYS
1	D	221	MET
1	D	247	LEU
1	E	57	ARG
1	E	87	GLN
1	E	137	MET
1	E	138	PHE
1	E	144	HIS
1	E	149	VAL
1	E	156	TYR
1	E	177	ARG
1	E	185	LEU
1	E	199	PRO

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Mol	Chain	Res	Type
1	E	205	VAL
1	E	211	MET
1	E	214	VAL
1	E	221	MET
1	E	225	THR
1	E	240	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (16) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	67	ASN
1	A	143	HIS
1	A	144	HIS
1	A	153	HIS
1	B	126	HIS
1	B	144	HIS
1	B	153	HIS
1	B	219	GLN
1	C	153	HIS
1	D	64	ASN
1	D	110	GLN
1	D	144	HIS
1	D	153	HIS
1	E	143	HIS
1	E	144	HIS
1	E	153	HIS

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 monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 10 ligands modelled in this entry, 5 are monoatomic - leaving 5 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
3	IPA	A	306	2	3,3,3	0.38	0	3,3,3	0.54	0
3	IPA	B	302	2	3,3,3	0.82	0	3,3,3	0.28	0
3	IPA	D	304	2	3,3,3	0.76	0	3,3,3	0.24	0
3	IPA	B	303	2	3,3,3	0.70	0	3,3,3	0.54	0
3	IPA	D	305	2	3,3,3	0.66	0	3,3,3	0.29	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.

4 monomers are involved in 9 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	306	IPA	1	0
3	D	304	IPA	1	0
3	B	303	IPA	5	0
3	D	305	IPA	2	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 (i)

6.1 Protein, DNA and RNA chains (i)

EDS was not executed - this section is therefore empty.

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

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates (i)

EDS was not executed - this section is therefore empty.

6.4 Ligands (i)

EDS was not executed - this section is therefore empty.

6.5 Other polymers (i)

EDS was not executed - this section is therefore empty.