Full wwPDB X-ray Structure Validation Report (i)

Feb 1, 2016 – 07:11 AM GMT

PDB ID	:	2ZU6
Title	:	crystal structure of the eIF4A-PDCD4 complex
Authors	:	Cho, Y.; Chang, J.H.; Sohn, S.Y.
Deposited on	:	2008-10-13
Resolution	:	2.80 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 (i) symbol.

The following versions of software and data (see references (1)) were used in the production of this report:

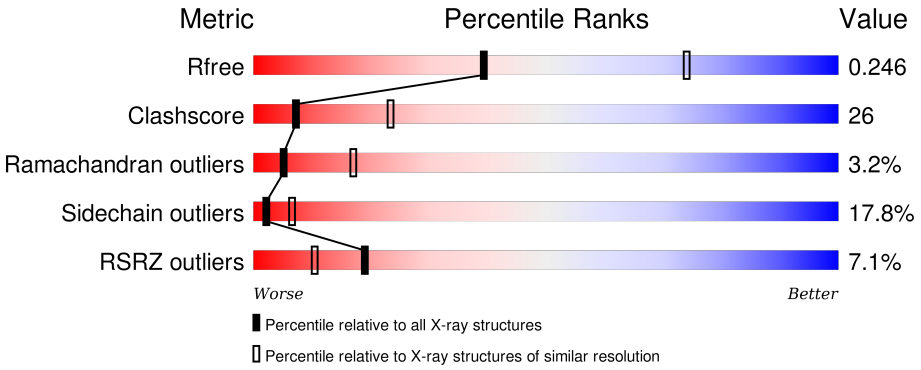
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	trunk26865

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 2.80 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	91344	2393 (2.80-2.80)
Clashscore	102246	2827 (2.80-2.80)
Ramachandran outliers	100387	2782 (2.80-2.80)
Sidechain outliers	100360	2784 (2.80-2.80)
RSRZ outliers	91569	2404 (2.80-2.80)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria. 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	388	3% 45% 35% 9% 12%
1	C	388	9% 40% 40% 11% • 10%
1	D	388	3% 47% 33% 9% • 11%
1	F	388	18% 31% 31% 7% • 30%
2	B	307	% 56% 32% • 7%

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Mol	Chain	Length	Quality of chain
2	E	307	

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	EDO	A	3	-	-	-	X

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 14986 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 Eukaryotic initiation factor 4A-I.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	343	Total	C	N	O	S	0	0	0
			2743	1734	477	514	18			
1	C	351	Total	C	N	O	S	0	0	0
			2819	1778	492	531	18			
1	D	345	Total	C	N	O	S	0	0	0
			2756	1742	480	516	18			
1	F	271	Total	C	N	O	S	0	0	0
			2196	1389	381	411	15			

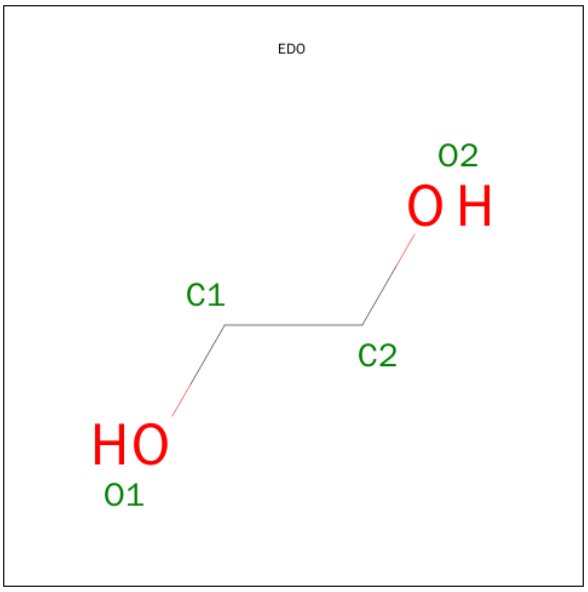
There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	19	MET	-	EXPRESSION TAG	UNP P60842
C	19	MET	-	EXPRESSION TAG	UNP P60842
D	19	MET	-	EXPRESSION TAG	UNP P60842
F	19	MET	-	EXPRESSION TAG	UNP P60842

- Molecule 2 is a protein called Programmed cell death protein 4.

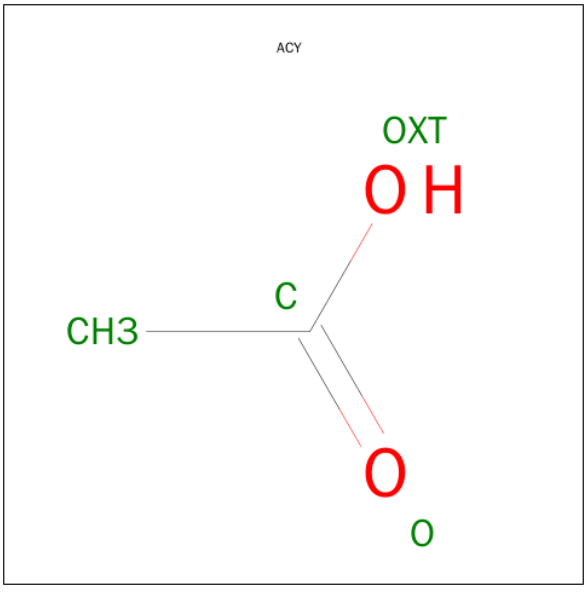
Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
2	B	284	Total	C	N	O	S	Se	0	0	0
			2218	1403	366	434	6	9			
2	E	282	Total	C	N	O	S	Se	0	0	0
			2201	1393	363	430	6	9			

- Molecule 3 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: $C_2H_6O_2$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total C O 4 2 2	0	0
3	A	1	Total C O 4 2 2	0	0
3	D	1	Total C O 4 2 2	0	0

- Molecule 4 is ACETIC ACID (three-letter code: ACY) (formula: $C_2H_4O_2$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total C O 4 2 2	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	D	1	Total C O 4 2 2	0	0

- Molecule 5 is water.

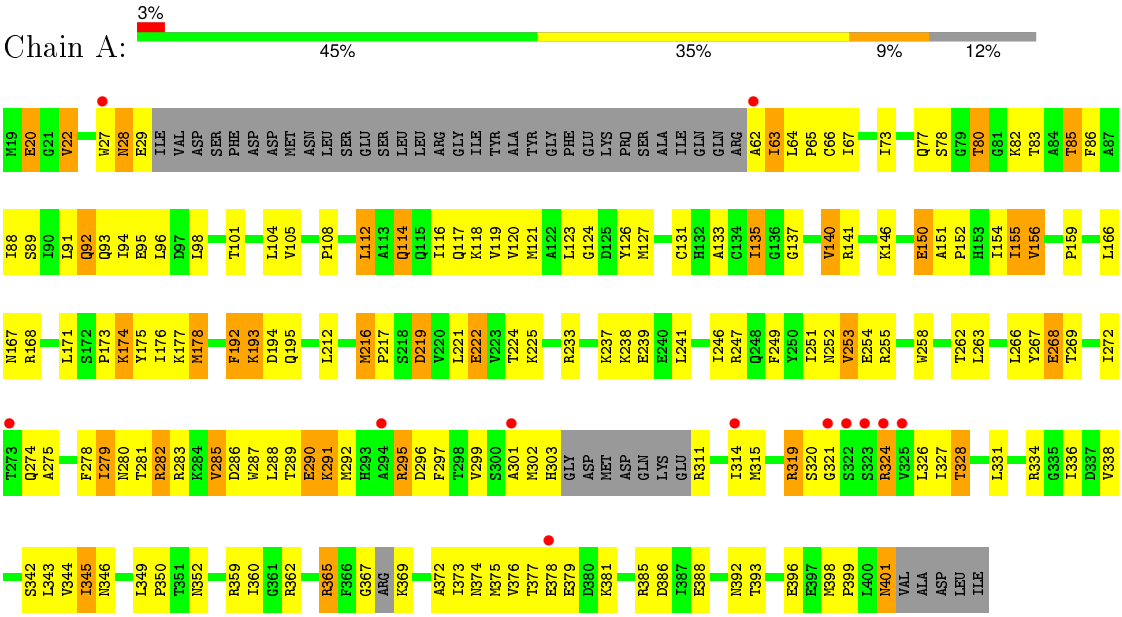
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	11	Total O 11 11	0	0
5	B	6	Total O 6 6	0	0
5	C	3	Total O 3 3	0	0
5	D	11	Total O 11 11	0	0
5	E	2	Total O 2 2	0	0

3 Residue-property plots (i)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density (RSRZ > 2). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

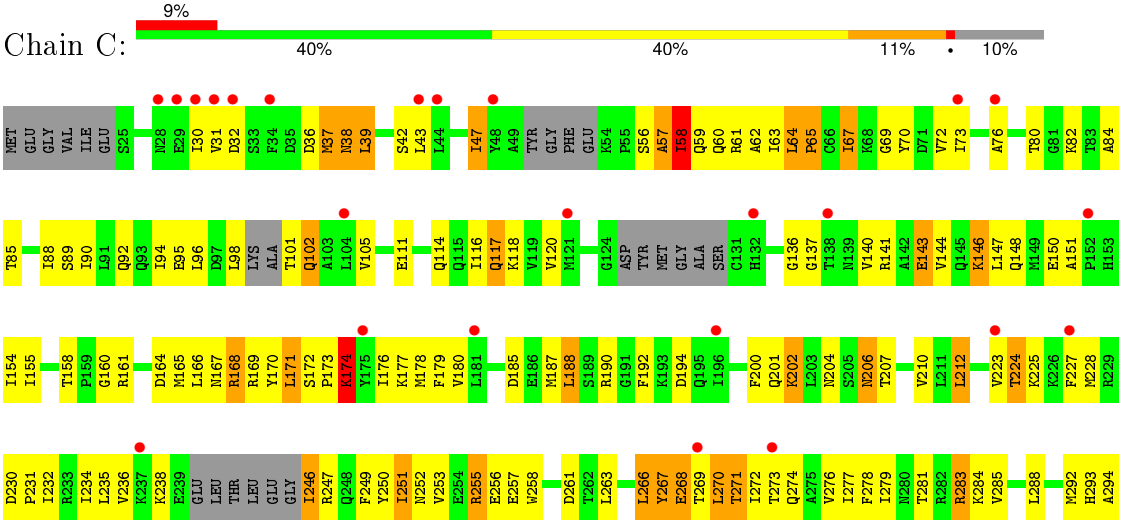
- Molecule 1: Eukaryotic initiation factor 4A-I

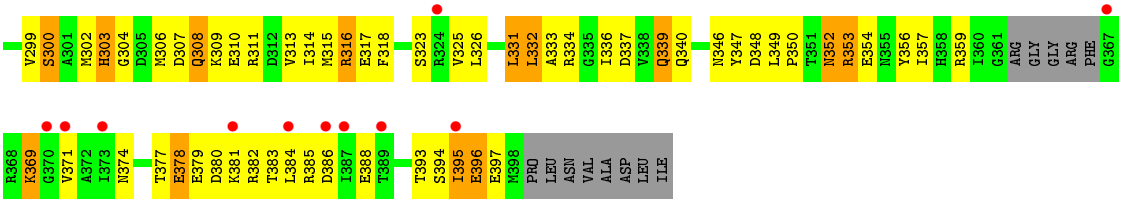
Chain A:



- Molecule 1: Eukaryotic initiation factor 4A-I

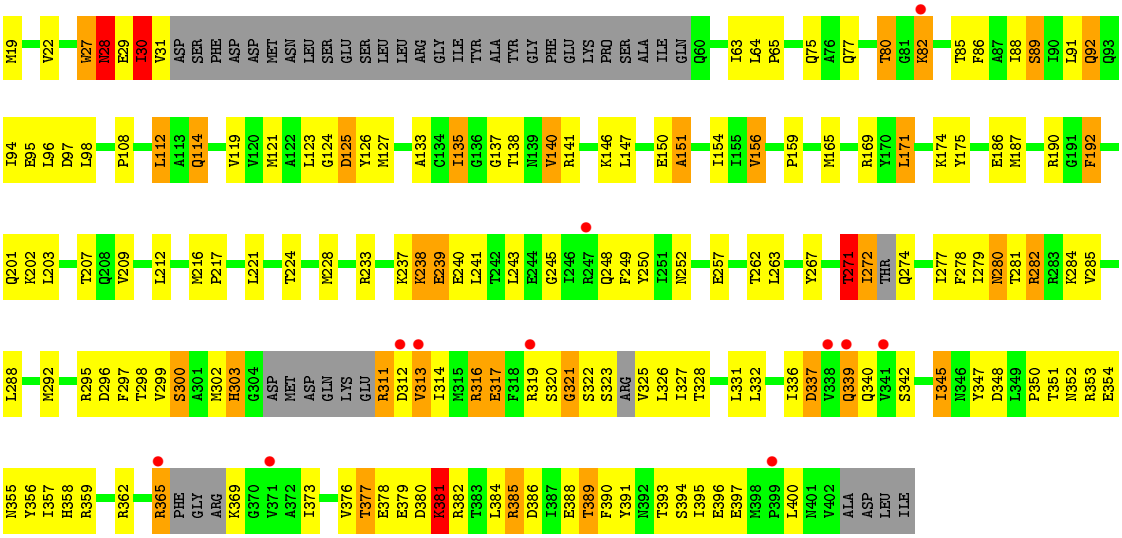
Chain C:





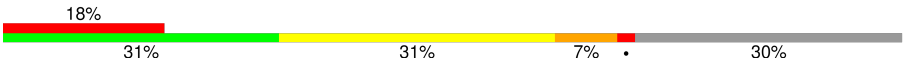
• Molecule 1: Eukaryotic initiation factor 4A-I

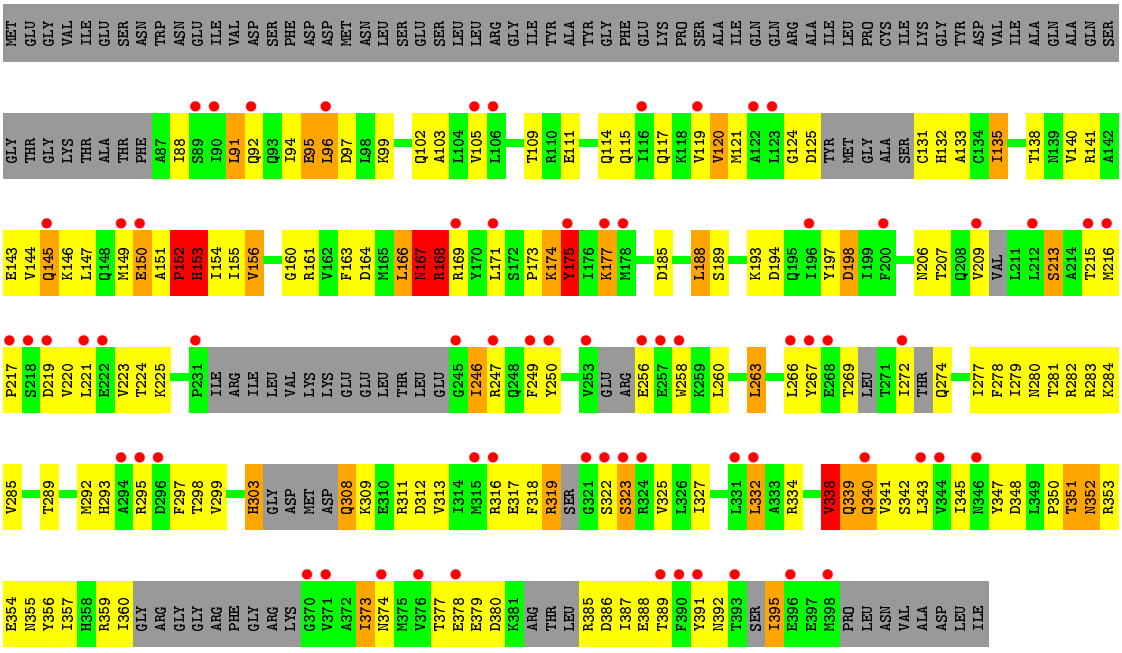
Chain D:



• Molecule 1: Eukaryotic initiation factor 4A-I

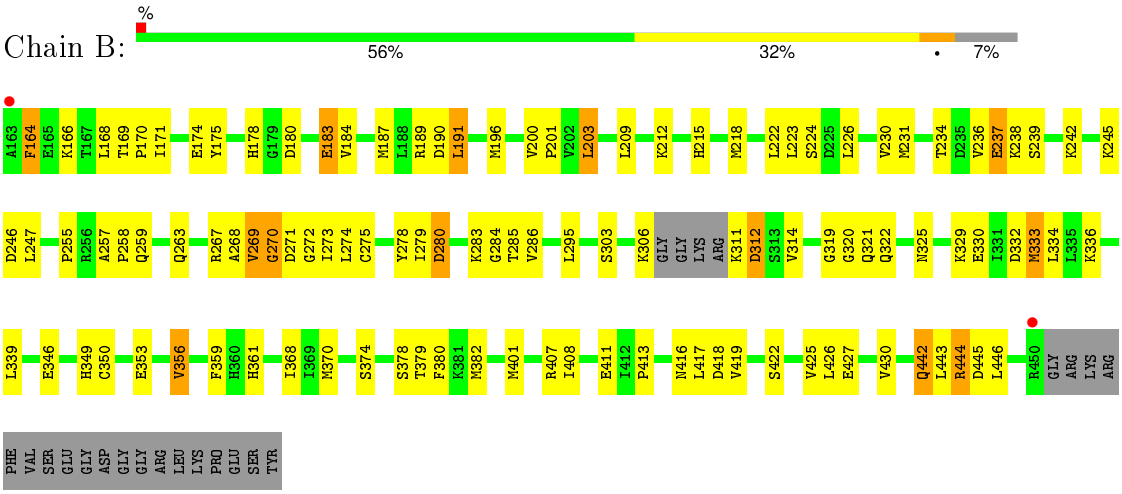
Chain F:





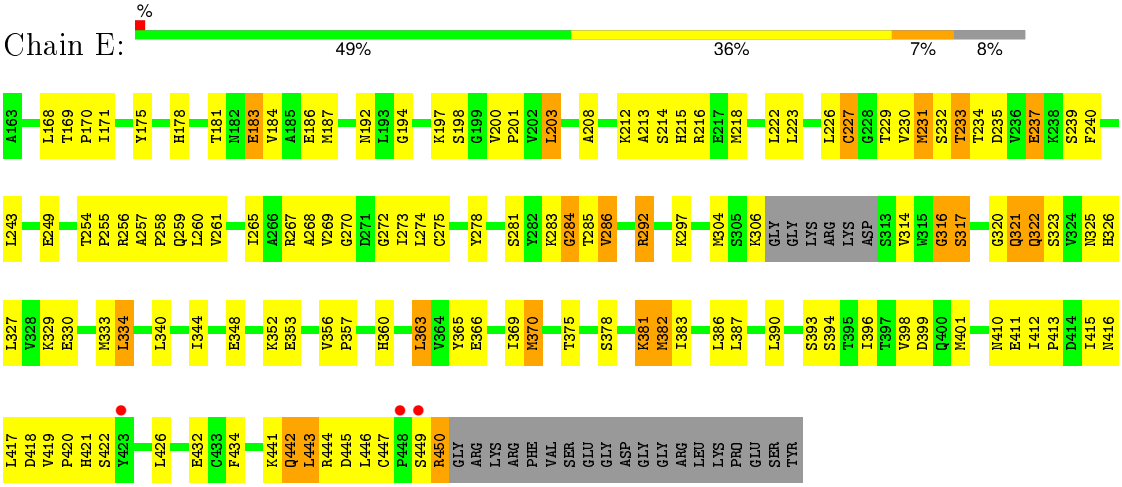
• Molecule 2: Programmed cell death protein 4

Chain B:



- Molecule 2: Programmed cell death protein 4

Chain E:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, α, β, γ	156.89Å 165.38Å 100.42Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	50.00 – 2.80 49.86 – 2.81	Depositor EDS
% Data completeness (in resolution range)	99.0 (50.00-2.80) 94.1 (49.86-2.81)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	0.06	Depositor
$< I/\sigma(I) >$ [1]	3.39 (at 2.81Å)	Xtriage
Refinement program	PHENIX	Depositor
R, R_{free}	0.248 , 0.294 0.239 , 0.246	Depositor DCC
R_{free} test set	3053 reflections (5.02%)	DCC
Wilson B-factor (Å^2)	62.1	Xtriage
Anisotropy	0.515	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.29 , 63.3	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Outliers	0 of 64546 reflections	Xtriage
F_o,F_c correlation	0.92	EDS
Total number of atoms	14986	wwPDB-VP
Average B, all atoms (Å^2)	88.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 7.83% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

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

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	0.77	2/2781 (0.1%)	0.84	4/3750 (0.1%)
1	C	0.41	0/2855	0.54	0/3846
1	D	0.72	0/2791	0.81	1/3761 (0.0%)
1	F	0.44	0/2218	0.54	0/2978
2	B	0.65	0/2244	0.73	1/3015 (0.0%)
2	E	0.67	1/2227 (0.0%)	0.75	1/2993 (0.0%)
All	All	0.63	3/15116 (0.0%)	0.71	7/20343 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	F	0	1
2	E	0	2
All	All	0	3

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	192	PHE	N-CA	7.02	1.60	1.46
2	E	227	CYS	CB-SG	-5.21	1.73	1.81
1	A	193	LYS	CE-NZ	-5.07	1.36	1.49

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	192	PHE	CB-CG-CD1	-8.22	115.05	120.80
2	E	334	LEU	CA-CB-CG	6.31	129.82	115.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	D	192	PHE	N-CA-C	5.92	126.97	111.00
1	A	22	VAL	CB-CA-C	-5.53	100.90	111.40
1	A	155	ILE	CG1-CB-CG2	-5.16	100.05	111.40
2	B	209	LEU	CB-CG-CD1	-5.14	102.26	111.00
1	A	193	LYS	N-CA-C	5.04	124.60	111.00

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	E	286	VAL	Peptide
2	E	316	GLY	Peptide
1	F	152	PRO	Peptide

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	2743	0	2792	160	0
1	C	2819	0	2865	202	0
1	D	2756	0	2811	136	0
1	F	2196	0	2220	122	0
2	B	2218	0	2231	80	0
2	E	2201	0	2214	117	0
3	A	8	0	12	1	0
3	D	4	0	6	0	0
4	A	4	0	3	1	0
4	D	4	0	3	0	0
5	A	11	0	0	0	0
5	B	6	0	0	0	0
5	C	3	0	0	1	0
5	D	11	0	0	1	0
5	E	2	0	0	1	0
All	All	14986	0	15157	782	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 26.

All (782) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:279:ILE:HD13	1:C:284:LYS:HB3	1.25	1.15
1:F:115:GLN:O	1:F:119:VAL:HG23	1.48	1.14
2:E:442:GLN:NE2	2:E:442:GLN:H	1.45	1.14
2:B:339:LEU:HD11	2:B:370:MSE:HE3	1.29	1.13
1:C:73:ILE:HD12	1:C:224:THR:HG21	1.22	1.13
2:E:286:VAL:HG21	2:E:292:ARG:HE	1.10	1.10
2:E:442:GLN:HE21	2:E:442:GLN:N	1.48	1.09
1:C:369:LYS:HA	1:C:369:LYS:HE2	1.36	1.08
1:A:77:GLN:OE1	1:A:238:LYS:HD3	1.50	1.08
1:D:389:THR:HG21	5:D:18:HOH:O	1.54	1.07
1:A:121:MET:CE	1:A:121:MET:HA	1.85	1.07
2:B:442:GLN:H	2:B:442:GLN:NE2	1.51	1.07
1:A:290:GLU:OE1	1:A:290:GLU:HA	1.55	1.06
2:B:442:GLN:N	2:B:442:GLN:HE21	1.54	1.05
1:C:378:GLU:HA	1:C:381:LYS:HD3	1.37	1.05
1:A:279:ILE:HD11	1:A:327:ILE:CG2	1.87	1.04
1:A:279:ILE:HD11	1:A:327:ILE:HG22	1.39	1.04
2:B:171:ILE:HG23	2:B:187:MSE:HE3	1.40	1.03
2:E:434:PHE:HE1	2:E:441:LYS:HA	1.22	1.03
1:A:350:PRO:HD3	1:A:359:ARG:NH1	1.73	1.02
1:C:272:ILE:HG21	1:C:274:GLN:HE21	1.20	1.01
1:C:272:ILE:HG21	1:C:274:GLN:NE2	1.76	1.00
1:C:147:LEU:HA	1:C:151:ALA:HB3	1.44	1.00
1:C:272:ILE:CG2	1:C:274:GLN:HE21	1.77	0.96
2:E:212:LYS:H	2:E:215:HIS:HD2	1.10	0.96
2:B:212:LYS:H	2:B:215:HIS:HD2	1.15	0.94
2:B:442:GLN:H	2:B:442:GLN:HE21	1.03	0.93
2:E:434:PHE:CE1	2:E:441:LYS:HA	2.03	0.93
1:D:300:SER:O	1:D:326:LEU:HD12	1.68	0.92
1:D:165:MET:HB3	1:D:171:LEU:HD22	1.52	0.92
1:D:377:THR:H	1:D:380:ASP:HB2	1.31	0.91
2:E:212:LYS:H	2:E:215:HIS:CD2	1.88	0.90
2:E:286:VAL:HG21	2:E:292:ARG:NE	1.86	0.90
1:D:351:THR:CB	2:E:321:GLN:HE22	1.85	0.90
1:A:62:ALA:HB1	1:A:88:ILE:HG21	1.54	0.89
1:C:147:LEU:HA	1:C:151:ALA:CB	2.00	0.89
1:A:94:ILE:HD11	1:A:154:ILE:HD11	1.53	0.89
1:C:58:ILE:HD12	1:C:236:VAL:HG23	1.52	0.89
1:D:281:THR:HG21	2:E:183:GLU:HG3	1.55	0.88
1:A:121:MET:HE2	1:A:121:MET:HA	1.52	0.87

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:395:ILE:O	1:F:395:ILE:HG13	1.71	0.87
1:F:94:ILE:HG12	1:F:95:GLU:H	1.40	0.87
1:D:312:ASP:O	1:D:316:ARG:HB2	1.75	0.87
1:C:82:LYS:HE2	1:C:212:LEU:HB3	1.57	0.87
1:D:295:ARG:HB2	1:D:297:PHE:HE2	1.39	0.87
1:A:377:THR:O	1:A:381:LYS:HG3	1.75	0.87
2:E:357:PRO:HA	2:E:360:HIS:CE1	2.10	0.86
1:C:73:ILE:HD12	1:C:224:THR:CG2	2.03	0.86
2:E:434:PHE:HE1	2:E:441:LYS:CA	1.89	0.85
1:C:172:SER:HB2	1:C:174:LYS:HD2	1.59	0.84
1:C:378:GLU:HA	1:C:381:LYS:CD	2.06	0.84
1:A:290:GLU:CA	1:A:290:GLU:OE1	2.26	0.83
1:A:222:GLU:OE1	1:A:222:GLU:HA	1.78	0.83
1:A:275:ALA:HB2	1:A:343:LEU:HD23	1.58	0.83
1:F:188:LEU:HD23	1:F:220:VAL:HG22	1.60	0.83
2:E:230:VAL:HG13	2:E:231:MSE:HG3	1.61	0.83
1:A:98:LEU:HD21	1:A:175:TYR:CD1	2.14	0.83
2:B:311:LYS:HG3	2:B:312:ASP:H	1.44	0.82
1:A:290:GLU:O	1:A:292:MET:N	2.13	0.81
1:A:295:ARG:HH11	1:A:295:ARG:HG3	1.45	0.81
1:A:350:PRO:HD3	1:A:359:ARG:HH11	1.45	0.80
1:D:351:THR:HB	2:E:321:GLN:HE22	1.46	0.79
1:D:28:ASN:HB2	1:D:30:ILE:HD12	1.64	0.79
1:C:352:ASN:HA	1:C:353:ARG:NH1	1.97	0.79
1:D:302:MET:HB2	1:D:328:THR:HG22	1.63	0.79
2:B:353:GLU:OE1	1:C:283:ARG:NH2	2.14	0.79
2:B:215:HIS:HA	2:B:218:MSE:HE3	1.63	0.78
1:C:270:LEU:HD12	1:C:272:ILE:H	1.47	0.78
1:C:73:ILE:CD1	1:C:224:THR:HG21	2.11	0.78
1:C:62:ALA:HA	1:C:65:PRO:HG2	1.66	0.78
1:F:188:LEU:HD12	1:F:193:LYS:HG2	1.64	0.78
1:A:141:ARG:NH2	2:E:281:SER:OG	2.16	0.78
1:A:290:GLU:C	1:A:292:MET:H	1.88	0.77
2:B:212:LYS:H	2:B:215:HIS:CD2	2.01	0.77
1:A:27:TRP:CZ3	1:A:29:GLU:HB2	2.19	0.77
2:B:339:LEU:HD11	2:B:370:MSE:CE	2.13	0.77
1:D:282:ARG:HH21	1:D:332:LEU:HD11	1.49	0.76
1:A:77:GLN:O	1:A:80:THR:HG22	1.85	0.76
2:E:412:ILE:HG23	2:E:413:PRO:HD3	1.68	0.76
1:C:270:LEU:HG	1:C:271:THR:H	1.51	0.76
1:D:75:GLN:HB2	1:D:216:MET:CE	2.16	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:377:THR:HG22	1:A:378:GLU:N	2.01	0.75
1:F:279:ILE:HD11	1:F:285:VAL:HG23	1.67	0.75
1:A:295:ARG:NH1	1:A:295:ARG:HG3	2.00	0.75
2:E:212:LYS:N	2:E:215:HIS:HD2	1.84	0.75
1:C:303:HIS:O	1:C:332:LEU:HD22	1.87	0.74
2:B:339:LEU:CD1	2:B:370:MSE:HE3	2.14	0.74
1:D:376:VAL:HG11	1:D:384:LEU:HD22	1.69	0.74
1:C:253:VAL:HG23	1:C:255:ARG:O	1.88	0.74
1:C:39:LEU:HB3	1:C:43:LEU:HD13	1.69	0.73
1:D:339:GLN:HB2	1:D:362:ARG:CG	2.19	0.73
1:C:353:ARG:H	1:C:353:ARG:HH11	1.35	0.72
1:D:174:LYS:HG2	1:D:175:TYR:CE2	2.24	0.72
1:F:279:ILE:HD11	1:F:285:VAL:CG2	2.19	0.72
1:F:274:GLN:HE22	1:F:342:SER:HB2	1.55	0.72
2:B:183:GLU:O	2:B:187:MSE:HG3	1.89	0.71
1:C:279:ILE:HD11	1:C:285:VAL:HG23	1.73	0.71
1:A:274:GLN:HA	1:A:324:ARG:O	1.90	0.71
1:D:357:ILE:HB	1:D:391:TYR:CE2	2.25	0.71
1:A:239:GLU:OE1	1:A:365:ARG:HG3	1.91	0.70
1:C:146:LYS:O	1:C:151:ALA:HB2	1.91	0.70
1:A:275:ALA:CB	1:A:343:LEU:HD23	2.22	0.70
1:C:369:LYS:CA	1:C:369:LYS:HE2	2.19	0.70
1:F:91:LEU:HD11	1:F:120:VAL:HG13	1.72	0.69
1:C:190:ARG:HH11	1:C:190:ARG:CG	2.05	0.69
1:F:91:LEU:O	1:F:94:ILE:HG22	1.92	0.69
1:D:295:ARG:HB2	1:D:297:PHE:CE2	2.26	0.69
1:A:108:PRO:HD2	1:A:112:LEU:HD12	1.73	0.69
1:D:388:GLU:HB2	1:D:395:ILE:HD12	1.73	0.68
2:B:269:VAL:O	2:B:272:GLY:N	2.21	0.68
1:F:299:VAL:HG23	1:F:325:VAL:HB	1.76	0.68
2:E:304:MSE:HA	1:F:293:HIS:CE1	2.29	0.68
1:F:278:PHE:HB3	1:F:359:ARG:HH21	1.59	0.68
1:C:309:LYS:HB3	1:C:310:GLU:OE1	1.93	0.68
2:B:166:LYS:HD3	2:B:166:LYS:N	2.07	0.68
1:C:58:ILE:HD13	1:C:76:ALA:HB2	1.76	0.67
1:D:353:ARG:HG3	1:D:353:ARG:HH11	1.59	0.67
1:F:167:ASN:HD22	1:F:168:ARG:N	1.92	0.67
1:A:62:ALA:CB	1:A:88:ILE:HG21	2.23	0.67
1:D:350:PRO:HD3	1:D:359:ARG:CZ	2.24	0.67
2:B:356:VAL:HG13	2:B:359:PHE:HB3	1.77	0.67
2:E:417:LEU:HB3	1:F:161:ARG:HB3	1.77	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:279:ILE:HD11	1:F:281:THR:O	1.94	0.67
1:F:278:PHE:HB3	1:F:359:ARG:NH2	2.10	0.67
1:C:313:VAL:O	1:C:316:ARG:HD2	1.94	0.66
2:E:442:GLN:HE21	2:E:442:GLN:H	0.72	0.66
1:C:148:GLN:HE22	1:C:170:TYR:HA	1.60	0.66
1:A:62:ALA:HB3	1:A:92:GLN:NE2	2.11	0.65
1:C:64:LEU:HD12	1:C:65:PRO:HD3	1.78	0.65
1:D:288:LEU:O	1:D:292:MET:HG2	1.96	0.65
1:C:279:ILE:HD12	1:C:281:THR:H	1.61	0.65
1:F:166:LEU:HG	1:F:171:LEU:HD23	1.79	0.65
2:B:426:LEU:O	2:B:430:VAL:HG23	1.95	0.65
1:D:108:PRO:HD2	1:D:112:LEU:HD12	1.79	0.65
1:C:270:LEU:HG	1:C:271:THR:N	2.11	0.65
1:F:338:VAL:HA	1:F:341:VAL:HG21	1.79	0.65
1:A:282:ARG:O	1:A:285:VAL:HG12	1.95	0.65
1:F:131:CYS:SG	1:F:132:HIS:N	2.69	0.65
1:F:272:ILE:HG21	1:F:274:GLN:HE21	1.62	0.65
1:A:251:ILE:HG22	1:A:253:VAL:HG23	1.78	0.64
1:D:385:ARG:NE	1:D:388:GLU:OE1	2.28	0.64
1:F:354:GLU:H	1:F:354:GLU:CD	2.01	0.64
1:D:75:GLN:HB2	1:D:216:MET:HE1	1.78	0.64
1:C:116:ILE:O	1:C:120:VAL:HG23	1.96	0.64
1:D:339:GLN:HB2	1:D:362:ARG:HG3	1.79	0.64
1:D:281:THR:CG2	2:E:183:GLU:HG3	2.25	0.64
2:E:240:PHE:CE1	2:E:265:ILE:HG13	2.33	0.64
1:F:132:HIS:CD2	1:F:146:LYS:NZ	2.66	0.64
1:D:302:MET:CB	1:D:328:THR:HG22	2.27	0.64
1:C:247:ARG:HB3	1:C:371:VAL:HG13	1.80	0.64
1:A:83:THR:HG22	1:A:85:THR:H	1.61	0.64
1:F:163:PHE:CE1	1:F:198:ASP:HB3	2.33	0.64
1:F:278:PHE:CB	1:F:359:ARG:HH21	2.11	0.63
1:D:250:TYR:HD2	1:D:395:ILE:HG22	1.61	0.63
2:B:418:ASP:OD2	1:C:161:ARG:NH1	2.30	0.63
2:E:240:PHE:CD1	2:E:265:ILE:HG13	2.34	0.63
1:A:94:ILE:CD1	1:A:154:ILE:HD11	2.28	0.63
1:A:222:GLU:CA	1:A:222:GLU:OE1	2.47	0.62
1:D:278:PHE:CG	1:D:359:ARG:HD3	2.34	0.62
1:A:78:SER:HA	3:A:3:EDO:H21	1.81	0.62
1:C:165:MET:HB3	1:C:171:LEU:HD22	1.79	0.62
1:A:343:LEU:HD11	1:A:373:ILE:HD12	1.80	0.62
1:A:174:LYS:HG2	1:A:175:TYR:CE2	2.35	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:27:TRP:HA	1:D:237:LYS:O	1.99	0.62
1:C:167:ASN:C	1:C:169:ARG:H	2.02	0.62
2:B:442:GLN:N	2:B:442:GLN:NE2	2.25	0.62
2:E:197:LYS:HD3	2:E:231:MSE:HA	1.81	0.62
1:C:64:LEU:N	1:C:65:PRO:HD2	2.14	0.62
2:B:175:TYR:HA	2:B:178:HIS:CE1	2.35	0.62
2:E:198:SER:O	2:E:239:SER:OG	2.15	0.62
1:C:303:HIS:H	1:C:303:HIS:CD2	2.18	0.62
1:C:279:ILE:HD11	1:C:281:THR:O	2.00	0.62
2:B:332:ASP:OD2	2:B:336:LYS:HE2	1.99	0.62
1:A:121:MET:HE3	1:A:121:MET:HA	1.79	0.62
1:A:252:ASN:OD1	1:A:252:ASN:O	2.18	0.62
1:A:290:GLU:C	1:A:292:MET:N	2.52	0.61
1:C:251:ILE:HG13	1:C:252:ASN:N	2.13	0.61
1:A:253:VAL:HG13	1:A:258:TRP:HB3	1.82	0.61
2:E:327:LEU:O	2:E:330:GLU:N	2.32	0.61
1:D:313:VAL:O	1:D:317:GLU:OE2	2.18	0.61
1:D:376:VAL:CG1	1:D:384:LEU:HD22	2.31	0.61
2:E:426:LEU:CD2	2:E:447:CYS:SG	2.89	0.61
2:E:426:LEU:HD23	2:E:447:CYS:SG	2.40	0.61
1:C:352:ASN:HA	1:C:353:ARG:HH12	1.63	0.61
1:C:31:VAL:HB	1:C:63:ILE:HG21	1.82	0.61
1:C:377:THR:HG23	1:C:379:GLU:H	1.66	0.61
1:D:30:ILE:HG21	1:D:64:LEU:HD21	1.83	0.61
1:A:289:THR:OG1	1:A:301:ALA:HB2	2.01	0.61
2:E:215:HIS:HA	2:E:218:MSE:HE3	1.82	0.61
1:D:239:GLU:HG2	1:D:365:ARG:HG3	1.83	0.61
1:F:103:ALA:HB3	1:F:154:ILE:HG12	1.83	0.60
1:C:266:LEU:O	1:C:270:LEU:N	2.34	0.60
1:F:332:LEU:O	1:F:332:LEU:HG	2.01	0.60
1:C:303:HIS:CE1	1:C:306:MET:HB2	2.36	0.60
1:C:30:ILE:HG22	1:C:61:ARG:HG2	1.81	0.60
1:C:279:ILE:CG1	1:C:285:VAL:HG23	2.31	0.60
1:D:388:GLU:HA	1:D:393:THR:HG22	1.83	0.60
1:F:164:ASP:O	1:F:167:ASN:HB3	2.01	0.60
1:F:102:GLN:HA	1:F:175:TYR:O	2.01	0.60
1:D:249:PHE:HD2	1:D:396:GLU:HB2	1.67	0.60
1:C:246:ILE:HG23	1:C:246:ILE:O	2.01	0.60
1:D:351:THR:HB	2:E:321:GLN:NE2	2.16	0.60
1:A:321:GLY:HA3	1:A:324:ARG:HD2	1.82	0.59
1:C:310:GLU:O	1:C:313:VAL:HG12	2.02	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:449:SER:O	2:E:450:ARG:C	2.39	0.59
2:B:212:LYS:N	2:B:215:HIS:HD2	1.92	0.59
1:C:388:GLU:OE2	1:C:394:SER:HA	2.01	0.59
1:C:58:ILE:HD12	1:C:236:VAL:CG2	2.30	0.59
1:D:339:GLN:CB	1:D:362:ARG:HG3	2.31	0.59
1:A:345:ILE:HD11	1:A:375:MET:CE	2.33	0.59
2:E:366:GLU:O	2:E:370:MSE:HG3	2.01	0.59
1:A:62:ALA:CB	1:A:88:ILE:CG2	2.81	0.59
1:D:64:LEU:HB3	1:D:65:PRO:HD2	1.85	0.59
1:C:250:TYR:OH	1:C:397:GLU:HG2	2.03	0.59
1:C:234:ILE:HG22	1:C:235:LEU:N	2.18	0.59
1:A:295:ARG:HB3	1:A:297:PHE:HE2	1.67	0.59
1:F:284:LYS:HE3	1:F:348:ASP:OD1	2.02	0.59
1:D:88:ILE:O	1:D:92:GLN:HG2	2.03	0.59
1:A:377:THR:CG2	1:A:378:GLU:N	2.65	0.59
1:A:114:GLN:HE21	1:A:114:GLN:CA	2.16	0.59
2:B:236:VAL:HG12	2:B:274:LEU:HD12	1.84	0.58
1:D:82:LYS:O	1:D:119:VAL:HG21	2.03	0.58
1:A:278:PHE:HB2	1:A:346:ASN:HD22	1.66	0.58
1:C:72:VAL:HG22	1:C:210:VAL:HG22	1.86	0.58
1:C:57:ALA:C	1:C:59:GLN:H	2.06	0.58
1:A:279:ILE:HD11	1:A:327:ILE:HG23	1.80	0.58
1:A:377:THR:O	1:A:381:LYS:CG	2.50	0.58
1:C:279:ILE:CD1	1:C:285:VAL:HG23	2.34	0.58
1:F:166:LEU:HA	1:F:171:LEU:HB3	1.85	0.58
1:F:279:ILE:HD13	1:F:284:LYS:HG2	1.85	0.58
1:C:249:PHE:CD2	1:C:397:GLU:O	2.57	0.58
1:C:271:THR:HG23	1:C:271:THR:O	2.03	0.58
2:E:383:ILE:O	2:E:387:LEU:HG	2.04	0.58
1:D:80:THR:O	1:D:86:PHE:HB2	2.04	0.57
1:F:132:HIS:CD2	1:F:146:LYS:HZ1	2.22	0.57
2:E:261:VAL:HG12	2:E:265:ILE:HD12	1.86	0.57
2:E:208:ALA:HB1	2:E:216:ARG:HG2	1.86	0.57
1:D:272:ILE:HB	1:D:274:GLN:N	2.20	0.57
1:D:249:PHE:CD2	1:D:396:GLU:HB2	2.39	0.57
2:B:187:MSE:O	2:B:191:LEU:HD13	2.04	0.57
1:A:319:ARG:NE	1:A:320:SER:HB2	2.20	0.57
1:F:168:ARG:HB2	1:F:168:ARG:NH1	2.19	0.57
1:F:168:ARG:HB2	1:F:168:ARG:HH11	1.70	0.57
1:C:288:LEU:O	1:C:292:MET:HG2	2.05	0.57
2:B:246:ASP:O	2:B:247:LEU:C	2.43	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:164:PHE:O	2:B:168:LEU:HD23	2.04	0.57
1:C:172:SER:HB2	1:C:174:LYS:CD	2.33	0.57
2:E:222:LEU:O	2:E:226:LEU:HG	2.05	0.57
2:E:268:ALA:HB3	2:E:274:LEU:HD22	1.86	0.57
1:F:99:LYS:CE	1:F:150:GLU:HB2	2.34	0.57
1:F:357:ILE:HG23	1:F:391:TYR:OH	2.05	0.56
1:D:357:ILE:HB	1:D:391:TYR:HE2	1.70	0.56
2:B:356:VAL:HG13	2:B:356:VAL:O	2.05	0.56
2:B:180:ASP:OD1	2:B:183:GLU:HB2	2.06	0.56
1:D:279:ILE:HD11	1:D:288:LEU:HD22	1.87	0.56
1:D:221:LEU:O	1:D:224:THR:HB	2.05	0.56
1:D:238:LYS:HB3	1:D:238:LYS:NZ	2.19	0.56
1:C:223:VAL:O	1:C:227:PHE:HB2	2.04	0.56
2:B:333:MSE:HA	2:B:333:MSE:HE3	1.88	0.56
1:C:105:VAL:HG13	1:C:180:VAL:HB	1.88	0.56
1:F:279:ILE:CG1	1:F:285:VAL:HG22	2.35	0.56
1:F:206:ASN:OD1	1:F:207:THR:N	2.38	0.56
1:C:333:ALA:HA	1:C:336:ILE:HG23	1.86	0.56
1:A:401:ASN:N	1:A:401:ASN:OD1	2.38	0.56
1:C:56:SER:HA	1:C:60:GLN:HE21	1.71	0.56
2:E:365:TYR:CZ	2:E:369:ILE:HD11	2.40	0.56
1:C:353:ARG:NH1	1:C:353:ARG:H	2.04	0.56
2:B:283:LYS:O	2:B:285:THR:HG23	2.06	0.56
1:F:154:ILE:HG22	1:F:155:ILE:N	2.20	0.56
1:D:352:ASN:HB3	1:D:355:ASN:ND2	2.21	0.56
1:F:94:ILE:HG12	1:F:95:GLU:N	2.18	0.55
1:C:314:ILE:HA	1:C:317:GLU:HG2	1.88	0.55
1:A:246:ILE:HD11	1:A:362:ARG:NE	2.21	0.55
1:A:279:ILE:CD1	1:A:327:ILE:CG2	2.74	0.55
1:C:114:GLN:O	1:C:117:GLN:HG3	2.07	0.55
1:C:101:THR:O	1:C:176:ILE:HG13	2.06	0.55
1:C:165:MET:CB	1:C:171:LEU:HD22	2.36	0.55
1:D:377:THR:N	1:D:380:ASP:HB2	2.14	0.55
1:F:272:ILE:HD12	1:F:272:ILE:H	1.70	0.55
1:A:319:ARG:HE	1:A:320:SER:HB2	1.72	0.55
1:F:377:THR:HG23	1:F:379:GLU:H	1.70	0.55
1:A:150:GLU:O	1:A:151:ALA:C	2.43	0.55
1:A:350:PRO:CD	1:A:359:ARG:NH1	2.60	0.55
1:A:377:THR:HG22	1:A:379:GLU:H	1.69	0.55
1:C:72:VAL:HG12	1:C:232:ILE:HB	1.88	0.55
1:A:280:ASN:ND2	1:A:359:ARG:HH22	2.05	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:193:LYS:HG2	1:A:194:ASP:N	2.22	0.55
1:A:219:ASP:OD1	1:A:219:ASP:N	2.37	0.55
1:C:177:LYS:HA	1:C:207:THR:HG22	1.89	0.55
1:D:353:ARG:HG3	1:D:353:ARG:NH1	2.22	0.55
2:B:280:ASP:OD2	2:B:280:ASP:N	2.40	0.55
1:C:143:GLU:O	1:C:146:LYS:HB3	2.07	0.54
1:C:31:VAL:HG21	1:C:64:LEU:HD21	1.90	0.54
1:F:103:ALA:HB3	1:F:154:ILE:HG23	1.89	0.54
1:C:395:ILE:O	1:C:395:ILE:HG12	2.06	0.54
1:C:167:ASN:O	1:C:169:ARG:N	2.39	0.54
1:D:165:MET:HB3	1:D:171:LEU:CD2	2.33	0.54
1:A:254:GLU:O	1:A:377:THR:HG23	2.08	0.54
1:F:95:GLU:OE2	1:F:97:ASP:HB3	2.07	0.54
2:B:356:VAL:CG1	2:B:356:VAL:O	2.56	0.54
1:F:318:PHE:HA	1:F:323:SER:OG	2.07	0.54
1:F:281:THR:O	1:F:285:VAL:HG23	2.07	0.54
2:E:387:LEU:HB3	2:E:401:MSE:HE1	1.90	0.54
1:A:114:GLN:NE2	1:A:114:GLN:HA	2.23	0.54
1:C:200:PHE:C	1:C:202:LYS:H	2.10	0.54
1:C:267:TYR:HA	1:C:270:LEU:HD23	1.88	0.54
1:C:300:SER:HB3	1:C:326:LEU:HD23	1.89	0.54
2:B:333:MSE:CA	2:B:333:MSE:HE3	2.38	0.54
1:C:384:LEU:HD23	1:C:384:LEU:C	2.28	0.54
1:D:63:ILE:HG23	1:D:92:GLN:HE22	1.73	0.53
1:D:209:VAL:HG12	1:D:228:MET:HE3	1.90	0.53
2:E:378:SER:OG	2:E:382:MSE:HE2	2.08	0.53
1:A:249:PHE:HA	1:A:396:GLU:O	2.08	0.53
2:E:320:GLY:C	2:E:322:GLN:H	2.12	0.53
1:C:333:ALA:HA	1:C:336:ILE:CG2	2.38	0.53
1:F:308:GLN:HB3	1:F:311:ARG:NH1	2.24	0.53
1:A:221:LEU:O	1:A:224:THR:HB	2.08	0.53
1:F:152:PRO:HG3	1:F:155:ILE:HD11	1.90	0.53
1:C:350:PRO:HG3	1:C:359:ARG:CZ	2.38	0.53
2:E:419:VAL:O	2:E:422:SER:HB3	2.08	0.53
1:D:281:THR:HG21	2:E:183:GLU:CG	2.36	0.53
2:E:171:ILE:HD11	2:E:187:MSE:HE2	1.90	0.53
1:C:65:PRO:O	1:C:70:TYR:HB2	2.09	0.53
1:D:320:SER:O	1:D:321:GLY:C	2.47	0.53
1:C:346:ASN:HD22	1:C:374:ASN:ND2	2.06	0.53
1:F:246:ILE:HG13	1:F:246:ILE:O	2.07	0.53
1:F:152:PRO:HB3	1:F:155:ILE:HD11	1.90	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:393:SER:O	2:E:394:SER:HB2	2.07	0.53
1:A:93:GLN:O	1:A:177:LYS:NZ	2.37	0.53
1:D:353:ARG:NE	2:E:322:GLN:O	2.42	0.52
1:A:344:VAL:O	1:A:372:ALA:HA	2.09	0.52
1:A:121:MET:HE2	1:A:124:GLY:HA3	1.89	0.52
1:D:278:PHE:HB3	1:D:359:ARG:NH1	2.24	0.52
1:F:207:THR:O	1:F:209:VAL:HG23	2.09	0.52
1:A:63:ILE:O	1:A:63:ILE:CG1	2.57	0.52
2:E:283:LYS:O	2:E:285:THR:HG23	2.08	0.52
1:C:303:HIS:N	1:C:303:HIS:CD2	2.78	0.52
1:C:206:ASN:ND2	1:C:206:ASN:H	2.07	0.52
1:C:251:ILE:CG1	1:C:252:ASN:N	2.72	0.52
1:D:352:ASN:HB3	1:D:355:ASN:HD22	1.73	0.52
1:D:356:TYR:O	1:D:359:ARG:HB2	2.10	0.52
1:A:80:THR:O	1:A:86:PHE:HB2	2.10	0.52
1:C:57:ALA:HB3	1:C:59:GLN:HE21	1.75	0.52
1:F:247:ARG:HG2	1:F:249:PHE:HE1	1.75	0.52
2:E:412:ILE:O	2:E:416:ASN:HB2	2.08	0.52
1:A:288:LEU:HG	1:A:288:LEU:O	2.10	0.52
1:F:279:ILE:CD1	1:F:281:THR:O	2.58	0.52
1:F:117:GLN:HG2	1:F:133:ALA:HB2	1.91	0.52
1:D:125:ASP:OD1	1:D:125:ASP:N	2.43	0.52
1:C:37:MET:HG2	1:C:39:LEU:HG	1.92	0.52
1:F:274:GLN:NE2	1:F:342:SER:HB2	2.23	0.52
2:E:201:PRO:HG2	2:E:239:SER:OG	2.10	0.52
2:E:390:LEU:HD13	2:E:396:ILE:HD12	1.92	0.52
2:B:169:THR:HB	2:B:170:PRO:HD3	1.92	0.52
2:E:356:VAL:O	2:E:356:VAL:HG13	2.10	0.52
2:E:269:VAL:O	2:E:272:GLY:N	2.42	0.52
1:C:167:ASN:C	1:C:169:ARG:N	2.63	0.52
1:F:105:VAL:HB	1:F:156:VAL:HB	1.92	0.52
1:C:173:PRO:C	1:C:176:ILE:HD13	2.31	0.51
1:D:278:PHE:CD1	1:D:359:ARG:HD3	2.45	0.51
1:C:61:ARG:HD2	1:C:234:ILE:HG23	1.91	0.51
1:A:63:ILE:O	1:A:63:ILE:HD12	2.10	0.51
2:E:233:THR:O	2:E:237:GLU:OE2	2.27	0.51
1:A:302:MET:HB3	1:A:328:THR:HG23	1.91	0.51
1:F:350:PRO:HG2	1:F:356:TYR:HB2	1.92	0.51
1:D:385:ARG:O	1:D:389:THR:HG22	2.10	0.51
1:A:377:THR:HG22	1:A:378:GLU:H	1.72	0.51
2:E:413:PRO:O	2:E:416:ASN:HB3	2.11	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:98:LEU:HD21	1:D:175:TYR:CD1	2.45	0.51
1:C:339:GLN:CD	1:C:340:GLN:H	2.14	0.51
1:F:115:GLN:O	1:F:119:VAL:CG2	2.39	0.51
2:B:269:VAL:O	2:B:271:ASP:N	2.44	0.51
1:F:154:ILE:CG2	1:F:155:ILE:N	2.73	0.51
1:A:167:ASN:CG	1:A:167:ASN:O	2.49	0.51
1:D:147:LEU:HG	1:D:171:LEU:HD11	1.93	0.51
1:D:377:THR:CG2	1:D:378:GLU:N	2.73	0.51
1:A:252:ASN:O	1:A:253:VAL:O	2.29	0.51
1:F:279:ILE:HG22	1:F:347:TYR:HB3	1.93	0.51
1:C:190:ARG:NH1	1:C:190:ARG:CG	2.69	0.51
1:C:166:LEU:HD23	1:C:171:LEU:HB3	1.92	0.51
1:A:116:ILE:O	1:A:120:VAL:HG23	2.11	0.51
1:C:37:MET:HE2	1:C:39:LEU:HD11	1.91	0.51
1:D:190:ARG:O	2:E:255:PRO:HG2	2.11	0.51
2:B:236:VAL:HG12	2:B:274:LEU:CD1	2.41	0.51
1:A:117:GLN:NE2	1:A:121:MET:HG3	2.25	0.51
1:C:251:ILE:HD12	1:C:252:ASN:H	1.75	0.51
1:C:315:MET:SD	1:C:337:ASP:OD2	2.69	0.51
1:A:252:ASN:HA	1:A:376:VAL:HG22	1.91	0.51
2:B:238:LYS:HE3	1:D:138:THR:O	2.10	0.51
1:C:168:ARG:C	1:C:170:TYR:H	2.13	0.51
1:C:57:ALA:C	1:C:59:GLN:N	2.63	0.51
1:F:308:GLN:HA	1:F:311:ARG:HD3	1.91	0.51
2:E:412:ILE:HA	2:E:415:ILE:HD12	1.92	0.51
1:D:77:GLN:O	1:D:80:THR:HG22	2.11	0.51
1:A:63:ILE:O	1:A:63:ILE:HG13	2.09	0.51
2:B:189:ARG:HG3	2:B:189:ARG:HH11	1.74	0.51
1:C:63:ILE:HG23	1:C:64:LEU:HG	1.93	0.51
1:F:279:ILE:HD12	1:F:281:THR:H	1.76	0.51
1:D:357:ILE:HG23	1:D:358:HIS:N	2.26	0.51
1:C:276:VAL:HG22	1:C:326:LEU:HB3	1.92	0.51
1:F:319:ARG:HB2	1:F:340:GLN:OE1	2.12	0.51
1:C:94:ILE:HG12	1:C:95:GLU:N	2.26	0.50
1:D:336:ILE:HG13	1:D:337:ASP:N	2.26	0.50
1:C:270:LEU:HD12	1:C:272:ILE:N	2.22	0.50
2:E:214:SER:O	2:E:218:MSE:HG3	2.11	0.50
1:A:302:MET:HB2	1:A:326:LEU:HD11	1.92	0.50
2:E:344:ILE:HG23	2:E:386:LEU:CD1	2.41	0.50
1:D:385:ARG:O	1:D:389:THR:CG2	2.60	0.50
1:C:246:ILE:CG2	1:C:246:ILE:O	2.60	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:345:ILE:HD13	1:A:345:ILE:C	2.32	0.50
1:A:126:TYR:N	1:A:126:TYR:CD2	2.79	0.50
1:D:280:ASN:ND2	1:D:348:ASP:HB2	2.27	0.50
2:E:283:LYS:O	2:E:284:GLY:C	2.50	0.50
1:A:96:LEU:HD13	1:A:127:MET:O	2.12	0.50
1:A:377:THR:CG2	1:A:378:GLU:H	2.25	0.50
2:E:257:ALA:N	2:E:258:PRO:CD	2.75	0.50
1:F:163:PHE:HE1	1:F:198:ASP:HB3	1.77	0.50
1:C:308:GLN:HA	1:C:311:ARG:HB2	1.94	0.50
1:F:117:GLN:HG2	1:F:133:ALA:CB	2.41	0.49
1:F:99:LYS:HE2	1:F:150:GLU:HB2	1.94	0.49
1:C:281:THR:OG1	1:C:284:LYS:HB2	2.12	0.49
1:C:279:ILE:HG22	1:C:347:TYR:HB3	1.95	0.49
1:A:63:ILE:HG23	1:A:64:LEU:HD22	1.94	0.49
2:B:334:LEU:HG	2:B:350:CYS:HB2	1.94	0.49
1:F:151:ALA:HB1	1:F:152:PRO:HD2	1.95	0.49
2:E:237:GLU:HG3	2:E:278:TYR:CD1	2.48	0.49
1:C:332:LEU:C	1:C:334:ARG:H	2.14	0.49
1:D:245:GLY:O	1:D:369:LYS:N	2.45	0.49
1:C:187:MET:O	1:C:192:PHE:HB2	2.13	0.49
1:C:143:GLU:HG3	1:C:144:VAL:N	2.27	0.49
1:A:114:GLN:HE21	1:A:114:GLN:HA	1.78	0.49
1:C:84:ALA:O	1:C:88:ILE:HG12	2.12	0.49
1:C:354:GLU:O	1:C:357:ILE:HG12	2.12	0.49
1:D:91:LEU:O	1:D:94:ILE:HD12	2.13	0.48
1:A:338:VAL:HG22	1:A:338:VAL:O	2.12	0.48
2:E:215:HIS:CE1	5:E:17:HOH:O	2.65	0.48
1:D:303:HIS:O	1:D:311:ARG:NH2	2.44	0.48
1:C:249:PHE:HD2	1:C:397:GLU:O	1.94	0.48
2:B:413:PRO:O	2:B:416:ASN:HB3	2.14	0.48
1:C:64:LEU:N	1:C:65:PRO:CD	2.76	0.48
1:C:377:THR:H	1:C:380:ASP:HB2	1.79	0.48
1:A:96:LEU:HD11	1:A:127:MET:HB3	1.95	0.48
1:F:285:VAL:HG13	1:F:327:ILE:HG22	1.95	0.48
1:F:343:LEU:HD11	1:F:373:ILE:HD11	1.94	0.48
1:D:108:PRO:O	1:D:190:ARG:NH1	2.46	0.48
1:C:168:ARG:O	1:C:170:TYR:N	2.46	0.48
2:E:344:ILE:HG23	2:E:386:LEU:HD13	1.95	0.48
1:F:188:LEU:CD1	1:F:193:LYS:HG2	2.37	0.48
1:A:27:TRP:O	1:A:28:ASN:C	2.53	0.48
1:D:88:ILE:O	1:D:89:SER:C	2.52	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:322:SER:O	1:D:323:SER:HB2	2.13	0.48
1:A:239:GLU:OE1	1:A:365:ARG:N	2.47	0.48
1:D:377:THR:HG23	1:D:378:GLU:N	2.29	0.48
1:A:268:GLU:O	1:A:269:THR:C	2.52	0.48
1:C:311:ARG:HH22	1:C:334:ARG:HB3	1.79	0.47
2:B:215:HIS:CA	2:B:218:MSE:HE3	2.39	0.47
1:C:353:ARG:HH11	1:C:353:ARG:N	2.08	0.47
1:C:332:LEU:C	1:C:334:ARG:N	2.68	0.47
1:F:167:ASN:C	1:F:169:ARG:H	2.18	0.47
2:B:419:VAL:HB	2:B:422:SER:HB3	1.96	0.47
1:C:293:HIS:O	1:C:294:ALA:C	2.52	0.47
1:A:346:ASN:HB2	1:A:374:ASN:HD22	1.79	0.47
1:F:339:GLN:C	1:F:341:VAL:H	2.17	0.47
1:F:197:TYR:HE2	1:F:223:VAL:HG22	1.80	0.47
2:E:353:GLU:OE2	1:F:283:ARG:NH2	2.37	0.47
1:D:271:THR:HG23	1:D:271:THR:O	2.14	0.47
1:C:190:ARG:HG3	1:C:190:ARG:NH1	2.29	0.47
1:C:190:ARG:HG2	1:C:190:ARG:HH11	1.75	0.47
2:B:236:VAL:CG1	2:B:274:LEU:HD12	2.45	0.47
1:F:385:ARG:HA	1:F:385:ARG:NE	2.29	0.47
2:E:184:VAL:HG11	2:E:222:LEU:HD11	1.97	0.47
2:E:411:GLU:O	2:E:415:ILE:HG13	2.15	0.47
1:C:302:MET:HE3	1:C:332:LEU:HD12	1.96	0.47
1:C:164:ASP:OD1	1:C:168:ARG:HD2	2.14	0.47
1:D:279:ILE:HD13	1:D:347:TYR:HB3	1.97	0.47
1:A:246:ILE:HD11	1:A:362:ARG:CZ	2.45	0.47
1:F:105:VAL:O	1:F:156:VAL:HA	2.15	0.47
1:A:173:PRO:HA	1:A:176:ILE:HD12	1.95	0.47
1:D:146:LYS:O	1:D:147:LEU:C	2.53	0.47
1:A:91:LEU:HA	1:A:94:ILE:HD12	1.95	0.47
1:C:247:ARG:HG2	1:C:249:PHE:HE1	1.79	0.47
1:C:331:LEU:O	1:C:333:ALA:N	2.48	0.47
1:F:308:GLN:CB	1:F:311:ARG:HH11	2.28	0.47
1:D:94:ILE:HD11	1:D:154:ILE:HD11	1.97	0.47
1:F:267:TYR:CE2	1:F:297:PHE:HD1	2.33	0.47
1:D:240:GLU:HB2	2:E:399:ASP:OD2	2.15	0.47
1:A:155:ILE:HG13	1:A:171:LEU:HD11	1.97	0.47
1:A:121:MET:CE	1:A:121:MET:CA	2.75	0.47
1:F:166:LEU:HD21	1:F:173:PRO:HG3	1.96	0.47
2:E:381:LYS:HG2	2:E:382:MSE:N	2.30	0.47
1:D:137:GLY:O	1:D:140:VAL:HG22	2.15	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:257:GLU:HG2	5:C:3:HOH:O	2.15	0.47
1:D:114:GLN:CA	1:D:114:GLN:HE21	2.28	0.47
2:B:189:ARG:C	2:B:191:LEU:H	2.18	0.46
1:F:96:LEU:HD21	1:F:153:HIS:HE1	1.80	0.46
1:D:382:ARG:H	1:D:382:ARG:HD2	1.80	0.46
1:F:144:VAL:CG1	1:F:145:GLN:N	2.78	0.46
1:C:314:ILE:O	1:C:318:PHE:N	2.44	0.46
1:D:311:ARG:HG3	1:D:314:ILE:CG2	2.46	0.46
1:D:159:PRO:HG2	1:D:192:PHE:CG	2.50	0.46
2:E:445:ASP:O	2:E:446:LEU:HD23	2.15	0.46
1:F:166:LEU:CD2	1:F:173:PRO:HG3	2.46	0.46
2:B:319:GLY:C	2:B:321:GLN:H	2.18	0.46
2:E:231:MSE:HE3	2:E:231:MSE:HB2	1.94	0.46
1:C:384:LEU:HD23	1:C:384:LEU:O	2.16	0.46
1:A:88:ILE:HD11	1:A:123:LEU:HD13	1.97	0.46
1:D:216:MET:N	1:D:217:PRO:CD	2.79	0.46
1:D:379:GLU:OE2	1:D:379:GLU:N	2.47	0.46
1:D:135:ILE:HA	1:D:135:ILE:HD12	1.61	0.46
1:C:279:ILE:HG13	1:C:285:VAL:HG23	1.97	0.46
1:C:37:MET:N	1:C:37:MET:SD	2.73	0.46
1:F:152:PRO:HB3	1:F:155:ILE:CD1	2.45	0.46
1:A:255:ARG:HB2	1:A:255:ARG:NH1	2.30	0.46
1:F:263:LEU:HD12	1:F:292:MET:SD	2.56	0.46
1:C:102:GLN:HA	1:C:176:ILE:HA	1.98	0.46
1:D:27:TRP:O	1:D:28:ASN:C	2.54	0.46
1:C:31:VAL:HB	1:C:63:ILE:CG2	2.46	0.46
1:A:73:ILE:HD11	1:A:224:THR:HG23	1.98	0.46
1:A:311:ARG:HB2	1:A:314:ILE:HG22	1.98	0.46
1:A:88:ILE:HD13	1:A:88:ILE:N	2.30	0.46
2:E:201:PRO:HB2	2:E:239:SER:HB3	1.97	0.46
1:A:114:GLN:NE2	1:A:114:GLN:CA	2.78	0.46
1:C:90:ILE:HD11	1:C:180:VAL:HG21	1.97	0.46
1:A:216:MET:N	1:A:217:PRO:CD	2.78	0.46
1:F:295:ARG:HD3	1:F:297:PHE:HE2	1.81	0.46
1:A:255:ARG:CB	1:A:255:ARG:HH11	2.29	0.46
1:C:378:GLU:CA	1:C:381:LYS:HD3	2.27	0.45
1:A:283:ARG:HH21	2:B:183:GLU:HG2	1.81	0.45
1:C:63:ILE:HG23	1:C:64:LEU:N	2.31	0.45
1:D:390:PHE:HD2	1:D:391:TYR:CD1	2.33	0.45
1:D:390:PHE:HD2	1:D:391:TYR:CE1	2.34	0.45
1:C:349:LEU:HD21	1:C:384:LEU:HD12	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:224:THR:HG22	1:A:225:LYS:N	2.31	0.45
1:A:82:LYS:O	1:A:119:VAL:HG21	2.16	0.45
1:A:101:THR:HA	1:A:152:PRO:O	2.16	0.45
1:C:117:GLN:HE21	1:C:118:LYS:HG3	1.82	0.45
1:F:141:ARG:HA	1:F:144:VAL:HG12	1.98	0.45
1:F:144:VAL:HG13	1:F:145:GLN:N	2.32	0.45
2:E:227:CYS:SG	2:E:273:ILE:HG22	2.57	0.45
2:E:175:TYR:HA	2:E:178:HIS:CE1	2.51	0.45
1:F:395:ILE:O	1:F:395:ILE:CG1	2.55	0.45
1:D:339:GLN:O	1:D:362:ARG:HD3	2.16	0.45
1:F:197:TYR:CE2	1:F:223:VAL:HG22	2.51	0.45
1:C:154:ILE:HG22	1:C:155:ILE:N	2.31	0.45
2:E:348:GLU:O	2:E:352:LYS:HD2	2.16	0.45
2:B:303:SER:O	2:B:306:LYS:HG3	2.16	0.45
2:E:442:GLN:NE2	2:E:442:GLN:N	2.28	0.45
1:C:37:MET:O	1:C:38:ASN:C	2.55	0.45
1:D:357:ILE:O	1:D:357:ILE:HG13	2.16	0.45
1:F:151:ALA:CB	1:F:152:PRO:HD2	2.46	0.45
2:B:339:LEU:HD22	2:B:382:MSE:HE3	1.98	0.45
2:B:184:VAL:HG11	2:B:222:LEU:HD11	1.99	0.45
2:E:417:LEU:O	1:F:160:GLY:HA3	2.17	0.45
2:E:426:LEU:HD21	2:E:447:CYS:SG	2.57	0.45
1:D:249:PHE:O	1:D:373:ILE:HA	2.16	0.45
1:D:238:LYS:CB	1:D:238:LYS:NZ	2.80	0.45
1:C:204:ASN:HB3	1:C:206:ASN:HD21	1.81	0.45
1:A:135:ILE:HD12	1:A:135:ILE:HA	1.77	0.45
1:C:136:GLY:HA2	1:C:140:VAL:CG1	2.47	0.45
1:A:253:VAL:HG12	1:A:254:GLU:N	2.31	0.45
2:E:420:PRO:C	2:E:422:SER:H	2.19	0.45
1:A:286:ASP:O	1:A:287:TRP:C	2.55	0.45
1:A:105:VAL:HB	1:A:156:VAL:HB	1.99	0.45
2:E:256:ARG:O	2:E:260:LEU:HD12	2.16	0.45
1:C:279:ILE:CD1	1:C:281:THR:O	2.64	0.45
1:A:367:GLY:O	1:A:369:LYS:HB3	2.16	0.45
1:F:260:LEU:O	1:F:260:LEU:HD12	2.17	0.45
1:F:266:LEU:HA	1:F:269:THR:HG22	1.98	0.45
1:A:238:LYS:HG2	1:A:239:GLU:O	2.16	0.45
1:A:166:LEU:HG	1:A:171:LEU:HD22	1.98	0.45
1:C:47:ILE:HA	1:C:47:ILE:HD13	1.78	0.45
2:B:370:MSE:O	2:B:374:SER:HB3	2.16	0.45
1:C:271:THR:O	1:C:271:THR:CG2	2.65	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:82:LYS:HG3	1:C:212:LEU:HD22	1.98	0.45
1:A:252:ASN:O	1:A:253:VAL:C	2.55	0.45
1:C:278:PHE:CG	1:C:359:ARG:HG2	2.51	0.45
2:E:390:LEU:HD13	2:E:396:ILE:CD1	2.47	0.45
1:C:194:ASP:N	1:C:194:ASP:OD2	2.50	0.45
2:E:363:LEU:C	2:E:363:LEU:HD13	2.37	0.45
1:F:219:ASP:OD1	1:F:219:ASP:N	2.49	0.45
1:A:238:LYS:CG	1:A:239:GLU:N	2.80	0.44
1:F:102:GLN:HG2	1:F:175:TYR:HB3	1.98	0.44
1:C:200:PHE:C	1:C:202:LYS:N	2.71	0.44
1:A:247:ARG:HD2	1:A:249:PHE:CZ	2.52	0.44
1:F:124:GLY:HA3	1:F:125:ASP:HA	1.72	0.44
1:C:172:SER:O	1:C:176:ILE:HD11	2.17	0.44
1:C:76:ALA:HB3	1:C:82:LYS:HD2	2.00	0.44
1:A:27:TRP:HA	1:A:237:LYS:O	2.16	0.44
1:F:303:HIS:O	1:F:332:LEU:HD22	2.17	0.44
1:A:155:ILE:HG23	1:A:155:ILE:HD12	1.78	0.44
2:E:434:PHE:HE1	2:E:441:LYS:N	2.15	0.44
1:F:279:ILE:HD11	1:F:285:VAL:HG22	1.98	0.44
1:C:36:ASP:C	1:C:38:ASN:H	2.21	0.44
1:D:267:TYR:HE1	1:D:325:VAL:HG21	1.83	0.44
2:B:425:VAL:O	2:B:426:LEU:C	2.56	0.44
1:F:177:LYS:C	1:F:207:THR:HG23	2.38	0.44
1:F:356:TYR:O	1:F:360:ILE:HG13	2.17	0.44
2:B:361:HIS:ND1	2:B:407:ARG:NH1	2.66	0.44
1:F:135:ILE:H	1:F:135:ILE:HG13	1.56	0.44
1:C:279:ILE:C	1:C:279:ILE:HD12	2.38	0.44
1:D:354:GLU:OE1	2:E:356:VAL:CG2	2.66	0.44
1:D:252:ASN:ND2	1:D:381:LYS:HD3	2.32	0.44
2:B:200:VAL:N	2:B:201:PRO:CD	2.81	0.44
2:B:368:ILE:HG21	2:B:408:ILE:HG13	2.00	0.44
1:D:297:PHE:HB2	1:D:299:VAL:HG23	1.99	0.44
2:B:269:VAL:O	2:B:270:GLY:C	2.55	0.44
1:D:114:GLN:HA	1:D:114:GLN:HE21	1.83	0.44
2:B:268:ALA:HB1	2:B:273:ILE:HG13	2.00	0.44
1:F:279:ILE:C	1:F:279:ILE:HD12	2.38	0.44
1:C:171:LEU:HD12	1:C:171:LEU:HA	1.92	0.44
2:E:197:LYS:HD2	2:E:235:ASP:OD2	2.17	0.44
1:D:280:ASN:N	1:D:280:ASN:HD22	2.16	0.44
2:E:169:THR:HB	2:E:170:PRO:HD3	2.00	0.44
1:C:270:LEU:CG	1:C:271:THR:N	2.79	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:303:HIS:O	1:C:332:LEU:CD2	2.64	0.43
1:C:348:ASP:O	1:C:359:ARG:NH2	2.50	0.43
1:D:354:GLU:OE1	2:E:356:VAL:HG22	2.18	0.43
1:C:277:ILE:HD12	1:C:325:VAL:HG11	2.01	0.43
2:E:443:LEU:HA	2:E:443:LEU:HD22	1.80	0.43
2:E:434:PHE:CE1	2:E:441:LYS:CA	2.80	0.43
1:A:280:ASN:HD21	1:A:359:ARG:HH22	1.65	0.43
1:A:253:VAL:HG13	1:A:258:TRP:CB	2.48	0.43
2:B:247:LEU:HD23	2:B:247:LEU:HA	1.75	0.43
1:D:140:VAL:O	1:D:141:ARG:C	2.56	0.43
2:E:168:LEU:CD1	2:E:200:VAL:HG22	2.48	0.43
1:A:377:THR:HG21	1:A:379:GLU:OE2	2.18	0.43
1:D:64:LEU:HB3	1:D:65:PRO:CD	2.48	0.43
1:C:39:LEU:HD12	1:C:39:LEU:H	1.83	0.43
1:C:337:ASP:HB3	1:C:339:GLN:OE1	2.18	0.43
1:D:322:SER:O	1:D:323:SER:CB	2.66	0.43
2:E:317:SER:HB3	2:E:326:HIS:HE1	1.83	0.43
1:C:137:GLY:O	1:C:140:VAL:HG13	2.18	0.43
1:A:295:ARG:HB3	1:A:297:PHE:CE2	2.51	0.43
1:C:249:PHE:CE2	1:C:397:GLU:O	2.71	0.43
2:B:418:ASP:OD1	1:C:158:THR:OG1	2.19	0.43
2:B:263:GLN:NE2	2:B:314:VAL:HG22	2.33	0.43
1:A:91:LEU:HD23	1:A:91:LEU:HA	1.85	0.43
1:C:352:ASN:HA	1:C:353:ARG:HH11	1.79	0.43
1:A:112:LEU:O	1:A:112:LEU:HD22	2.19	0.43
1:A:345:ILE:HD11	1:A:375:MET:HE3	1.99	0.43
1:C:268:GLU:H	1:C:268:GLU:HG2	1.59	0.43
1:C:224:THR:HG22	1:C:228:MET:SD	2.58	0.43
2:E:226:LEU:HD22	2:E:230:VAL:HG11	2.00	0.43
2:E:226:LEU:O	2:E:230:VAL:HG12	2.19	0.43
1:D:353:ARG:HH21	2:E:323:SER:HA	1.83	0.43
1:A:216:MET:N	1:A:217:PRO:HD3	2.34	0.43
1:A:133:ALA:HA	1:A:156:VAL:O	2.18	0.43
1:D:95:GLU:O	1:D:97:ASP:N	2.51	0.43
1:A:117:GLN:HG2	1:A:131:CYS:SG	2.58	0.43
1:A:141:ARG:HH22	2:E:281:SER:HG	1.63	0.43
1:F:277:ILE:HB	1:F:327:ILE:HG12	2.00	0.43
2:E:322:GLN:HE21	2:E:322:GLN:HB3	1.40	0.43
2:E:418:ASP:OD1	1:F:161:ARG:HD2	2.19	0.43
1:D:121:MET:CE	1:D:121:MET:HA	2.49	0.43
2:E:257:ALA:O	2:E:261:VAL:HG23	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:308:GLN:HA	1:F:311:ARG:HB2	2.01	0.43
1:A:267:TYR:CE1	1:A:272:ILE:HD11	2.54	0.43
2:B:444:ARG:HD2	2:B:445:ASP:OD1	2.19	0.43
1:A:159:PRO:HG2	1:A:192:PHE:HB3	2.01	0.43
1:A:192:PHE:CE1	2:B:255:PRO:HD3	2.53	0.43
1:A:399:PRO:HB2	1:A:401:ASN:OD1	2.18	0.43
1:A:281:THR:HG21	2:B:183:GLU:HG3	2.01	0.43
1:D:237:LYS:HD3	1:D:237:LYS:HA	1.91	0.43
1:D:190:ARG:HH21	2:E:254:THR:HG23	1.84	0.43
1:F:185:ASP:H	1:F:213:SER:HG	1.66	0.43
1:C:67:ILE:HD12	1:C:89:SER:HA	2.01	0.43
1:D:277:ILE:HG12	1:D:345:ILE:HG23	2.01	0.43
1:C:385:ARG:HA	1:C:385:ARG:HD3	1.67	0.43
1:A:252:ASN:C	1:A:253:VAL:O	2.56	0.42
2:E:265:ILE:O	2:E:268:ALA:N	2.52	0.42
1:C:234:ILE:CG2	1:C:235:LEU:N	2.82	0.42
2:E:370:MSE:HE2	2:E:383:ILE:HD11	2.00	0.42
1:D:339:GLN:N	1:D:339:GLN:HE21	2.17	0.42
2:B:333:MSE:O	2:B:333:MSE:HE3	2.18	0.42
1:C:140:VAL:HA	1:C:143:GLU:HB3	1.99	0.42
1:A:352:ASN:OD1	2:B:320:GLY:HA3	2.19	0.42
2:B:349:HIS:O	2:B:353:GLU:HG3	2.20	0.42
2:E:441:LYS:O	2:E:442:GLN:C	2.57	0.42
1:A:282:ARG:HA	1:A:285:VAL:HB	2.01	0.42
1:A:278:PHE:HB2	1:A:346:ASN:ND2	2.33	0.42
1:C:267:TYR:HA	1:C:270:LEU:CD2	2.49	0.42
1:A:295:ARG:CG	1:A:295:ARG:HH11	2.18	0.42
1:F:354:GLU:N	1:F:354:GLU:CD	2.69	0.42
2:E:382:MSE:O	2:E:383:ILE:C	2.57	0.42
1:C:384:LEU:C	1:C:386:ASP:N	2.72	0.42
1:A:63:ILE:O	1:A:63:ILE:CD1	2.66	0.42
1:D:388:GLU:HB2	1:D:395:ILE:CD1	2.46	0.42
1:A:251:ILE:HD11	1:A:398:MET:CE	2.48	0.42
1:F:152:PRO:CB	1:F:155:ILE:HD11	2.49	0.42
1:A:178:MET:HE3	1:A:178:MET:HB3	1.74	0.42
1:C:188:LEU:HD13	1:C:188:LEU:HA	1.84	0.42
2:B:346:GLU:HG2	1:C:281:THR:HG21	2.01	0.42
1:F:279:ILE:HG13	1:F:285:VAL:HG22	2.00	0.42
1:F:308:GLN:HB3	1:F:311:ARG:HH11	1.83	0.42
1:C:278:PHE:CD1	1:C:359:ARG:HG2	2.54	0.42
1:D:250:TYR:CE1	1:D:397:GLU:HG3	2.55	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:166:LEU:HA	1:C:166:LEU:HD23	1.91	0.42
1:C:178:MET:HE3	1:C:179:PHE:H	1.84	0.42
2:B:346:GLU:OE1	1:C:283:ARG:HD2	2.19	0.42
1:A:346:ASN:HD21	1:A:359:ARG:HD3	1.84	0.42
1:C:353:ARG:O	1:C:356:TYR:N	2.50	0.42
1:F:167:ASN:O	1:F:169:ARG:N	2.53	0.42
1:D:203:LEU:HD13	1:D:207:THR:HG21	2.02	0.42
1:F:352:ASN:N	1:F:352:ASN:OD1	2.53	0.42
1:A:29:GLU:OE2	1:A:29:GLU:HA	2.19	0.42
2:B:174:GLU:O	2:B:175:TYR:C	2.58	0.42
1:C:253:VAL:CG2	1:C:255:ARG:O	2.64	0.41
1:D:108:PRO:CG	1:D:186:GLU:HB2	2.50	0.41
2:E:398:VAL:O	2:E:401:MSE:HB2	2.20	0.41
1:D:354:GLU:CG	2:E:356:VAL:HG23	2.50	0.41
2:B:237:GLU:HG2	2:B:278:TYR:CD1	2.54	0.41
1:C:147:LEU:HA	1:C:151:ALA:HB2	1.98	0.41
1:C:316:ARG:H	1:C:316:ARG:HG3	1.64	0.41
1:C:331:LEU:C	1:C:333:ALA:H	2.23	0.41
2:B:239:SER:O	2:B:242:LYS:HB3	2.20	0.41
2:B:279:ILE:HG23	2:B:295:LEU:HD22	2.02	0.41
1:C:396:GLU:H	1:C:396:GLU:CD	2.23	0.41
1:A:251:ILE:CG2	1:A:253:VAL:HG23	2.48	0.41
1:C:39:LEU:HD22	1:C:43:LEU:HD21	2.02	0.41
2:E:304:MSE:HA	1:F:293:HIS:ND1	2.36	0.41
1:F:308:GLN:CB	1:F:311:ARG:NH1	2.83	0.41
1:D:336:ILE:HG13	1:D:337:ASP:H	1.85	0.41
1:C:230:ASP:HA	1:C:231:PRO:HD3	1.77	0.41
2:B:417:LEU:O	1:C:160:GLY:HA3	2.20	0.41
2:E:329:LYS:O	2:E:333:MSE:HB2	2.20	0.41
1:A:279:ILE:CG1	1:A:285:VAL:HG23	2.50	0.41
2:E:197:LYS:HB3	2:E:235:ASP:OD2	2.20	0.41
1:C:56:SER:HA	1:C:60:GLN:NE2	2.35	0.41
1:D:121:MET:HE1	1:D:124:GLY:HA3	2.03	0.41
2:E:340:LEU:O	1:F:351:THR:OG1	2.27	0.41
1:A:388:GLU:HG2	1:A:393:THR:O	2.20	0.41
2:B:379:THR:O	2:B:380:PHE:C	2.57	0.41
2:B:330:GLU:HA	2:B:330:GLU:OE2	2.21	0.41
1:C:168:ARG:C	1:C:170:TYR:N	2.74	0.41
1:C:346:ASN:HD22	1:C:374:ASN:HD21	1.66	0.41
1:C:369:LYS:HA	1:C:369:LYS:CE	2.26	0.41
1:A:146:LYS:HG3	1:A:150:GLU:CD	2.41	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:369:LYS:HA	1:D:369:LYS:HD3	1.87	0.41
1:D:187:MET:HB2	1:D:187:MET:HE2	1.95	0.41
2:B:226:LEU:HD22	2:B:230:VAL:HG11	2.03	0.41
1:D:279:ILE:HG21	1:D:284:LYS:HG2	2.02	0.41
1:C:204:ASN:N	1:C:204:ASN:ND2	2.67	0.41
1:F:247:ARG:HG2	1:F:249:PHE:CE1	2.53	0.41
1:A:20:GLU:OE2	1:A:20:GLU:HA	2.21	0.41
2:E:292:ARG:HG3	2:E:292:ARG:O	2.19	0.41
1:A:288:LEU:O	1:A:292:MET:CG	2.68	0.41
1:C:272:ILE:HG22	1:C:274:GLN:HE21	1.73	0.41
1:D:267:TYR:CZ	1:D:297:PHE:HD1	2.39	0.41
1:C:176:ILE:O	1:C:207:THR:HG22	2.21	0.41
2:E:304:MSE:HE2	2:E:304:MSE:HB3	1.92	0.41
1:C:310:GLU:O	1:C:313:VAL:CG1	2.68	0.41
2:E:378:SER:O	2:E:382:MSE:HG2	2.21	0.41
1:A:64:LEU:HA	1:A:65:PRO:HD3	1.95	0.41
1:D:311:ARG:HG3	1:D:314:ILE:HG21	2.02	0.41
2:E:203:LEU:HA	2:E:203:LEU:HD23	1.67	0.41
2:B:203:LEU:HD23	2:B:203:LEU:HA	1.74	0.41
1:A:137:GLY:O	1:A:140:VAL:HG22	2.20	0.41
1:D:267:TYR:CE2	1:D:297:PHE:HD1	2.39	0.40
1:C:37:MET:HE3	1:C:39:LEU:HD21	2.04	0.40
2:E:365:TYR:CZ	2:E:369:ILE:CD1	3.03	0.40
1:D:381:LYS:HB2	1:D:382:ARG:HH11	1.86	0.40
1:C:185:ASP:OD1	1:C:185:ASP:N	2.55	0.40
1:C:154:ILE:CG2	1:C:155:ILE:N	2.84	0.40
2:E:317:SER:HB3	2:E:326:HIS:CE1	2.57	0.40
2:B:257:ALA:N	2:B:258:PRO:CD	2.84	0.40
1:D:133:ALA:HA	1:D:156:VAL:O	2.22	0.40
1:A:288:LEU:O	1:A:292:MET:HG3	2.20	0.40
2:B:183:GLU:OE1	2:B:187:MSE:HE2	2.21	0.40
1:F:374:ASN:OD1	1:F:395:ILE:HD13	2.21	0.40
2:B:231:MSE:HE3	2:B:236:VAL:HG22	2.03	0.40
1:D:150:GLU:O	1:D:151:ALA:C	2.59	0.40
1:A:98:LEU:HD21	1:A:175:TYR:HD1	1.75	0.40
1:D:28:ASN:O	1:D:28:ASN:ND2	2.44	0.40
2:E:411:GLU:O	2:E:411:GLU:HG2	2.21	0.40
1:F:277:ILE:HG12	1:F:345:ILE:HD12	2.02	0.40
1:F:155:ILE:HG13	1:F:171:LEU:HD11	2.03	0.40
2:B:283:LYS:O	2:B:284:GLY:C	2.59	0.40
1:A:89:SER:HB3	4:A:1:ACY:C	2.51	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:285:VAL:HG22	1:D:327:ILE:HG22	2.04	0.40
2:E:213:ALA:O	2:E:214:SER:C	2.59	0.40
1:F:152:PRO:CG	1:F:155:ILE:HD11	2.51	0.40
2:E:333:MSE:HG3	1:F:282:ARG:CZ	2.52	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	335/388 (86%)	297 (89%)	31 (9%)	7 (2%)	9 29
1	C	339/388 (87%)	265 (78%)	60 (18%)	14 (4%)	3 11
1	D	333/388 (86%)	288 (86%)	32 (10%)	13 (4%)	4 12
1	F	247/388 (64%)	198 (80%)	37 (15%)	12 (5%)	3 8
2	B	280/307 (91%)	250 (89%)	26 (9%)	4 (1%)	14 42
2	E	278/307 (91%)	226 (81%)	44 (16%)	8 (3%)	6 19
All	All	1812/2166 (84%)	1524 (84%)	230 (13%)	58 (3%)	5 17

All (58) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	28	ASN
1	A	253	VAL
1	A	291	LYS
1	A	296	ASP
2	B	270	GLY
1	C	174	LYS
1	D	27	TRP
1	F	153	HIS

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Mol	Chain	Res	Type
1	F	167	ASN
1	F	174	LYS
1	A	95	GLU
1	C	38	ASN
1	C	58	ILE
1	C	168	ARG
1	C	331	LEU
1	C	332	LEU
1	D	28	ASN
1	D	96	LEU
1	D	271	THR
1	D	321	GLY
1	D	381	LYS
2	E	192	ASN
2	E	284	GLY
2	E	321	GLN
1	F	309	LYS
1	A	92	GLN
2	B	190	ASP
2	B	269	VAL
2	B	312	ASP
1	C	57	ALA
1	C	69	GLY
1	C	96	LEU
1	D	89	SER
2	E	194	GLY
1	F	149	MET
1	F	152	PRO
1	F	338	VAL
1	A	268	GLU
1	C	201	GLN
1	D	126	TYR
2	E	421	HIS
1	F	175	TYR
1	F	340	GLN
1	D	296	ASP
2	E	270	GLY
1	F	168	ARG
1	C	85	THR
1	C	238	LYS
1	C	304	GLY
1	D	298	THR

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Mol	Chain	Res	Type
1	D	337	ASP
2	E	186	GLU
1	F	322	SER
1	C	65	PRO
1	F	217	PRO
2	E	316	GLY
1	D	30	ILE
1	D	151	ALA

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	303/342 (89%)	251 (83%)	52 (17%)	2 7
1	C	314/342 (92%)	256 (82%)	58 (18%)	2 6
1	D	305/342 (89%)	249 (82%)	56 (18%)	2 6
1	F	245/342 (72%)	177 (72%)	68 (28%)	0 1
2	B	251/259 (97%)	223 (89%)	28 (11%)	7 22
2	E	249/259 (96%)	215 (86%)	34 (14%)	4 13
All	All	1667/1886 (88%)	1371 (82%)	296 (18%)	2 6

All (296) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	20	GLU
1	A	22	VAL
1	A	63	ILE
1	A	66	CYS
1	A	67	ILE
1	A	80	THR
1	A	85	THR
1	A	104	LEU
1	A	112	LEU
1	A	114	GLN

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Mol	Chain	Res	Type
1	A	118	LYS
1	A	135	ILE
1	A	140	VAL
1	A	150	GLU
1	A	156	VAL
1	A	168	ARG
1	A	174	LYS
1	A	178	MET
1	A	195	GLN
1	A	212	LEU
1	A	216	MET
1	A	219	ASP
1	A	222	GLU
1	A	233	ARG
1	A	241	LEU
1	A	262	THR
1	A	263	LEU
1	A	266	LEU
1	A	279	ILE
1	A	282	ARG
1	A	285	VAL
1	A	290	GLU
1	A	291	LYS
1	A	295	ARG
1	A	299	VAL
1	A	303	HIS
1	A	315	MET
1	A	319	ARG
1	A	324	ARG
1	A	328	THR
1	A	331	LEU
1	A	334	ARG
1	A	336	ILE
1	A	342	SER
1	A	345	ILE
1	A	349	LEU
1	A	360	ILE
1	A	365	ARG
1	A	385	ARG
1	A	386	ASP
1	A	392	ASN
1	A	401	ASN

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Mol	Chain	Res	Type
2	B	164	PHE
2	B	183	GLU
2	B	191	LEU
2	B	196	MSE
2	B	203	LEU
2	B	223	LEU
2	B	224	SER
2	B	234	THR
2	B	237	GLU
2	B	245	LYS
2	B	259	GLN
2	B	267	ARG
2	B	275	CYS
2	B	280	ASP
2	B	286	VAL
2	B	322	GLN
2	B	325	ASN
2	B	329	LYS
2	B	333	MSE
2	B	356	VAL
2	B	378	SER
2	B	401	MSE
2	B	411	GLU
2	B	427	GLU
2	B	442	GLN
2	B	443	LEU
2	B	444	ARG
2	B	446	LEU
1	C	32	ASP
1	C	37	MET
1	C	39	LEU
1	C	42	SER
1	C	47	ILE
1	C	58	ILE
1	C	64	LEU
1	C	67	ILE
1	C	80	THR
1	C	92	GLN
1	C	98	LEU
1	C	102	GLN
1	C	111	GLU
1	C	117	GLN

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Mol	Chain	Res	Type
1	C	141	ARG
1	C	143	GLU
1	C	146	LYS
1	C	150	GLU
1	C	171	LEU
1	C	174	LYS
1	C	188	LEU
1	C	202	LYS
1	C	206	ASN
1	C	212	LEU
1	C	224	THR
1	C	225	LYS
1	C	246	ILE
1	C	251	ILE
1	C	255	ARG
1	C	256	GLU
1	C	258	TRP
1	C	261	ASP
1	C	263	LEU
1	C	266	LEU
1	C	267	TYR
1	C	268	GLU
1	C	269	THR
1	C	270	LEU
1	C	271	THR
1	C	273	THR
1	C	283	ARG
1	C	299	VAL
1	C	300	SER
1	C	303	HIS
1	C	307	ASP
1	C	308	GLN
1	C	316	ARG
1	C	323	SER
1	C	339	GLN
1	C	352	ASN
1	C	353	ARG
1	C	369	LYS
1	C	378	GLU
1	C	382	ARG
1	C	383	THR
1	C	393	THR

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Mol	Chain	Res	Type
1	C	395	ILE
1	C	396	GLU
1	D	19	MET
1	D	22	VAL
1	D	28	ASN
1	D	29	GLU
1	D	30	ILE
1	D	31	VAL
1	D	80	THR
1	D	82	LYS
1	D	85	THR
1	D	92	GLN
1	D	112	LEU
1	D	114	GLN
1	D	123	LEU
1	D	125	ASP
1	D	127	MET
1	D	135	ILE
1	D	140	VAL
1	D	156	VAL
1	D	169	ARG
1	D	171	LEU
1	D	201	GLN
1	D	202	LYS
1	D	212	LEU
1	D	233	ARG
1	D	238	LYS
1	D	239	GLU
1	D	241	LEU
1	D	243	LEU
1	D	248	GLN
1	D	257	GLU
1	D	262	THR
1	D	263	LEU
1	D	271	THR
1	D	272	ILE
1	D	280	ASN
1	D	282	ARG
1	D	300	SER
1	D	303	HIS
1	D	311	ARG
1	D	313	VAL

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Mol	Chain	Res	Type
1	D	316	ARG
1	D	317	GLU
1	D	319	ARG
1	D	331	LEU
1	D	339	GLN
1	D	340	GLN
1	D	342	SER
1	D	345	ILE
1	D	365	ARG
1	D	377	THR
1	D	381	LYS
1	D	385	ARG
1	D	386	ASP
1	D	389	THR
1	D	394	SER
1	D	400	LEU
2	E	181	THR
2	E	183	GLU
2	E	203	LEU
2	E	223	LEU
2	E	229	THR
2	E	231	MSE
2	E	232	SER
2	E	233	THR
2	E	234	THR
2	E	237	GLU
2	E	243	LEU
2	E	249	GLU
2	E	259	GLN
2	E	267	ARG
2	E	275	CYS
2	E	292	ARG
2	E	297	LYS
2	E	306	LYS
2	E	314	VAL
2	E	317	SER
2	E	322	GLN
2	E	325	ASN
2	E	334	LEU
2	E	363	LEU
2	E	370	MSE
2	E	375	THR

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Mol	Chain	Res	Type
2	E	381	LYS
2	E	382	MSE
2	E	410	ASN
2	E	432	GLU
2	E	442	GLN
2	E	443	LEU
2	E	444	ARG
2	E	450	ARG
1	F	88	ILE
1	F	91	LEU
1	F	92	GLN
1	F	95	GLU
1	F	96	LEU
1	F	109	THR
1	F	111	GLU
1	F	114	GLN
1	F	120	VAL
1	F	121	MET
1	F	135	ILE
1	F	138	THR
1	F	140	VAL
1	F	143	GLU
1	F	145	GLN
1	F	147	LEU
1	F	150	GLU
1	F	153	HIS
1	F	156	VAL
1	F	166	LEU
1	F	167	ASN
1	F	168	ARG
1	F	174	LYS
1	F	175	TYR
1	F	177	LYS
1	F	188	LEU
1	F	189	SER
1	F	194	ASP
1	F	198	ASP
1	F	213	SER
1	F	215	THR
1	F	216	MET
1	F	221	LEU
1	F	224	THR

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Mol	Chain	Res	Type
1	F	225	LYS
1	F	246	ILE
1	F	250	TYR
1	F	256	GLU
1	F	258	TRP
1	F	263	LEU
1	F	280	ASN
1	F	289	THR
1	F	298	THR
1	F	303	HIS
1	F	308	GLN
1	F	312	ASP
1	F	313	VAL
1	F	316	ARG
1	F	317	GLU
1	F	319	ARG
1	F	323	SER
1	F	332	LEU
1	F	334	ARG
1	F	338	VAL
1	F	339	GLN
1	F	351	THR
1	F	352	ASN
1	F	353	ARG
1	F	355	ASN
1	F	373	ILE
1	F	378	GLU
1	F	380	ASP
1	F	386	ASP
1	F	387	ILE
1	F	388	GLU
1	F	389	THR
1	F	392	ASN
1	F	395	ILE

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (64) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	92	GLN
1	A	114	GLN
1	A	115	GLN
1	A	145	GLN

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Mol	Chain	Res	Type
1	A	195	GLN
1	A	280	ASN
1	A	346	ASN
1	A	374	ASN
1	A	392	ASN
2	B	173	GLN
2	B	215	HIS
2	B	263	GLN
2	B	290	GLN
2	B	321	GLN
2	B	322	GLN
2	B	326	HIS
2	B	349	HIS
2	B	442	GLN
1	C	59	GLN
1	C	60	GLN
1	C	75	GLN
1	C	92	GLN
1	C	114	GLN
1	C	117	GLN
1	C	145	GLN
1	C	148	GLN
1	C	201	GLN
1	C	204	ASN
1	C	206	ASN
1	C	248	GLN
1	C	252	ASN
1	C	274	GLN
1	C	280	ASN
1	C	303	HIS
1	C	358	HIS
1	C	374	ASN
1	D	92	GLN
1	D	114	GLN
1	D	115	GLN
1	D	204	ASN
1	D	248	GLN
1	D	252	ASN
1	D	280	ASN
1	D	293	HIS
1	D	339	GLN
1	D	355	ASN

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Mol	Chain	Res	Type
1	D	358	HIS
2	E	215	HIS
2	E	321	GLN
2	E	322	GLN
2	E	360	HIS
2	E	421	HIS
2	E	442	GLN
1	F	114	GLN
1	F	132	HIS
1	F	145	GLN
1	F	148	GLN
1	F	153	HIS
1	F	167	ASN
1	F	201	GLN
1	F	248	GLN
1	F	280	ASN
1	F	355	ASN
1	F	358	HIS

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 carbohydrates in this entry.

5.6 Ligand geometry

5 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	$\#\|Z\| > 2$
4	ACY	A	1	-	1,3,3	1.84	0	0,3,3	0.00	-
3	EDO	A	2	-	3,3,3	0.54	0	2,2,2	0.33	0
3	EDO	A	3	-	3,3,3	0.60	0	2,2,2	0.27	0
3	EDO	D	1	-	3,3,3	0.54	0	2,2,2	0.57	0
4	ACY	D	2	-	1,3,3	1.29	0	0,3,3	0.00	-

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
4	ACY	A	1	-	-	0/0/0/0	0/0/0/0
3	EDO	A	2	-	-	0/1/1/1	0/0/0/0
3	EDO	A	3	-	-	0/1/1/1	0/0/0/0
3	EDO	D	1	-	-	0/1/1/1	0/0/0/0
4	ACY	D	2	-	-	0/0/0/0	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.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	1	ACY	1	0
3	A	3	EDO	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	343/388 (88%)	0.23	12 (3%) 48 35	30, 64, 115, 161	0
1	C	351/388 (90%)	0.64	35 (9%) 9 4	56, 125, 160, 163	0
1	D	345/388 (88%)	0.16	11 (3%) 51 39	31, 68, 116, 160	0
1	F	271/388 (69%)	1.26	68 (25%) 1 0	69, 122, 155, 161	0
2	B	275/307 (89%)	-0.01	2 (0%) 89 84	36, 65, 90, 108	0
2	E	273/307 (88%)	-0.03	3 (1%) 82 74	37, 70, 92, 108	0
All	All	1858/2166 (85%)	0.37	131 (7%) 19 10	30, 84, 149, 163	0

All (131) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	48	TYR	7.9
1	F	175	TYR	6.9
1	C	389	THR	5.5
1	F	212	LEU	5.4
1	F	331	LEU	5.3
1	F	316	ARG	5.3
1	C	43	LEU	5.0
1	F	390	PHE	5.0
1	F	315	MET	4.8
1	F	371	VAL	4.7
1	C	175	TYR	4.7
1	F	89	SER	4.6
1	F	257	GLU	4.4
1	F	294	ALA	4.1
1	F	216	MET	4.1
1	F	122	ALA	4.0
1	C	384	LEU	3.9
1	F	209	VAL	3.7
1	C	324	ARG	3.7

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Mol	Chain	Res	Type	RSRZ
1	F	324	ARG	3.7
1	D	313	VAL	3.6
1	F	215	THR	3.6
1	F	343	LEU	3.6
1	C	237	LYS	3.6
1	F	396	GLU	3.5
1	F	256	GLU	3.5
1	C	395	ILE	3.5
1	F	398	MET	3.5
1	F	123	LEU	3.4
1	F	196	ILE	3.3
1	F	258	TRP	3.3
1	A	62	ALA	3.3
1	C	227	PHE	3.3
1	F	92	GLN	3.2
1	F	249	PHE	3.2
1	F	378	GLU	3.2
1	D	341	VAL	3.2
1	A	294	ALA	3.1
1	F	332	LEU	3.1
1	C	32	ASP	3.1
1	F	218	SER	3.1
1	F	150	GLU	3.1
1	F	90	ILE	3.1
1	F	374	ASN	3.1
1	D	339	GLN	3.0
1	F	268	GLU	3.0
1	C	121	MET	3.0
1	A	314	ILE	3.0
1	F	177	LYS	2.9
1	F	116	ILE	2.9
1	C	138	THR	2.9
1	F	169	ARG	2.9
1	F	219	ASP	2.9
1	F	344	VAL	2.9
1	C	373	ILE	2.9
1	C	269	THR	2.9
1	F	247	ARG	2.9
1	F	376	VAL	2.8
2	E	423	TYR	2.8
1	D	319	ARG	2.8
1	F	272	ILE	2.8

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Mol	Chain	Res	Type	RSRZ
1	F	389	THR	2.8
1	C	386	ASP	2.8
1	F	178	MET	2.8
1	C	28	ASN	2.7
1	C	76	ALA	2.7
1	F	245	GLY	2.7
1	D	399	PRO	2.7
2	B	450	ARG	2.7
1	C	44	LEU	2.7
1	C	29	GLU	2.7
1	A	323	SER	2.7
1	F	370	GLY	2.7
1	F	119	VAL	2.7
1	A	325	VAL	2.6
1	F	266	LEU	2.6
1	F	231	PRO	2.6
1	C	223	VAL	2.6
1	C	370	GLY	2.6
1	C	181	LEU	2.5
1	C	31	VAL	2.5
1	F	106	LEU	2.5
1	C	367	GLY	2.5
1	F	391	TYR	2.5
1	F	222	GLU	2.5
1	C	73	ILE	2.5
1	F	296	ASP	2.5
1	A	322	SER	2.5
1	A	324	ARG	2.5
1	D	312	ASP	2.5
1	C	152	PRO	2.4
1	F	322	SER	2.4
1	F	295	ARG	2.4
1	C	371	VAL	2.4
1	F	253	VAL	2.4
1	F	217	PRO	2.4
2	E	448	PRO	2.4
1	F	346	ASN	2.4
1	C	387	ILE	2.4
1	F	393	THR	2.4
1	D	371	VAL	2.3
1	C	104	LEU	2.3
1	C	132	HIS	2.3

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Mol	Chain	Res	Type	RSRZ
1	F	250	TYR	2.3
1	D	338	VAL	2.3
1	F	171	LEU	2.3
1	F	321	GLY	2.2
1	F	267	TYR	2.2
1	A	321	GLY	2.2
1	C	381	LYS	2.2
1	F	105	VAL	2.2
2	E	449	SER	2.2
1	F	96	LEU	2.2
1	A	273	THR	2.2
1	F	221	LEU	2.2
1	C	273	THR	2.2
1	D	247	ARG	2.2
1	A	27	TRP	2.1
1	A	301	ALA	2.1
1	C	30	ILE	2.1
1	F	323	SER	2.1
1	F	340	GLN	2.1
1	C	196	ILE	2.1
1	C	34	PHE	2.1
1	A	378	GLU	2.1
1	D	365	ARG	2.1
1	D	82	LYS	2.0
1	F	149	MET	2.0
1	F	145	GLN	2.0
2	B	163	ALA	2.0
1	F	200	PHE	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, 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	LLDF	B-factors(Å^2)	Q<0.9
3	EDO	A	3	4/4	0.89	0.32	3.91	57,62,64,66	0
3	EDO	D	1	4/4	0.91	0.24	1.48	67,68,69,69	0
4	ACY	A	1	4/4	0.83	0.22	0.41	78,78,79,79	0
4	ACY	D	2	4/4	0.83	0.37	-	75,75,76,76	0
3	EDO	A	2	4/4	0.81	0.22	-	81,83,84,85	0

6.5 Other polymers

There are no such residues in this entry.