Full wwPDB X-ray Structure Validation Report ⓘ

Feb 6, 2021 – 08:05 AM GMT

PDB ID	:	6TC0
Title	:	Crystal structure of MMS19-CIAO1-CIAO2B CIA targeting complex
Authors	:	Kassube, S.A.; Thoma, N.H.
Deposited on	:	2019-11-04
Resolution	:	3.60 Å(reported)

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

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the ⓘ symbol.

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

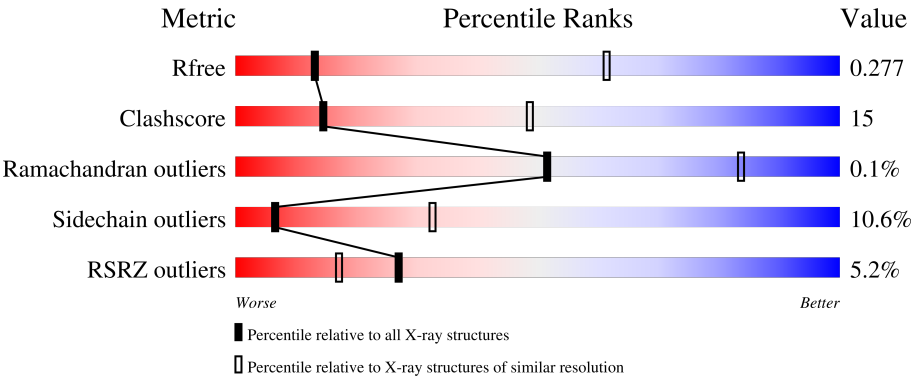
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.16
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.16

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 3.60 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}	130704	1257 (3.70-3.50)
Clashscore	141614	1353 (3.70-3.50)
Ramachandran outliers	138981	1307 (3.70-3.50)
Sidechain outliers	138945	1307 (3.70-3.50)
RSRZ outliers	127900	1161 (3.70-3.50)

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

Mol	Chain	Length	Quality of chain
1	A	338	3% 81% 17%
1	D	338	27% 83% 16%
2	B	159	4% 72% 23%
2	E	159	6% 77% 19%
3	C	1035	2% 58% 32% 6%

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Mol	Chain	Length	Quality of chain
3	F	1035	

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 22972 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 Probable cytosolic iron-sulfur protein assembly protein Ciao1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	336	Total	C	N	O	S	0	0	0
			2613	1629	455	516	13			
1	D	336	Total	C	N	O	S	0	0	0
			2613	1629	455	516	13			

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-2	GLY	-	expression tag	UNP Q7K1Y4
A	-1	GLY	-	expression tag	UNP Q7K1Y4
A	0	GLY	-	expression tag	UNP Q7K1Y4
A	1	ARG	-	expression tag	UNP Q7K1Y4
D	-2	GLY	-	expression tag	UNP Q7K1Y4
D	-1	GLY	-	expression tag	UNP Q7K1Y4
D	0	GLY	-	expression tag	UNP Q7K1Y4
D	1	ARG	-	expression tag	UNP Q7K1Y4

- Molecule 2 is a protein called MIP18 family protein galla-2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	154	Total	C	N	O	S	0	0	0
			1223	765	217	238	3			
2	E	154	Total	C	N	O	S	0	0	0
			1223	765	217	238	3			

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	-2	GLY	-	expression tag	UNP Q9VTC4
B	-1	GLY	-	expression tag	UNP Q9VTC4
B	0	GLY	-	expression tag	UNP Q9VTC4
B	1	ARG	-	expression tag	UNP Q9VTC4

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Chain	Residue	Modelled	Actual	Comment	Reference
E	-2	GLY	-	expression tag	UNP Q9VTC4
E	-1	GLY	-	expression tag	UNP Q9VTC4
E	0	GLY	-	expression tag	UNP Q9VTC4
E	1	ARG	-	expression tag	UNP Q9VTC4

- Molecule 3 is a protein called MMS19 nucleotide excision repair protein homolog.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	994	Total	C	N	O	S	0	0	0
			7669	4888	1311	1424	46			
3	F	989	Total	C	N	O	S	0	0	0
			7631	4862	1306	1418	45			

There are 8 discrepancies between the modelled and reference sequences:

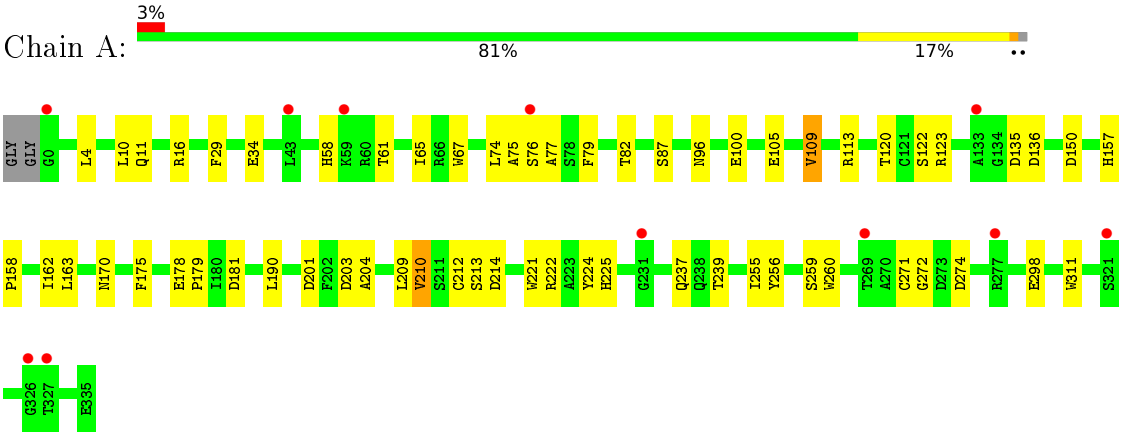
Chain	Residue	Modelled	Actual	Comment	Reference
C	-3	GLY	-	expression tag	UNP Q9D071
C	-2	GLY	-	expression tag	UNP Q9D071
C	-1	GLY	-	expression tag	UNP Q9D071
C	0	ARG	-	expression tag	UNP Q9D071
F	-3	GLY	-	expression tag	UNP Q9D071
F	-2	GLY	-	expression tag	UNP Q9D071
F	-1	GLY	-	expression tag	UNP Q9D071
F	0	ARG	-	expression tag	UNP Q9D071

3 Residue-property plots (i)

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

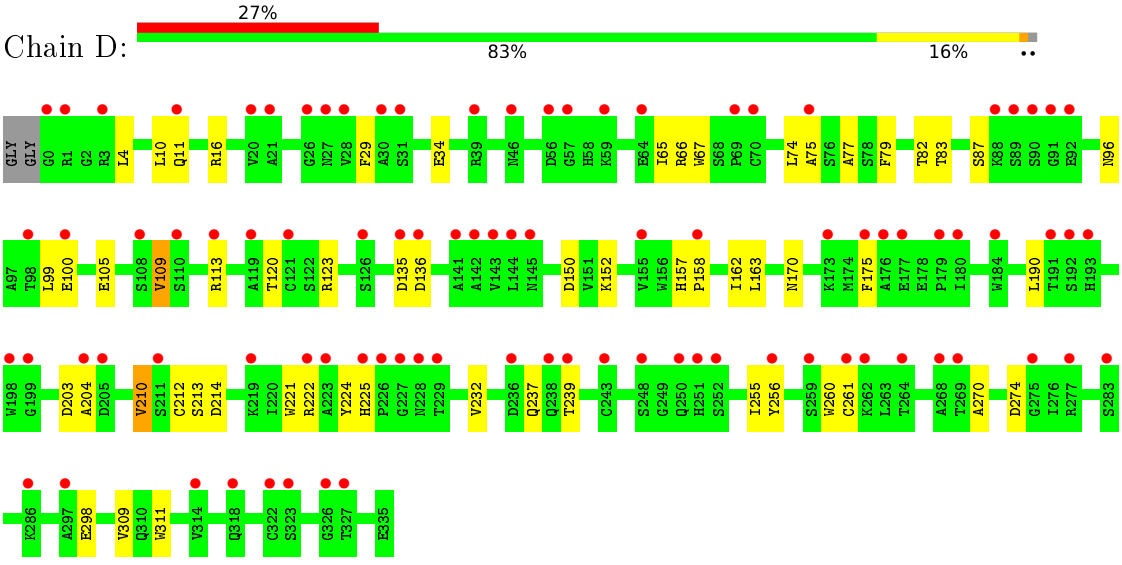
• Molecule 1: Probable cytosolic iron-sulfur protein assembly protein Ciao1

Chain A:



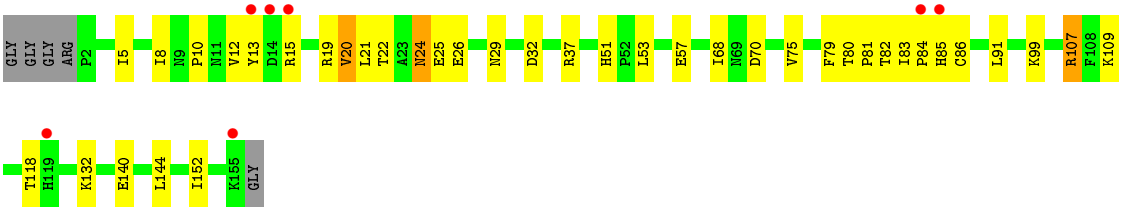
• Molecule 1: Probable cytosolic iron-sulfur protein assembly protein Ciao1

Chain D:



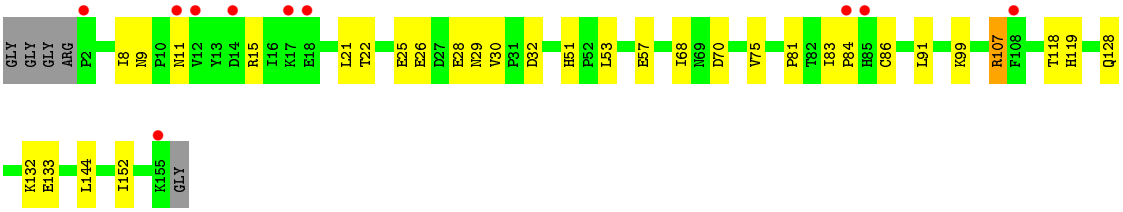
• Molecule 2: MIP18 family protein galla-2

Chain B:



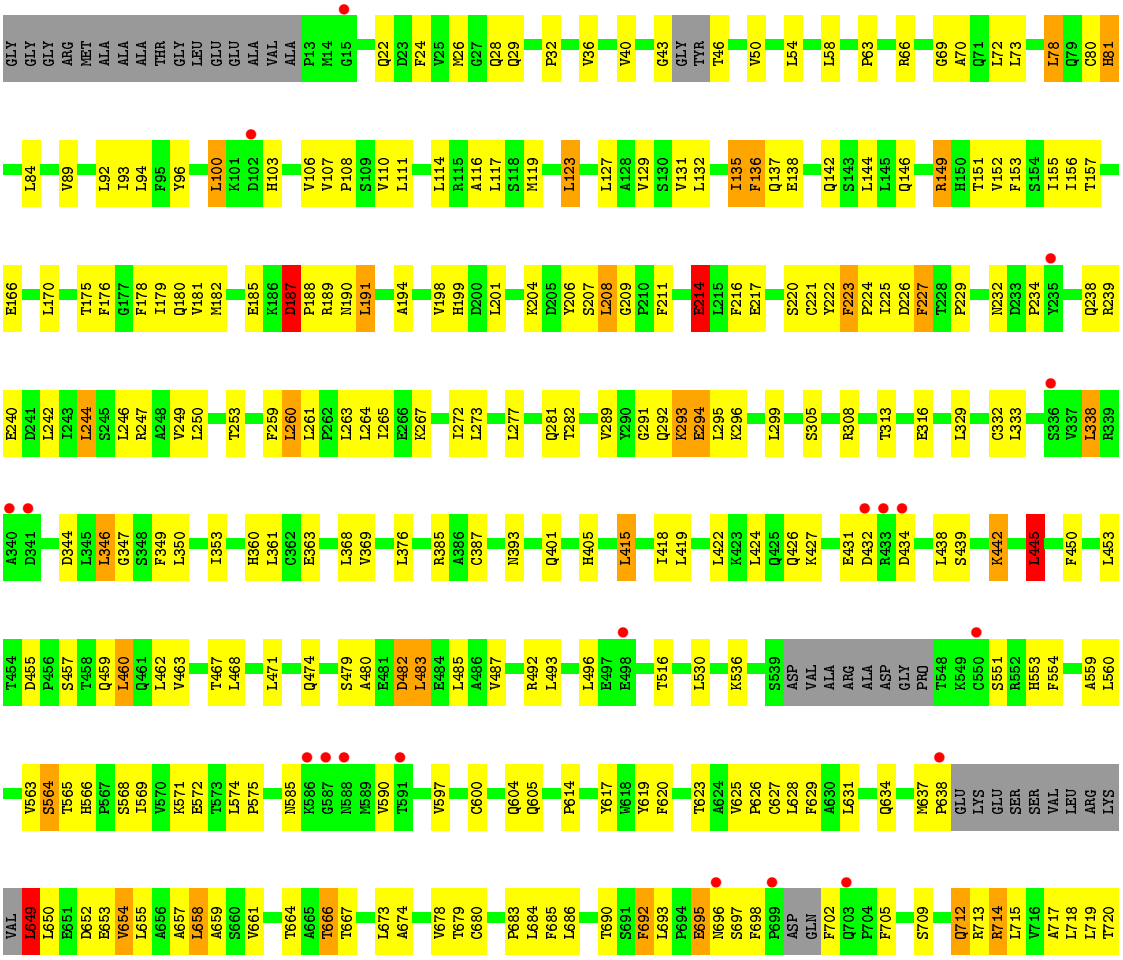
• Molecule 2: MIP18 family protein galla-2

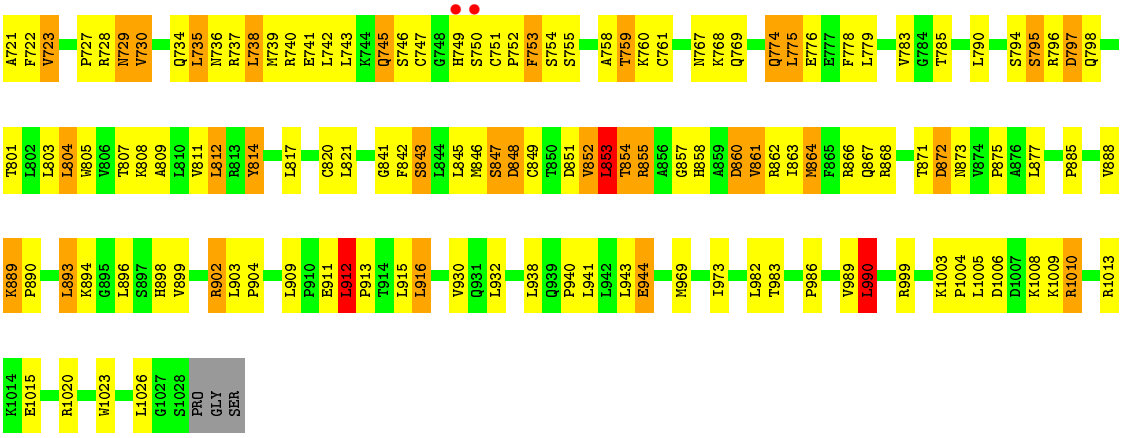
Chain E:



• Molecule 3: MMS19 nucleotide excision repair protein homolog

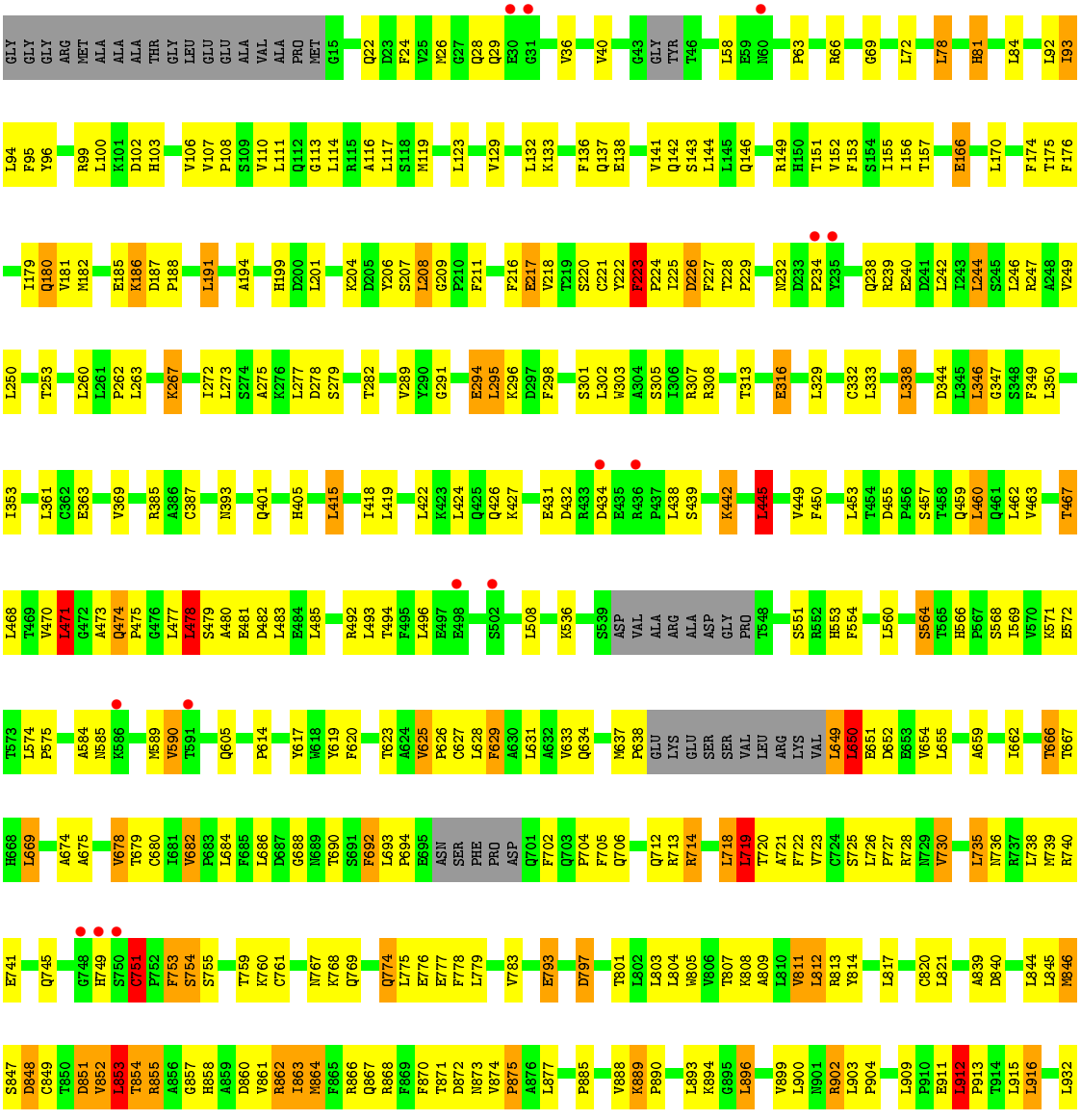
Chain C:

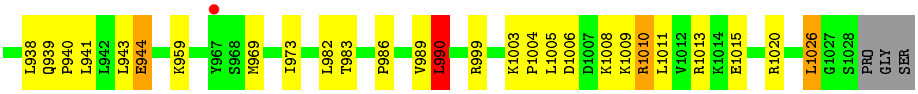




• Molecule 3: MMS19 nucleotide excision repair protein homolog

Chain F:




L938
Q939
P940
L941
L942
L943
E944
K959
Y967
S968
M969
I973
L982
T983
P986
V989
L990
R999
K1003
P1004
L1005
D1006
D1007
K1008
K1009
R1010
L1011
V1012
R1013
K1014
E1015
R1020
L1026
G1027
S1028
PRO
GLY
SER

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	107.40Å 140.70Å 327.33Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	20.00 – 3.60 20.00 – 3.60	Depositor EDS
% Data completeness (in resolution range)	100.0 (20.00-3.60) 100.0 (20.00-3.60)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.45 (at 3.62Å)	Xtriage
Refinement program	CNS, PHENIX 1.16_3549	Depositor
R, R_{free}	0.258 , 0.277 0.258 , 0.277	Depositor DCC
R_{free} test set	2900 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å^2)	175.8	Xtriage
Anisotropy	0.105	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.24 , 108.4	EDS
L-test for twinning[2]	$< \|L\| > = 0.40$, $< L^2 > = 0.23$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	22972	wwPDB-VP
Average B, all atoms (Å^2)	211.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.63% 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, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$\|Z\|>5$	RMSZ	#$\|Z\|>5$
1	A	0.38	0/2679	0.62	0/3649
1	D	0.42	0/2679	0.65	0/3649
2	B	0.54	0/1244	0.79	4/1694 (0.2%)
2	E	0.46	0/1244	0.80	5/1694 (0.3%)
3	C	0.45	2/7816 (0.0%)	0.74	15/10614 (0.1%)
3	F	0.45	2/7775 (0.0%)	0.74	18/10558 (0.2%)
All	All	0.45	4/23437 (0.0%)	0.72	42/31858 (0.1%)

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	187	ASP	CB-CG	-6.12	1.38	1.51
3	F	751	CYS	CB-SG	-6.12	1.71	1.82
3	F	217	GLU	CB-CG	-5.33	1.42	1.52
3	C	214	GLU	CB-CG	-5.18	1.42	1.52

All (42) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	C	735	LEU	CB-CG-CD2	-11.56	91.34	111.00
3	C	804	LEU	CB-CG-CD1	-10.07	93.89	111.00
3	C	208	LEU	CA-CB-CG	9.09	136.20	115.30
3	F	208	LEU	CA-CB-CG	8.94	135.86	115.30
3	F	718	LEU	CB-CG-CD1	-8.65	96.29	111.00
3	C	990	LEU	CA-CB-CG	8.54	134.94	115.30
3	F	990	LEU	CA-CB-CG	8.24	134.25	115.30
3	C	471	LEU	CA-CB-CG	7.70	133.02	115.30
2	E	107	ARG	NE-CZ-NH1	-7.62	116.49	120.30
3	F	445	LEU	CA-CB-CG	7.43	132.39	115.30
3	F	735	LEU	CB-CG-CD2	-7.40	98.43	111.00
3	C	445	LEU	CA-CB-CG	7.31	132.12	115.30
3	C	649	LEU	CA-CB-CG	7.13	131.69	115.30
2	E	21	LEU	CB-CG-CD2	7.09	123.05	111.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	F	719	LEU	CA-CB-CG	7.06	131.55	115.30
3	C	144	LEU	CA-CB-CG	6.92	131.21	115.30
3	F	471	LEU	CB-CG-CD1	6.89	122.72	111.00
3	F	144	LEU	CA-CB-CG	6.85	131.06	115.30
3	F	853	LEU	CA-CB-CG	6.80	130.95	115.30
3	F	478	LEU	CA-CB-CG	6.69	130.69	115.30
3	C	853	LEU	CA-CB-CG	6.51	130.26	115.30
3	F	912	LEU	CA-CB-CG	6.48	130.20	115.30
3	F	650	LEU	CB-CG-CD1	-6.43	100.08	111.00
2	E	15	ARG	NE-CZ-NH2	-6.41	117.09	120.30
2	E	21	LEU	CA-CB-CG	-6.39	100.59	115.30
3	F	1026	LEU	CB-CG-CD1	-6.38	100.15	111.00
3	F	471	LEU	CA-CB-CG	6.37	129.95	115.30
3	F	916	LEU	CA-CB-CG	6.21	129.59	115.30
2	B	20	VAL	CG1-CB-CG2	6.17	120.78	110.90
3	C	912	LEU	CA-CB-CG	6.13	129.41	115.30
3	F	862	ARG	NE-CZ-NH2	-6.06	117.27	120.30
3	C	916	LEU	CA-CB-CG	5.97	129.03	115.30
3	C	814	TYR	CA-CB-CG	5.91	124.62	113.40
2	B	107	ARG	NE-CZ-NH1	-5.89	117.36	120.30
3	C	191	LEU	CB-CG-CD2	-5.86	101.03	111.00
3	F	191	LEU	CB-CG-CD2	-5.52	101.62	111.00
3	C	136	PHE	CB-CG-CD1	-5.40	117.02	120.80
2	B	107	ARG	CD-NE-CZ	5.37	131.12	123.60
2	B	13	TYR	C-N-CA	5.34	135.05	121.70
2	E	107	ARG	CD-NE-CZ	5.14	130.80	123.60
3	C	655	LEU	CB-CG-CD2	-5.05	102.41	111.00
3	F	1026	LEU	CD1-CG-CD2	5.01	125.52	110.50

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	2613	0	2480	38	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	D	2613	0	2480	32	0
2	B	1223	0	1230	52	0
2	E	1223	0	1230	39	0
3	C	7669	0	7810	296	0
3	F	7631	0	7774	300	0
All	All	22972	0	23004	706	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 15.

All (706) 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)
3:F:226:ASP:HB3	3:F:239:ARG:HD3	1.20	1.19
3:C:226:ASP:HB2	3:C:239:ARG:HD2	1.21	1.12
3:F:751:CYS:SG	3:F:754:SER:N	2.26	1.09
3:F:769:GLN:O	3:F:813:ARG:NH2	1.83	1.09
3:F:474:GLN:N	3:F:474:GLN:OE1	1.93	1.00
3:C:604:GLN:HB2	3:C:661:VAL:HG22	1.44	0.98
2:B:8:ILE:HG21	2:E:144:LEU:HD13	1.42	0.98
3:F:877:LEU:HD13	3:F:896:LEU:HG	1.47	0.97
3:F:474:GLN:H	3:F:474:GLN:CD	1.64	0.96
3:C:629:PHE:HB2	3:C:693:LEU:HD22	1.43	0.96
3:F:846:MET:O	3:F:866:ARG:NH1	1.98	0.96
3:C:746:SER:HB2	3:C:759:THR:HG22	1.46	0.95
3:C:629:PHE:HE1	3:C:697:SER:HB3	1.32	0.94
3:F:760:LYS:NZ	3:F:851:ASP:OD1	2.01	0.94
3:F:751:CYS:SG	3:F:755:SER:N	2.41	0.93
1:D:113:ARG:HD3	1:D:158:PRO:O	1.71	0.90
3:C:760:LYS:NZ	3:C:851:ASP:OD1	2.05	0.89
3:C:685:PHE:C	3:C:705:PHE:HE2	1.74	0.89
2:B:26:GLU:HG2	3:C:1010:ARG:HB2	1.55	0.88
3:F:735:LEU:HD21	3:F:769:GLN:NE2	1.90	0.87
3:C:629:PHE:CE1	3:C:697:SER:HB3	2.10	0.86
1:A:113:ARG:HD3	1:A:158:PRO:O	1.75	0.86
3:C:247:ARG:HG2	3:C:282:THR:HG22	1.57	0.86
3:C:216:PHE:O	3:C:220:SER:OG	1.94	0.86
3:C:873:ASN:HD21	3:C:877:LEU:HD12	1.38	0.85
3:F:735:LEU:HD21	3:F:769:GLN:HE22	1.40	0.85
3:F:814:TYR:HD2	3:F:862:ARG:HG3	1.38	0.85
3:F:216:PHE:O	3:F:220:SER:OG	1.95	0.84

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:58:LEU:HD11	3:C:73:LEU:HD11	1.59	0.84
2:B:19:ARG:O	2:B:37:ARG:NH2	2.10	0.83
2:E:107:ARG:NH2	3:F:1006:ASP:OD1	2.12	0.83
3:F:426:GLN:HE22	3:F:474:GLN:HB3	1.43	0.83
3:C:862:ARG:HA	3:F:217:GLU:OE1	1.78	0.82
3:F:226:ASP:CB	3:F:239:ARG:HD3	2.05	0.82
3:F:720:THR:HG22	3:F:761:CYS:HB2	1.60	0.82
3:C:734:GLN:HE21	3:C:737:ARG:HD2	1.45	0.82
3:C:597:VAL:HG23	3:C:654:VAL:HG23	1.62	0.81
3:F:713:ARG:HE	3:F:749:HIS:HD2	1.28	0.81
3:C:735:LEU:HD21	3:C:769:GLN:NE2	1.96	0.81
3:C:702:PHE:CZ	3:C:712:GLN:HB3	2.15	0.81
2:B:53:LEU:HD11	2:E:53:LEU:HD11	1.63	0.80
3:F:805:TRP:HZ3	3:F:852:VAL:HG21	1.45	0.79
3:C:659:ALA:HB1	3:C:721:ALA:HB2	1.65	0.78
3:F:871:THR:O	3:F:875:PRO:HD2	1.83	0.78
3:F:24:PHE:CE1	3:F:72:LEU:HD13	2.19	0.78
3:C:750:SER:HA	3:C:798:GLN:HG2	1.64	0.78
3:C:132:LEU:HD23	3:C:132:LEU:H	1.49	0.77
3:C:178:PHE:HA	3:C:181:VAL:HG22	1.65	0.77
3:C:191:LEU:HD21	3:C:222:TYR:HE2	1.50	0.77
3:F:625:VAL:HG12	3:F:692:PHE:HE1	1.50	0.77
3:F:848:ASP:N	3:F:848:ASP:OD2	2.15	0.77
1:A:87:SER:OG	1:A:96:ASN:OD1	2.02	0.77
1:D:87:SER:OG	1:D:96:ASN:OD1	2.01	0.77
2:B:107:ARG:NH2	3:C:1006:ASP:OD1	2.17	0.77
3:F:625:VAL:HG23	3:F:626:PRO:HD3	1.67	0.76
3:C:199:HIS:HB2	3:C:249:VAL:HG12	1.67	0.76
3:C:291:GLY:N	3:C:294:GLU:OE2	2.17	0.76
3:C:686:LEU:HA	3:C:705:PHE:CE2	2.20	0.75
3:C:855:ARG:HD2	3:C:855:ARG:H	1.51	0.75
3:F:704:PRO:HG3	3:F:712:GLN:HB3	1.68	0.75
1:D:225:HIS:HA	1:D:239:THR:HG22	1.67	0.74
3:F:199:HIS:HB2	3:F:249:VAL:HG12	1.68	0.74
3:C:191:LEU:HD21	3:C:222:TYR:CE2	2.23	0.74
2:E:22:THR:O	2:E:26:GLU:HG3	1.87	0.74
1:A:272:GLY:O	2:B:109:LYS:NZ	2.20	0.74
1:D:256:TYR:CZ	2:E:132:LYS:HE2	2.22	0.74
3:F:229:PRO:HG2	3:F:232:ASN:O	1.88	0.74
3:C:747:CYS:HA	3:C:798:GLN:HB3	1.70	0.73
1:A:225:HIS:HA	1:A:239:THR:HG22	1.70	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:F:247:ARG:HG2	3:F:282:THR:HG22	1.70	0.73
3:C:182:MET:SD	3:C:194:ALA:HB1	2.27	0.73
3:F:855:ARG:HD2	3:F:855:ARG:H	1.52	0.73
2:B:84:PRO:HG3	2:E:118:THR:HA	1.69	0.73
3:F:267:LYS:HE2	3:F:275:ALA:HA	1.71	0.73
3:F:726:LEU:HB3	3:F:730:VAL:HG11	1.71	0.72
3:C:705:PHE:HD1	3:C:741:GLU:CD	1.91	0.72
3:C:797:ASP:N	3:C:797:ASP:OD1	2.22	0.72
3:F:473:ALA:N	3:F:474:GLN:OE1	2.23	0.72
2:B:144:LEU:HD13	2:E:8:ILE:HG21	1.72	0.72
2:B:32:ASP:HB2	3:C:1013:ARG:NH2	2.04	0.72
3:F:426:GLN:NE2	3:F:474:GLN:HB3	2.05	0.72
3:F:805:TRP:CZ3	3:F:852:VAL:HG21	2.24	0.72
3:F:457:SER:HB2	3:F:460:LEU:HB2	1.72	0.71
3:C:188:PRO:HG3	3:C:227:PHE:HZ	1.55	0.71
3:F:678:VAL:O	3:F:682:VAL:HG23	1.90	0.71
3:C:294:GLU:N	3:C:294:GLU:OE1	2.23	0.71
3:F:474:GLN:N	3:F:474:GLN:CD	2.29	0.71
3:F:848:ASP:OD1	3:F:855:ARG:NH2	2.23	0.71
3:C:714:ARG:HG2	3:C:753:PHE:CZ	2.26	0.71
3:F:690:THR:HB	3:F:693:LEU:HD11	1.72	0.71
3:F:814:TYR:CD2	3:F:862:ARG:HG3	2.23	0.71
3:C:746:SER:O	3:C:755:SER:HB2	1.90	0.71
3:F:807:THR:HG22	3:F:821:LEU:HB3	1.73	0.71
3:C:457:SER:HB2	3:C:460:LEU:HB2	1.73	0.70
3:F:226:ASP:HB3	3:F:239:ARG:CD	2.12	0.70
3:C:292:GLN:N	3:C:293:LYS:HZ3	1.90	0.70
3:F:702:PHE:HA	3:F:712:GLN:NE2	2.05	0.70
3:F:659:ALA:HB1	3:F:721:ALA:HB2	1.73	0.70
3:C:217:GLU:HG3	3:F:863:ILE:HD13	1.72	0.70
3:F:103:HIS:HB3	3:F:106:VAL:HB	1.74	0.70
2:B:12:VAL:HA	2:B:15:ARG:HD2	1.73	0.69
3:F:81:HIS:CE1	3:F:119:MET:HB3	2.28	0.69
3:C:223:PHE:CE1	3:C:267:LYS:HG3	2.28	0.69
3:C:223:PHE:HE1	3:C:267:LYS:HG3	1.57	0.69
3:F:182:MET:HG3	3:F:194:ALA:HB1	1.75	0.69
3:C:559:ALA:O	3:C:563:VAL:HG12	1.93	0.68
3:C:751:CYS:SG	3:C:752:PRO:HD2	2.33	0.68
3:F:797:ASP:OD1	3:F:797:ASP:N	2.23	0.68
3:F:81:HIS:HE1	3:F:119:MET:HB3	1.58	0.68
3:C:735:LEU:HD21	3:C:769:GLN:HE22	1.56	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:F:24:PHE:CE1	3:F:29:GLN:HB2	2.29	0.67
3:F:751:CYS:HG	3:F:755:SER:H	1.41	0.67
3:F:650:LEU:HD12	3:F:654:VAL:HG13	1.75	0.67
3:F:713:ARG:NE	3:F:749:HIS:HD2	1.91	0.67
3:F:221:CYS:HG	3:F:222:TYR:HD1	1.42	0.67
3:C:629:PHE:HE1	3:C:697:SER:CB	2.05	0.67
3:C:807:THR:HG22	3:C:821:LEU:HB3	1.74	0.67
2:B:24:ASN:OD1	2:B:24:ASN:N	2.26	0.67
3:C:81:HIS:HE1	3:C:119:MET:HB3	1.60	0.67
3:F:560:LEU:O	3:F:564:SER:OG	2.14	0.66
3:F:188:PRO:HG3	3:F:227:PHE:HZ	1.59	0.66
3:C:685:PHE:C	3:C:705:PHE:CE2	2.65	0.66
3:C:81:HIS:CE1	3:C:119:MET:HB3	2.31	0.66
3:C:229:PRO:HG2	3:C:232:ASN:O	1.95	0.66
3:C:808:LYS:HB2	3:C:845:LEU:CD2	2.25	0.66
3:C:866:ARG:HB3	3:C:903:LEU:HD22	1.78	0.65
3:F:714:ARG:HG2	3:F:753:PHE:HE1	1.62	0.65
3:F:191:LEU:HD21	3:F:222:TYR:HE2	1.62	0.65
3:C:803:LEU:O	3:C:807:THR:HG23	1.97	0.65
3:F:191:LEU:HD21	3:F:222:TYR:CE2	2.31	0.65
3:F:625:VAL:HG12	3:F:692:PHE:CE1	2.30	0.65
2:B:118:THR:HA	2:E:84:PRO:HG3	1.78	0.65
3:C:226:ASP:HB2	3:C:239:ARG:CD	2.12	0.65
3:F:107:VAL:HG23	3:F:108:PRO:HD3	1.79	0.65
3:C:812:LEU:HB3	3:C:861:VAL:HG23	1.77	0.65
3:C:625:VAL:HB	3:C:626:PRO:HD3	1.77	0.65
2:B:118:THR:CA	2:E:84:PRO:HG3	2.27	0.65
3:F:24:PHE:CG	3:F:72:LEU:HD22	2.32	0.64
1:A:61:THR:OG1	2:B:140:GLU:OE2	2.14	0.64
3:C:873:ASN:ND2	3:C:877:LEU:HD12	2.12	0.64
3:F:78:LEU:HD12	3:F:116:ALA:HB2	1.79	0.64
3:F:267:LYS:HD2	3:F:279:SER:HB3	1.78	0.64
3:C:727:PRO:HA	3:C:858:HIS:ND1	2.13	0.64
3:C:739:MET:HG3	3:C:778:PHE:HE1	1.63	0.64
2:B:8:ILE:O	2:B:10:PRO:HD3	1.97	0.64
3:C:103:HIS:HB3	3:C:106:VAL:HB	1.79	0.64
3:C:734:GLN:NE2	3:C:737:ARG:HD2	2.13	0.64
2:B:68:ILE:HG13	2:B:75:VAL:HG22	1.80	0.64
2:B:57:GLU:O	2:E:51:HIS:HE1	1.81	0.63
3:F:240:GLU:HG3	3:F:244:LEU:HD12	1.80	0.63
3:C:720:THR:HG22	3:C:761:CYS:HB2	1.80	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:54:LEU:HD13	3:C:73:LEU:CD2	2.29	0.63
3:F:22:GLN:O	3:F:26:MET:HG2	1.98	0.63
3:F:675:ALA:O	3:F:678:VAL:HG23	1.98	0.63
3:C:132:LEU:HA	3:C:135:ILE:HG23	1.80	0.63
3:C:221:CYS:HG	3:C:222:TYR:HD1	1.47	0.62
2:B:32:ASP:HB2	3:C:1013:ARG:HH22	1.64	0.62
3:C:714:ARG:HG2	3:C:753:PHE:HZ	1.63	0.62
1:D:152:LYS:NZ	2:E:133:GLU:OE1	2.21	0.62
3:C:940:PRO:O	3:C:944:GLU:HG2	2.00	0.62
3:C:768:LYS:HD3	3:C:858:HIS:O	1.97	0.62
3:C:93:ILE:HG13	3:C:117:LEU:HD13	1.80	0.62
2:E:83:ILE:HG23	2:E:84:PRO:HD2	1.82	0.62
3:F:626:PRO:HA	3:F:629:PHE:HD2	1.64	0.62
3:F:439:SER:HA	3:F:442:LYS:HD2	1.81	0.62
3:F:803:LEU:O	3:F:807:THR:HG23	2.00	0.62
3:C:299:LEU:HD21	3:C:349:PHE:CD1	2.34	0.62
3:C:127:LEU:O	3:C:131:VAL:HG23	2.00	0.61
3:F:415:LEU:HD22	3:F:463:VAL:HG12	1.82	0.61
2:E:99:LYS:HB2	2:E:152:ILE:HD12	1.83	0.61
3:F:768:LYS:HD3	3:F:858:HIS:O	1.99	0.61
3:C:652:ASP:HB3	3:C:714:ARG:NH2	2.15	0.61
2:B:83:ILE:HG12	2:E:81:PRO:O	2.01	0.61
3:F:226:ASP:OD2	3:F:239:ARG:NH1	2.34	0.61
2:B:26:GLU:HG3	2:B:32:ASP:CG	2.20	0.61
3:C:713:ARG:NH1	3:C:749:HIS:HB2	2.16	0.61
2:B:26:GLU:HG3	2:B:32:ASP:OD2	2.00	0.61
3:C:211:PHE:HA	3:C:214:GLU:OE2	2.01	0.61
3:F:847:SER:HB2	3:F:902:ARG:HE	1.65	0.61
3:C:70:ALA:HA	3:C:73:LEU:HD12	1.83	0.61
2:E:32:ASP:HB2	3:F:1013:ARG:NH2	2.16	0.61
3:F:851:ASP:N	3:F:851:ASP:OD2	2.29	0.61
2:B:51:HIS:HE1	2:E:57:GLU:O	1.84	0.60
3:F:940:PRO:O	3:F:944:GLU:HG2	1.99	0.60
3:C:750:SER:HA	3:C:798:GLN:CG	2.32	0.60
3:F:675:ALA:O	3:F:679:THR:HG23	2.01	0.60
3:C:807:THR:HG22	3:C:821:LEU:CB	2.30	0.60
3:F:631:LEU:HD23	3:F:718:LEU:CD1	2.31	0.60
3:C:217:GLU:HG3	3:F:863:ILE:CD1	2.31	0.60
3:F:471:LEU:O	3:F:474:GLN:NE2	2.35	0.60
3:F:807:THR:HG22	3:F:821:LEU:CB	2.31	0.60
1:D:190:LEU:HD23	1:D:221:TRP:CD2	2.37	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:107:VAL:HG23	3:C:108:PRO:HD3	1.84	0.59
3:C:146:GLN:NE2	3:C:187:ASP:HB2	2.17	0.59
3:C:623:THR:HA	3:C:626:PRO:HD2	1.83	0.59
3:F:740:ARG:NH2	3:F:777:GLU:OE2	2.35	0.59
3:C:739:MET:HG3	3:C:778:PHE:CE1	2.38	0.59
3:C:717:ALA:O	3:C:720:THR:OG1	2.14	0.59
3:F:650:LEU:HD11	3:F:655:LEU:HG	1.84	0.59
3:F:470:VAL:O	3:F:474:GLN:HG3	2.02	0.59
3:F:899:VAL:O	3:F:903:LEU:HG	2.02	0.59
3:F:631:LEU:HD23	3:F:718:LEU:HD11	1.85	0.59
3:C:78:LEU:HD12	3:C:116:ALA:HB2	1.83	0.59
3:C:938:LEU:HA	3:C:941:LEU:HD12	1.85	0.59
3:C:234:PRO:HD3	3:F:427:LYS:HG2	1.85	0.59
3:C:415:LEU:HD22	3:C:463:VAL:HG12	1.85	0.58
3:F:674:ALA:O	3:F:678:VAL:HG22	2.03	0.58
3:C:182:MET:HG3	3:C:194:ALA:HB1	1.84	0.58
3:C:69:GLY:O	3:C:73:LEU:HG	2.03	0.58
2:E:81:PRO:HG2	2:E:119:HIS:HB2	1.85	0.58
3:F:93:ILE:HG13	3:F:117:LEU:HD13	1.85	0.58
3:F:739:MET:HG3	3:F:778:PHE:HE1	1.68	0.58
1:A:203:ASP:OD2	1:A:204:ALA:N	2.32	0.58
3:C:808:LYS:NZ	3:C:847:SER:O	2.36	0.58
3:F:714:ARG:HG2	3:F:753:PHE:CE1	2.38	0.58
1:A:222:ARG:HG2	1:A:224:TYR:CE1	2.38	0.58
3:C:560:LEU:O	3:C:564:SER:OG	2.22	0.58
3:F:226:ASP:CG	3:F:239:ARG:HH11	2.07	0.58
3:F:793:GLU:N	3:F:793:GLU:OE2	2.37	0.58
3:C:240:GLU:HG3	3:C:244:LEU:HD12	1.85	0.58
2:B:84:PRO:CG	2:E:118:THR:HA	2.34	0.57
3:F:182:MET:SD	3:F:194:ALA:HB1	2.44	0.57
2:B:99:LYS:HB2	2:B:152:ILE:HD12	1.86	0.57
2:E:9:ASN:OD1	2:E:11:ASN:HB2	2.04	0.57
3:F:751:CYS:SG	3:F:753:PHE:N	2.77	0.57
1:D:210:VAL:HG22	1:D:260:TRP:CE3	2.40	0.57
3:F:938:LEU:HA	3:F:941:LEU:HD12	1.85	0.57
1:A:190:LEU:HD23	1:A:221:TRP:CD2	2.40	0.57
2:B:22:THR:O	2:B:26:GLU:OE1	2.23	0.57
2:E:68:ILE:HG13	2:E:75:VAL:HG22	1.86	0.57
3:F:267:LYS:HD3	3:F:275:ALA:O	2.05	0.57
2:B:29:ASN:HA	3:C:1009:LYS:HE3	1.86	0.57
3:C:728:ARG:NE	3:F:180:GLN:HE21	2.02	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:854:THR:HG23	3:C:857:GLY:HA3	1.87	0.57
3:F:111:LEU:HD22	3:F:152:VAL:HG22	1.87	0.57
3:F:226:ASP:CB	3:F:239:ARG:HH11	2.17	0.57
3:F:854:THR:HG23	3:F:857:GLY:HA3	1.86	0.57
3:C:24:PHE:CE2	3:C:72:LEU:HB2	2.40	0.56
2:B:29:ASN:HA	3:C:1009:LYS:CE	2.34	0.56
3:F:751:CYS:SG	3:F:754:SER:CA	2.93	0.56
3:C:713:ARG:HH12	3:C:749:HIS:HB2	1.70	0.56
1:A:256:TYR:CZ	2:B:132:LYS:HE2	2.41	0.56
3:C:422:LEU:HD21	3:C:445:LEU:HD11	1.88	0.56
3:F:422:LEU:HD21	3:F:445:LEU:HD11	1.87	0.56
3:C:738:LEU:O	3:C:742:LEU:HG	2.06	0.56
3:F:247:ARG:HH11	3:F:282:THR:HG23	1.71	0.56
3:C:1008:LYS:HG3	3:C:1009:LYS:HD2	1.87	0.56
3:C:680:CYS:C	3:C:683:PRO:HD2	2.26	0.56
3:C:153:PHE:HA	3:C:156:ILE:HD12	1.88	0.56
3:F:129:VAL:HG23	3:F:166:GLU:HG2	1.87	0.56
3:F:839:ALA:HB1	3:F:894:LYS:HB3	1.88	0.56
3:C:969:MET:HG3	3:C:1009:LYS:HD3	1.88	0.55
3:C:563:VAL:HG22	3:C:569:ILE:HG21	1.88	0.55
3:C:151:THR:O	3:C:155:ILE:HG13	2.05	0.55
3:C:146:GLN:HE21	3:C:187:ASP:HB2	1.70	0.55
3:C:805:TRP:HZ3	3:C:852:VAL:HG21	1.71	0.55
2:B:8:ILE:HD11	2:E:91:LEU:HD22	1.87	0.55
3:C:482:ASP:OD1	3:C:482:ASP:N	2.40	0.55
3:C:627:CYS:O	3:C:631:LEU:HD12	2.06	0.55
3:F:682:VAL:HG12	3:F:738:LEU:HD12	1.88	0.55
3:F:704:PRO:HB3	3:F:712:GLN:HB3	1.88	0.55
3:C:973:ILE:HG23	3:C:1015:GLU:HG3	1.88	0.55
3:C:211:PHE:HD1	3:C:214:GLU:OE1	1.90	0.55
3:C:333:LEU:HB3	3:C:346:LEU:HB3	1.89	0.55
3:C:736:ASN:O	3:C:740:ARG:HG3	2.06	0.55
3:F:361:LEU:HA	3:F:369:VAL:HG23	1.88	0.55
3:F:704:PRO:CG	3:F:712:GLN:HB3	2.36	0.55
3:C:727:PRO:O	3:C:730:VAL:HG13	2.07	0.55
1:A:11:GLN:HE21	3:C:999:ARG:NH2	2.05	0.55
1:A:271:CYS:SG	1:A:272:GLY:N	2.80	0.55
3:C:709:SER:HB2	3:C:712:GLN:CD	2.28	0.55
3:C:96:TYR:HD1	3:C:110:VAL:HG13	1.72	0.55
1:A:210:VAL:HG22	1:A:260:TRP:CE3	2.43	0.54
1:A:190:LEU:HD23	1:A:221:TRP:CE3	2.43	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:F:153:PHE:CE1	3:F:185:GLU:HG3	2.42	0.54
3:F:713:ARG:HE	3:F:749:HIS:CD2	2.18	0.54
1:A:77:ALA:HB2	1:A:109:VAL:HG22	1.89	0.54
3:F:574:LEU:HD13	3:F:623:THR:HG21	1.89	0.54
3:C:72:LEU:HG	3:C:72:LEU:O	2.07	0.54
1:D:212:CYS:HB2	1:D:255:ILE:HB	1.90	0.54
3:F:471:LEU:C	3:F:474:GLN:CD	2.66	0.54
1:A:212:CYS:HB2	1:A:255:ILE:HB	1.88	0.54
3:C:50:VAL:O	3:C:54:LEU:HD12	2.06	0.54
3:F:426:GLN:HE22	3:F:475:PRO:HD2	1.73	0.54
3:C:247:ARG:NH1	3:C:281:GLN:HB3	2.23	0.54
3:C:680:CYS:HB3	3:C:692:PHE:CD1	2.43	0.54
2:B:26:GLU:OE1	2:B:26:GLU:N	2.39	0.54
3:C:226:ASP:CB	3:C:239:ARG:HD2	2.15	0.54
3:C:349:PHE:CZ	3:C:353:ILE:HD11	2.43	0.54
3:C:695:GLU:HA	3:C:698:PHE:CZ	2.43	0.54
3:C:702:PHE:CE1	3:C:712:GLN:HB3	2.42	0.54
3:C:401:GLN:HE21	3:C:405:HIS:HE1	1.56	0.54
3:C:188:PRO:HG3	3:C:227:PHE:CZ	2.39	0.54
3:F:1008:LYS:HG3	3:F:1009:LYS:HD2	1.89	0.54
3:F:153:PHE:HA	3:F:156:ILE:HD12	1.89	0.53
3:C:684:LEU:HD13	3:C:690:THR:HG22	1.89	0.53
1:D:77:ALA:HB2	1:D:109:VAL:HG22	1.90	0.53
2:E:22:THR:HG21	3:F:1010:ARG:NH1	2.24	0.53
3:F:873:ASN:ND2	3:F:899:VAL:HG11	2.24	0.53
3:F:973:ILE:HG23	3:F:1015:GLU:HG3	1.91	0.53
3:C:790:LEU:O	3:C:796:ARG:NE	2.42	0.53
1:D:222:ARG:HG2	1:D:224:TYR:CE1	2.43	0.53
3:C:614:PRO:HA	3:C:617:TYR:CE2	2.44	0.53
3:C:1005:LEU:HD11	3:C:1020:ARG:HD2	1.91	0.53
1:A:109:VAL:HG13	1:A:120:THR:HG22	1.90	0.52
3:C:338:LEU:HG	3:C:385:ARG:HH12	1.73	0.52
3:F:96:TYR:HD1	3:F:110:VAL:HG13	1.74	0.52
3:C:182:MET:CG	3:C:194:ALA:HB1	2.39	0.52
2:B:84:PRO:HG3	2:E:118:THR:CA	2.38	0.52
3:F:779:LEU:HD22	3:F:817:LEU:HD23	1.91	0.52
3:F:779:LEU:O	3:F:783:VAL:HG23	2.09	0.52
1:A:82:THR:HG22	1:A:100:GLU:HG2	1.89	0.52
3:C:153:PHE:HE1	3:C:185:GLU:HG2	1.74	0.52
3:C:659:ALA:HB2	3:C:718:LEU:HD23	1.90	0.52
3:F:855:ARG:H	3:F:855:ARG:CD	2.19	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:32:ASP:HB2	3:F:1013:ARG:HH22	1.74	0.52
3:F:450:PHE:HA	3:F:453:LEU:HD12	1.91	0.52
3:C:347:GLY:HA2	3:C:350:LEU:HD12	1.91	0.52
2:B:19:ARG:C	2:B:37:ARG:HH22	2.10	0.52
3:C:1023:TRP:CE3	3:C:1026:LEU:HD11	2.45	0.52
3:C:808:LYS:HG2	3:C:812:LEU:HD11	1.92	0.52
3:F:623:THR:C	3:F:626:PRO:HD2	2.30	0.52
1:D:190:LEU:HD23	1:D:221:TRP:CE3	2.45	0.52
3:F:182:MET:CG	3:F:194:ALA:HB1	2.40	0.52
3:F:442:LYS:HD3	3:F:477:LEU:O	2.09	0.52
3:F:902:ARG:C	3:F:904:PRO:HD3	2.31	0.52
3:F:132:LEU:HD21	3:F:174:PHE:CD1	2.44	0.52
3:F:333:LEU:HB3	3:F:346:LEU:HB3	1.92	0.52
2:B:5:ILE:HD12	2:E:128:GLN:HB3	1.91	0.51
3:C:415:LEU:HA	3:C:418:ILE:HD12	1.92	0.51
3:F:678:VAL:HG13	3:F:722:PHE:HE2	1.76	0.51
3:C:695:GLU:HA	3:C:698:PHE:CE1	2.46	0.51
2:B:118:THR:HA	2:E:84:PRO:CG	2.40	0.51
3:F:151:THR:O	3:F:155:ILE:HG13	2.10	0.51
3:F:726:LEU:HB3	3:F:730:VAL:CG1	2.38	0.51
3:C:188:PRO:CG	3:C:227:PHE:HZ	2.21	0.51
3:C:867:GLN:O	3:C:871:THR:HG23	2.10	0.51
3:F:338:LEU:HG	3:F:385:ARG:HH12	1.76	0.51
3:F:551:SER:HA	3:F:554:PHE:HD2	1.75	0.51
2:B:82:THR:O	2:B:83:ILE:HB	2.10	0.51
3:C:361:LEU:HA	3:C:369:VAL:HG23	1.93	0.51
3:C:92:LEU:HB3	3:C:117:LEU:HD11	1.92	0.51
3:C:774:GLN:O	3:C:778:PHE:HD2	1.93	0.51
3:C:779:LEU:O	3:C:783:VAL:HG23	2.11	0.51
3:C:851:ASP:OD2	3:C:851:ASP:N	2.28	0.51
3:C:890:PRO:HA	3:C:893:LEU:HD12	1.93	0.51
3:F:896:LEU:HD22	3:F:900:LEU:HD11	1.92	0.51
3:C:779:LEU:HD22	3:C:817:LEU:HD23	1.91	0.50
1:A:157:HIS:HB2	1:A:162:ILE:HB	1.93	0.50
3:C:28:GLN:O	3:C:32:PRO:HD2	2.11	0.50
3:C:776:GLU:HA	3:C:779:LEU:HD12	1.93	0.50
1:D:82:THR:HG22	1:D:100:GLU:HG2	1.93	0.50
3:F:471:LEU:C	3:F:474:GLN:NE2	2.64	0.50
3:F:736:ASN:OD1	3:F:740:ARG:NE	2.44	0.50
3:C:666:THR:HG21	3:C:722:PHE:CD1	2.46	0.50
3:C:767:ASN:HB2	3:C:809:ALA:HB1	1.94	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:299:LEU:HD23	3:C:299:LEU:C	2.32	0.50
3:F:424:LEU:HD23	3:F:427:LYS:HD2	1.93	0.50
3:F:625:VAL:HG23	3:F:626:PRO:CD	2.40	0.50
3:F:669:LEU:HD23	3:F:674:ALA:HA	1.93	0.50
3:C:294:GLU:H	3:C:294:GLU:CD	2.00	0.50
3:C:24:PHE:CZ	3:C:72:LEU:HB2	2.47	0.50
3:C:24:PHE:CE1	3:C:72:LEU:HD13	2.47	0.50
3:F:141:VAL:HG21	3:F:181:VAL:HG22	1.94	0.50
3:F:774:GLN:O	3:F:778:PHE:HD2	1.95	0.50
3:C:360:HIS:NE2	3:C:368:LEU:HB3	2.27	0.50
3:C:40:VAL:HG11	3:C:80:CYS:SG	2.52	0.50
3:C:769:GLN:HB3	3:C:775:LEU:HD12	1.94	0.50
3:F:808:LYS:HB2	3:F:845:LEU:CD2	2.42	0.50
3:F:566:HIS:HD2	3:F:568:SER:H	1.60	0.49
3:F:58:LEU:HD21	3:F:69:GLY:HA3	1.94	0.49
3:C:180:GLN:NE2	3:F:728:ARG:HH11	2.09	0.49
3:C:566:HIS:HB3	3:C:569:ILE:HD12	1.93	0.49
3:F:223:PHE:HB3	3:F:224:PRO:CD	2.42	0.49
3:F:614:PRO:HA	3:F:617:TYR:CE2	2.45	0.49
3:C:902:ARG:C	3:C:904:PRO:HD3	2.31	0.49
3:F:1005:LEU:HD11	3:F:1020:ARG:HD2	1.94	0.49
3:F:303:TRP:CZ2	3:F:307:ARG:HD3	2.48	0.49
3:F:401:GLN:HE21	3:F:405:HIS:HE1	1.60	0.49
3:F:808:LYS:HB2	3:F:845:LEU:HD23	1.94	0.49
2:B:12:VAL:HG22	2:B:15:ARG:CZ	2.42	0.49
1:D:135:ASP:OD2	1:D:136:ASP:N	2.45	0.49
3:F:713:ARG:NE	3:F:749:HIS:CD2	2.76	0.49
2:B:80:THR:HG21	2:E:83:ILE:HG23	1.95	0.49
2:B:85:HIS:CD2	2:E:118:THR:HG22	2.48	0.49
3:F:141:VAL:HG21	3:F:181:VAL:HG13	1.94	0.49
1:A:213:SER:OG	1:A:214:ASP:N	2.46	0.49
3:F:634:GLN:OE1	3:F:650:LEU:HD22	2.12	0.49
3:F:983:THR:HA	3:F:990:LEU:HD11	1.95	0.49
3:C:709:SER:HB2	3:C:712:GLN:HG3	1.95	0.48
3:C:801:THR:O	3:C:805:TRP:HD1	1.95	0.48
3:F:739:MET:HG3	3:F:778:PHE:CE1	2.47	0.48
2:E:83:ILE:H	2:E:86:CYS:HB2	1.77	0.48
3:F:590:VAL:HG11	3:F:649:LEU:HD13	1.95	0.48
3:C:899:VAL:O	3:C:903:LEU:HG	2.12	0.48
3:F:228:THR:HG22	3:F:229:PRO:HD2	1.95	0.48
3:F:862:ARG:HA	3:F:862:ARG:HD3	1.51	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:F:478:LEU:CD2	3:F:482:ASP:HB2	2.44	0.48
3:C:705:PHE:CD1	3:C:741:GLU:CD	2.81	0.48
3:C:735:LEU:HD23	3:C:774:GLN:HE22	1.78	0.48
3:C:983:THR:HA	3:C:990:LEU:HD11	1.95	0.48
1:D:4:LEU:HD23	1:D:298:GLU:HB2	1.95	0.48
3:F:684:LEU:HD12	3:F:692:PHE:CZ	2.49	0.48
3:C:149:ARG:NE	3:C:185:GLU:OE1	2.47	0.48
3:F:874:VAL:HG11	3:F:915:LEU:HD21	1.94	0.48
2:B:70:ASP:OD2	2:B:107:ARG:NH1	2.46	0.48
3:C:131:VAL:O	3:C:135:ILE:HG22	2.13	0.48
3:C:292:GLN:N	3:C:293:LYS:NZ	2.60	0.48
3:C:551:SER:HA	3:C:554:PHE:HD2	1.79	0.48
1:A:163:LEU:HB3	1:A:175:PHE:HB2	1.95	0.48
3:C:129:VAL:HG23	3:C:166:GLU:HB3	1.96	0.48
3:C:566:HIS:HD2	3:C:568:SER:H	1.61	0.48
3:F:267:LYS:CD	3:F:279:SER:HB3	2.44	0.48
3:F:63:PRO:HA	3:F:66:ARG:HD2	1.96	0.47
1:D:163:LEU:HB3	1:D:175:PHE:HB2	1.96	0.47
3:F:132:LEU:HD21	3:F:174:PHE:CE1	2.49	0.47
3:C:100:LEU:HB2	3:C:110:VAL:HG11	1.96	0.47
1:D:157:HIS:HB2	1:D:162:ILE:HB	1.96	0.47
3:F:221:CYS:SG	3:F:222:TYR:HD1	2.38	0.47
3:F:571:LYS:HA	3:F:619:TYR:CE2	2.49	0.47
3:C:111:LEU:HD22	3:C:152:VAL:HG22	1.95	0.47
3:C:634:GLN:NE2	3:C:650:LEU:HD23	2.29	0.47
3:F:188:PRO:HB3	3:F:242:LEU:HD11	1.95	0.47
3:C:96:TYR:CD1	3:C:110:VAL:HG13	2.49	0.47
3:F:153:PHE:HE1	3:F:185:GLU:HG3	1.79	0.47
3:F:704:PRO:CB	3:F:712:GLN:HB3	2.43	0.47
3:F:705:PHE:CD1	3:F:741:GLU:HB3	2.49	0.47
3:F:864:MET:O	3:F:867:GLN:HG2	2.14	0.47
3:C:804:LEU:HD21	3:C:841:GLY:HA3	1.95	0.47
2:E:25:GLU:HB3	2:E:32:ASP:OD1	2.15	0.47
3:F:149:ARG:NE	3:F:185:GLU:OE1	2.48	0.47
3:F:267:LYS:NZ	3:F:278:ASP:HB2	2.30	0.47
3:F:650:LEU:HD12	3:F:654:VAL:CG1	2.41	0.47
3:F:95:PHE:CZ	3:F:99:ARG:HG3	2.50	0.47
1:A:16:ARG:HG2	1:A:34:GLU:HB2	1.95	0.47
3:C:625:VAL:HG13	3:C:692:PHE:CE1	2.50	0.47
3:C:58:LEU:HD21	3:C:69:GLY:HA3	1.96	0.47
1:D:16:ARG:HG2	1:D:34:GLU:HB2	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:F:291:GLY:H	3:F:294:GLU:HG2	1.78	0.47
3:F:574:LEU:HD11	3:F:620:PHE:CD1	2.50	0.47
2:E:70:ASP:OD2	2:E:107:ARG:NH1	2.47	0.47
3:C:450:PHE:HA	3:C:453:LEU:HD12	1.96	0.47
3:F:629:PHE:O	3:F:633:VAL:HG23	2.14	0.47
3:F:767:ASN:HB2	3:F:809:ALA:HB1	1.96	0.47
3:F:854:THR:OG1	3:F:857:GLY:N	2.48	0.47
3:C:424:LEU:HD23	3:C:427:LYS:HD2	1.96	0.47
3:C:571:LYS:HA	3:C:619:TYR:CE2	2.50	0.47
1:D:109:VAL:HG13	1:D:120:THR:HG22	1.96	0.47
3:C:426:GLN:NE2	3:C:474:GLN:HG2	2.30	0.47
3:C:679:THR:O	3:C:683:PRO:HG2	2.15	0.47
1:D:261:CYS:HB2	1:D:311:TRP:CG	2.50	0.47
1:A:4:LEU:HD23	1:A:298:GLU:HB2	1.97	0.46
3:C:795:SER:HB3	3:C:798:GLN:OE1	2.15	0.46
3:C:24:PHE:CD1	3:C:29:GLN:HA	2.49	0.46
1:D:203:ASP:OD2	1:D:204:ALA:N	2.41	0.46
2:E:99:LYS:HD3	2:E:152:ILE:HG23	1.96	0.46
3:C:617:TYR:OH	3:F:143:SER:HB2	2.15	0.46
3:C:63:PRO:HA	3:C:66:ARG:HD2	1.97	0.46
2:B:79:PHE:CE2	2:B:81:PRO:HG3	2.51	0.46
1:D:237:GLN:CD	1:D:237:GLN:H	2.19	0.46
2:E:26:GLU:OE2	3:F:1011:LEU:HG	2.15	0.46
3:F:626:PRO:HA	3:F:629:PHE:CD2	2.48	0.46
3:F:678:VAL:HG13	3:F:722:PHE:CE2	2.50	0.46
3:F:714:ARG:HD3	3:F:753:PHE:HE1	1.81	0.46
3:F:813:ARG:O	3:F:813:ARG:HG2	2.15	0.46
3:F:188:PRO:HG3	3:F:227:PHE:CZ	2.46	0.46
3:F:866:ARG:HB3	3:F:903:LEU:HD22	1.97	0.46
3:C:625:VAL:HG12	3:C:693:LEU:HD23	1.97	0.46
3:C:739:MET:HA	3:C:742:LEU:HD12	1.97	0.46
2:B:99:LYS:HD3	2:B:152:ILE:HG23	1.98	0.46
1:A:259:SER:HG	1:A:311:TRP:HD1	1.62	0.45
3:C:480:ALA:HA	3:C:483:LEU:CD1	2.46	0.45
3:F:678:VAL:CG1	3:F:722:PHE:HE2	2.29	0.45
3:F:804:LEU:HD13	3:F:844:LEU:HD23	1.98	0.45
1:A:135:ASP:OD2	1:A:136:ASP:N	2.49	0.45
3:F:96:TYR:CD1	3:F:110:VAL:HG13	2.51	0.45
3:F:492:ARG:HH21	3:F:493:LEU:HD21	1.81	0.45
3:F:755:SER:O	3:F:759:THR:HG23	2.16	0.45
3:F:81:HIS:CE1	3:F:119:MET:CB	2.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:5:ILE:HB	2:E:128:GLN:OE1	2.16	0.45
3:C:43:GLY:O	3:C:46:THR:HG23	2.16	0.45
3:C:863:ILE:HG22	3:C:864:MET:SD	2.56	0.45
1:D:10:LEU:HD12	1:D:29:PHE:HZ	1.81	0.45
3:F:24:PHE:CD1	3:F:72:LEU:HD22	2.51	0.45
3:C:209:GLY:C	3:C:211:PHE:H	2.20	0.45
3:F:347:GLY:HA2	3:F:350:LEU:HD12	1.97	0.45
3:C:36:VAL:O	3:C:40:VAL:HG23	2.17	0.45
3:C:685:PHE:HB3	3:C:705:PHE:CZ	2.51	0.45
3:C:685:PHE:CD2	3:C:719:LEU:HD22	2.51	0.45
3:F:24:PHE:CD2	3:F:72:LEU:HD22	2.52	0.45
3:C:709:SER:HB2	3:C:712:GLN:CG	2.46	0.45
3:C:712:GLN:HA	3:C:715:LEU:HD12	1.98	0.45
3:C:713:ARG:NH1	3:C:745:GLN:NE2	2.65	0.45
3:C:843:SER:HG	3:C:898:HIS:CG	2.35	0.45
3:F:426:GLN:NE2	3:F:475:PRO:HD2	2.32	0.45
2:B:25:GLU:CD	2:B:25:GLU:H	2.20	0.45
3:C:214:GLU:CG	3:F:862:ARG:HH12	2.30	0.45
3:C:188:PRO:HB3	3:C:242:LEU:HD11	1.98	0.45
3:F:221:CYS:SG	3:F:222:TYR:CD1	3.10	0.45
1:A:178:GLU:OE1	1:A:181:ASP:HB2	2.17	0.45
3:C:24:PHE:CE1	3:C:29:GLN:HB3	2.52	0.45
3:C:650:LEU:C	3:C:650:LEU:HD12	2.37	0.45
3:C:729:ASN:N	3:C:729:ASN:OD1	2.50	0.45
2:E:9:ASN:HD21	2:E:11:ASN:HD22	1.65	0.45
3:F:650:LEU:HD11	3:F:655:LEU:CG	2.47	0.45
3:F:675:ALA:HA	3:F:678:VAL:CG2	2.47	0.45
3:C:211:PHE:HD1	3:C:214:GLU:CD	2.20	0.45
3:C:649:LEU:HB2	3:C:650:LEU:H	1.60	0.45
3:F:566:HIS:HB3	3:F:569:ILE:HD12	1.99	0.45
3:C:574:LEU:HD11	3:C:620:PHE:CD1	2.52	0.44
3:F:182:MET:HG2	3:F:182:MET:O	2.17	0.44
3:F:209:GLY:C	3:F:211:PHE:H	2.20	0.44
3:F:619:TYR:O	3:F:623:THR:HG23	2.17	0.44
3:F:688:GLY:O	3:F:690:THR:HG23	2.17	0.44
3:F:713:ARG:HD2	3:F:745:GLN:NE2	2.31	0.44
3:C:650:LEU:O	3:C:650:LEU:HD12	2.17	0.44
3:C:728:ARG:HH12	3:C:860:ASP:HB2	1.83	0.44
2:E:28:GLU:HB3	2:E:30:VAL:HG23	1.99	0.44
3:F:480:ALA:HA	3:F:483:LEU:HD12	2.00	0.44
1:A:10:LEU:HD12	1:A:29:PHE:HZ	1.83	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:805:TRP:CZ3	3:C:852:VAL:HG21	2.50	0.44
1:D:123:ARG:HA	1:D:150:ASP:OD1	2.17	0.44
3:F:223:PHE:HB3	3:F:224:PRO:HD3	2.00	0.44
1:A:79:PHE:HA	1:A:105:GLU:HB3	2.00	0.44
2:B:25:GLU:N	2:B:25:GLU:OE1	2.40	0.44
2:B:91:LEU:HD22	2:E:8:ILE:HD11	1.99	0.44
3:C:479:SER:HB3	3:C:482:ASP:OD2	2.18	0.44
3:F:349:PHE:CZ	3:F:353:ILE:HD11	2.53	0.44
3:F:415:LEU:HA	3:F:418:ILE:HD12	1.99	0.44
3:C:745:GLN:HG2	3:C:758:ALA:HB2	1.99	0.44
3:C:855:ARG:CD	3:C:855:ARG:H	2.19	0.44
3:F:308:ARG:HH11	3:F:308:ARG:HG3	1.83	0.44
3:F:727:PRO:O	3:F:730:VAL:HG13	2.17	0.44
2:B:82:THR:O	2:B:86:CYS:HB2	2.18	0.44
3:C:674:ALA:O	3:C:678:VAL:HG23	2.17	0.44
3:F:267:LYS:HG2	3:F:275:ALA:HB1	2.00	0.44
3:F:627:CYS:O	3:F:631:LEU:HD13	2.17	0.44
3:F:637:MET:HB3	3:F:638:PRO:HD3	2.00	0.44
3:F:625:VAL:CG1	3:F:692:PHE:CE1	3.00	0.44
1:A:256:TYR:CE1	2:B:132:LYS:HE2	2.53	0.43
3:C:153:PHE:CE1	3:C:185:GLU:HG2	2.53	0.43
3:C:516:THR:HG23	3:C:565:THR:HB	2.00	0.43
1:A:11:GLN:HE21	3:C:999:ARG:CZ	2.30	0.43
1:D:79:PHE:HA	1:D:105:GLU:HB3	2.01	0.43
3:C:221:CYS:SG	3:C:222:TYR:CD1	3.11	0.43
3:C:89:VAL:HG11	3:C:123:LEU:HB3	2.00	0.43
3:C:911:GLU:HB3	3:C:915:LEU:HD23	1.99	0.43
3:F:262:PRO:HG3	3:F:298:PHE:CE1	2.53	0.43
3:C:152:VAL:HA	3:C:155:ILE:HD12	1.99	0.43
3:C:182:MET:HG3	3:C:194:ALA:CB	2.48	0.43
1:D:83:THR:HB	1:D:99:LEU:HB2	2.00	0.43
3:F:631:LEU:HD23	3:F:718:LEU:HD13	2.00	0.43
3:F:808:LYS:HE2	3:F:812:LEU:HD21	2.00	0.43
3:F:890:PRO:HA	3:F:893:LEU:HD12	1.99	0.43
1:A:178:GLU:HA	1:A:179:PRO:HD3	1.82	0.43
3:C:885:PRO:O	3:C:889:LYS:HB2	2.19	0.43
3:F:877:LEU:HD13	3:F:896:LEU:CG	2.34	0.43
1:A:58:HIS:NE2	1:A:76:SER:OG	2.38	0.43
3:C:743:LEU:HB3	3:C:785:THR:HG21	2.00	0.43
3:C:912:LEU:N	3:C:913:PRO:HD2	2.33	0.43
3:F:1003:LYS:HB3	3:F:1004:PRO:HD3	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:F:969:MET:HG3	3:F:1009:LYS:HD3	1.99	0.43
3:F:188:PRO:CG	3:F:227:PHE:HZ	2.29	0.43
3:F:793:GLU:CD	3:F:793:GLU:H	2.22	0.43
3:C:227:PHE:N	3:C:227:PHE:CD2	2.86	0.43
3:C:299:LEU:HD21	3:C:349:PHE:CG	2.53	0.43
3:F:227:PHE:CD2	3:F:227:PHE:N	2.86	0.43
3:F:361:LEU:HD23	3:F:369:VAL:HG22	2.00	0.43
3:C:178:PHE:HE2	3:C:198:VAL:HG23	1.84	0.43
3:C:693:LEU:HD23	3:C:693:LEU:HA	1.74	0.43
3:C:854:THR:OG1	3:C:857:GLY:N	2.51	0.43
3:C:361:LEU:HD11	3:C:376:LEU:HD11	2.01	0.43
3:F:36:VAL:O	3:F:40:VAL:HG23	2.19	0.43
3:C:187:ASP:CG	3:C:190:ASN:H	2.22	0.43
3:C:22:GLN:O	3:C:26:MET:HE2	2.17	0.43
3:C:360:HIS:CD2	3:C:368:LEU:HB3	2.54	0.43
3:C:81:HIS:CE1	3:C:119:MET:CB	3.01	0.43
1:D:11:GLN:HE21	3:F:999:ARG:HH22	1.67	0.43
1:A:122:SER:OG	1:A:123:ARG:N	2.52	0.43
2:B:32:ASP:CB	3:C:1013:ARG:HH22	2.29	0.43
3:C:221:CYS:SG	3:C:222:TYR:HD1	2.40	0.43
3:C:483:LEU:O	3:C:487:VAL:HG23	2.19	0.43
3:C:637:MET:HB3	3:C:638:PRO:HD3	2.01	0.43
3:C:659:ALA:HB1	3:C:721:ALA:CB	2.42	0.43
3:C:712:GLN:HG2	3:C:712:GLN:H	0.88	0.42
3:C:848:ASP:OD2	3:C:848:ASP:N	2.51	0.42
3:F:152:VAL:HA	3:F:155:ILE:HD12	2.01	0.42
3:F:808:LYS:O	3:F:811:VAL:N	2.47	0.42
3:F:911:GLU:HB3	3:F:915:LEU:HD23	2.01	0.42
3:C:260:LEU:HD13	3:C:264:LEU:HD11	2.01	0.42
3:C:308:ARG:HH11	3:C:308:ARG:HG3	1.84	0.42
3:C:597:VAL:HG23	3:C:654:VAL:CG2	2.43	0.42
3:C:625:VAL:HG12	3:C:693:LEU:CD2	2.49	0.42
3:F:459:GLN:HA	3:F:462:LEU:HD12	2.01	0.42
3:F:590:VAL:HG21	3:F:649:LEU:HD13	2.02	0.42
3:F:680:CYS:HB3	3:F:692:PHE:CD1	2.54	0.42
3:C:872:ASP:O	3:C:875:PRO:HD2	2.19	0.42
3:F:107:VAL:CG2	3:F:108:PRO:HD3	2.48	0.42
3:F:182:MET:HG3	3:F:194:ALA:CB	2.46	0.42
3:F:714:ARG:CG	3:F:753:PHE:HE1	2.28	0.42
3:F:92:LEU:HB3	3:F:117:LEU:HD11	2.00	0.42
3:F:298:PHE:CD2	3:F:298:PHE:N	2.88	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:F:847:SER:HB2	3:F:902:ARG:NE	2.34	0.42
3:C:492:ARG:HH21	3:C:493:LEU:HD21	1.82	0.42
3:C:572:GLU:O	3:C:575:PRO:HD2	2.20	0.42
3:C:628:LEU:HD23	3:C:718:LEU:HD13	2.01	0.42
3:C:719:LEU:O	3:C:723:VAL:HG23	2.19	0.42
1:D:224:TYR:CE2	1:D:232:VAL:HG21	2.55	0.42
2:E:29:ASN:HA	3:F:1009:LYS:HE3	2.02	0.42
3:F:986:PRO:O	3:F:989:VAL:HG22	2.19	0.42
3:C:176:PHE:HA	3:C:179:ILE:HD12	2.02	0.42
3:C:187:ASP:OD1	3:C:189:ARG:HB3	2.19	0.42
3:C:804:LEU:HA	3:C:804:LEU:HD23	1.55	0.42
3:F:584:ALA:HA	3:F:589:MET:HB2	2.00	0.42
3:C:216:PHE:CE2	3:C:259:PHE:HB3	2.54	0.42
3:C:600:CYS:SG	3:C:658:LEU:HD22	2.60	0.42
3:F:176:PHE:HA	3:F:179:ILE:HD12	2.00	0.42
3:C:459:GLN:HA	3:C:462:LEU:HD12	2.02	0.42
3:C:625:VAL:HB	3:C:626:PRO:CD	2.46	0.42
3:C:661:VAL:O	3:C:664:THR:OG1	2.32	0.42
3:C:986:PRO:O	3:C:989:VAL:HG22	2.20	0.42
3:F:650:LEU:HG	3:F:650:LEU:O	2.14	0.42
3:F:662:ILE:O	3:F:666:THR:OG1	2.37	0.42
3:F:713:ARG:HD2	3:F:745:GLN:HE21	1.84	0.42
3:F:721:ALA:O	3:F:725:SER:OG	2.32	0.42
3:F:912:LEU:N	3:F:913:PRO:HD2	2.35	0.42
1:A:123:ARG:HA	1:A:150:ASP:OD1	2.20	0.42
3:F:719:LEU:HD11	3:F:738:LEU:HD21	2.01	0.42
3:C:1003:LYS:HB3	3:C:1004:PRO:HD3	2.02	0.42
3:C:750:SER:HA	3:C:798:GLN:CD	2.39	0.42
3:C:187:ASP:HA	3:C:188:PRO:HD3	1.83	0.41
3:C:201:LEU:O	3:C:206:TYR:HB2	2.20	0.41
2:B:118:THR:O	2:E:84:PRO:HG3	2.20	0.41
3:F:96:TYR:CE1	3:F:113:GLY:HA3	2.56	0.41
3:F:201:LEU:O	3:F:206:TYR:HB2	2.20	0.41
3:F:909:LEU:O	3:F:912:LEU:HB2	2.19	0.41
3:C:479:SER:HB3	3:C:482:ASP:CG	2.41	0.41
3:C:749:HIS:O	3:C:749:HIS:ND1	2.52	0.41
3:C:894:LYS:HG2	3:C:930:VAL:HG21	2.02	0.41
3:F:896:LEU:HD22	3:F:900:LEU:CD1	2.50	0.41
3:F:692:PHE:HD2	3:F:692:PHE:H	1.67	0.41
3:C:702:PHE:HZ	3:C:712:GLN:HB3	1.77	0.41
3:C:853:LEU:H	3:C:853:LEU:HD22	1.85	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:F:753:PHE:CD2	3:F:753:PHE:C	2.93	0.41
1:A:65:ILE:HA	1:A:75:ALA:O	2.20	0.41
3:F:467:THR:O	3:F:471:LEU:HB2	2.21	0.41
3:F:702:PHE:HA	3:F:712:GLN:HE22	1.83	0.41
3:F:720:THR:HG22	3:F:761:CYS:CB	2.41	0.41
3:C:223:PHE:CD1	3:C:224:PRO:HD3	2.56	0.41
3:C:293:LYS:H	3:C:293:LYS:NZ	2.18	0.41
3:C:439:SER:HA	3:C:442:LYS:HD2	2.03	0.41
3:C:889:LYS:N	3:C:890:PRO:CD	2.84	0.41
1:D:270:ALA:HB2	1:D:309:VAL:HG13	2.02	0.41
1:D:65:ILE:HA	1:D:75:ALA:O	2.21	0.41
3:F:24:PHE:CD1	3:F:29:GLN:HA	2.56	0.41
3:F:572:GLU:O	3:F:575:PRO:HD2	2.21	0.41
3:F:885:PRO:O	3:F:889:LYS:HB2	2.20	0.41
3:F:939:GLN:HB3	3:F:940:PRO:HD3	2.01	0.41
3:C:629:PHE:HZ	3:C:696:ASN:HB2	1.86	0.41
3:F:303:TRP:CH2	3:F:307:ARG:HD3	2.56	0.41
3:F:736:ASN:O	3:F:740:ARG:HG3	2.20	0.41
3:C:695:GLU:N	3:C:695:GLU:OE1	2.53	0.41
3:F:246:LEU:HD22	3:F:250:LEU:HD11	2.02	0.41
3:F:713:ARG:O	3:F:754:SER:OG	2.36	0.41
3:F:870:PHE:HB2	3:F:903:LEU:HD13	2.02	0.41
3:C:187:ASP:OD2	3:C:190:ASN:CB	2.69	0.41
3:C:246:LEU:HD22	3:C:250:LEU:HD11	2.02	0.41
3:F:186:LYS:HD2	3:F:186:LYS:N	2.35	0.41
3:F:814:TYR:HE1	3:F:868:ARG:CG	2.34	0.41
1:A:190:LEU:N	1:A:190:LEU:HD12	2.35	0.41
3:C:427:LYS:HG2	3:F:234:PRO:HD3	2.03	0.41
1:D:213:SER:OG	1:D:214:ASP:N	2.54	0.41
3:F:449:VAL:O	3:F:453:LEU:HG	2.20	0.41
3:F:651:GLU:H	3:F:654:VAL:HG11	1.86	0.41
3:F:714:ARG:HD3	3:F:753:PHE:CE1	2.55	0.41
3:F:776:GLU:HA	3:F:779:LEU:HD12	2.02	0.41
3:F:801:THR:O	3:F:805:TRP:HD1	2.04	0.41
3:C:735:LEU:HG	3:C:778:PHE:CZ	2.55	0.41
3:F:191:LEU:HD23	3:F:191:LEU:HA	1.85	0.41
3:F:678:VAL:O	3:F:680:CYS:N	2.54	0.41
3:F:889:LYS:N	3:F:890:PRO:CD	2.84	0.41
1:A:237:GLN:CD	1:A:237:GLN:H	2.20	0.40
3:C:261:LEU:O	3:C:265:ILE:HG13	2.22	0.40
3:F:629:PHE:CD2	3:F:694:PRO:HD2	2.56	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:F:846:MET:HA	3:F:846:MET:CE	2.51	0.40
1:A:67:TRP:CD2	1:A:74:LEU:HD13	2.56	0.40
2:B:12:VAL:HG22	2:B:15:ARG:NH1	2.37	0.40
3:C:214:GLU:HG3	3:F:862:ARG:HH12	1.85	0.40
3:C:909:LEU:O	3:C:912:LEU:HB2	2.20	0.40
3:F:182:MET:O	3:F:218:VAL:HG11	2.21	0.40
3:F:494:THR:HG22	3:F:508:LEU:HG	2.01	0.40
3:F:690:THR:HB	3:F:693:LEU:CD1	2.47	0.40
3:F:809:ALA:HA	3:F:812:LEU:CD1	2.52	0.40
1:A:201:ASP:O	1:A:209:LEU:HD12	2.21	0.40
2:B:83:ILE:HG22	2:B:85:HIS:H	1.87	0.40
1:D:66:ARG:HD3	1:D:66:ARG:HA	1.81	0.40
3:F:295:LEU:N	3:F:295:LEU:HD23	2.36	0.40
2:B:20:VAL:O	2:B:20:VAL:HG13	2.21	0.40
3:C:530:LEU:HD13	3:C:560:LEU:HG	2.02	0.40
3:C:652:ASP:HB3	3:C:714:ARG:HH21	1.82	0.40
3:C:657:ALA:O	3:C:661:VAL:HG23	2.22	0.40
3:C:848:ASP:HB3	3:C:855:ARG:HH21	1.87	0.40
1:D:67:TRP:CD2	1:D:74:LEU:HD13	2.56	0.40
3:F:316:GLU:H	3:F:316:GLU:HG3	1.67	0.40
3:C:625:VAL:HG13	3:C:692:PHE:CD1	2.57	0.40
3:F:853:LEU:H	3:F:853:LEU:HD22	1.86	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	334/338 (99%)	320 (96%)	14 (4%)	0	100	100
1	D	334/338 (99%)	322 (96%)	12 (4%)	0	100	100
2	B	152/159 (96%)	148 (97%)	4 (3%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
2	E	152/159 (96%)	148 (97%)	4 (3%)	0	100 100
3	C	984/1035 (95%)	936 (95%)	47 (5%)	1 (0%)	51 83
3	F	979/1035 (95%)	930 (95%)	48 (5%)	1 (0%)	51 83
All	All	2935/3064 (96%)	2804 (96%)	129 (4%)	2 (0%)	51 83

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	C	223	PHE
3	F	223	PHE

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	284/284 (100%)	280 (99%)	4 (1%)	67 85
1	D	284/284 (100%)	280 (99%)	4 (1%)	67 85
2	B	141/142 (99%)	139 (99%)	2 (1%)	67 85
2	E	141/142 (99%)	141 (100%)	0	100 100
3	C	859/887 (97%)	734 (85%)	125 (15%)	3 20
3	F	854/887 (96%)	717 (84%)	137 (16%)	2 16
All	All	2563/2626 (98%)	2291 (89%)	272 (11%)	6 32

All (272) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	109	VAL
1	A	170	ASN
1	A	210	VAL
1	A	274	ASP
2	B	21	LEU
2	B	24	ASN

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Mol	Chain	Res	Type
3	C	78	LEU
3	C	81	HIS
3	C	84	LEU
3	C	94	LEU
3	C	100	LEU
3	C	114	LEU
3	C	123	LEU
3	C	135	ILE
3	C	136	PHE
3	C	137	GLN
3	C	138	GLU
3	C	142	GLN
3	C	149	ARG
3	C	157	THR
3	C	170	LEU
3	C	175	THR
3	C	187	ASP
3	C	204	LYS
3	C	207	SER
3	C	208	LEU
3	C	214	GLU
3	C	225	ILE
3	C	227	PHE
3	C	238	GLN
3	C	244	LEU
3	C	253	THR
3	C	260	LEU
3	C	263	LEU
3	C	272	ILE
3	C	273	LEU
3	C	277	LEU
3	C	289	VAL
3	C	293	LYS
3	C	294	GLU
3	C	295	LEU
3	C	296	LYS
3	C	305	SER
3	C	313	THR
3	C	316	GLU
3	C	329	LEU
3	C	332	CYS
3	C	338	LEU

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Mol	Chain	Res	Type
3	C	344	ASP
3	C	346	LEU
3	C	363	GLU
3	C	387	CYS
3	C	393	ASN
3	C	415	LEU
3	C	419	LEU
3	C	431	GLU
3	C	432	ASP
3	C	434	ASP
3	C	438	LEU
3	C	442	LYS
3	C	445	LEU
3	C	455	ASP
3	C	460	LEU
3	C	467	THR
3	C	468	LEU
3	C	482	ASP
3	C	483	LEU
3	C	485	LEU
3	C	496	LEU
3	C	536	LYS
3	C	553	HIS
3	C	564	SER
3	C	585	ASN
3	C	590	VAL
3	C	605	GLN
3	C	649	LEU
3	C	653	GLU
3	C	654	VAL
3	C	658	LEU
3	C	666	THR
3	C	667	THR
3	C	673	LEU
3	C	692	PHE
3	C	695	GLU
3	C	712	GLN
3	C	714	ARG
3	C	723	VAL
3	C	729	ASN
3	C	730	VAL
3	C	738	LEU

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Mol	Chain	Res	Type
3	C	745	GLN
3	C	753	PHE
3	C	754	SER
3	C	759	THR
3	C	774	GLN
3	C	775	LEU
3	C	794	SER
3	C	795	SER
3	C	797	ASP
3	C	811	VAL
3	C	812	LEU
3	C	814	TYR
3	C	820	CYS
3	C	842	PHE
3	C	843	SER
3	C	846	MET
3	C	847	SER
3	C	848	ASP
3	C	849	CYS
3	C	852	VAL
3	C	853	LEU
3	C	854	THR
3	C	855	ARG
3	C	860	ASP
3	C	861	VAL
3	C	864	MET
3	C	868	ARG
3	C	872	ASP
3	C	888	VAL
3	C	889	LYS
3	C	893	LEU
3	C	896	LEU
3	C	902	ARG
3	C	912	LEU
3	C	916	LEU
3	C	932	LEU
3	C	943	LEU
3	C	944	GLU
3	C	982	LEU
3	C	990	LEU
3	C	1010	ARG
1	D	109	VAL

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Mol	Chain	Res	Type
1	D	170	ASN
1	D	210	VAL
1	D	274	ASP
3	F	28	GLN
3	F	78	LEU
3	F	81	HIS
3	F	84	LEU
3	F	93	ILE
3	F	94	LEU
3	F	100	LEU
3	F	102	ASP
3	F	114	LEU
3	F	123	LEU
3	F	133	LYS
3	F	136	PHE
3	F	137	GLN
3	F	138	GLU
3	F	142	GLN
3	F	146	GLN
3	F	157	THR
3	F	166	GLU
3	F	170	LEU
3	F	175	THR
3	F	180	GLN
3	F	186	LYS
3	F	187	ASP
3	F	204	LYS
3	F	207	SER
3	F	208	LEU
3	F	223	PHE
3	F	225	ILE
3	F	226	ASP
3	F	238	GLN
3	F	244	LEU
3	F	253	THR
3	F	260	LEU
3	F	263	LEU
3	F	267	LYS
3	F	272	ILE
3	F	273	LEU
3	F	277	LEU
3	F	289	VAL

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Mol	Chain	Res	Type
3	F	294	GLU
3	F	295	LEU
3	F	296	LYS
3	F	301	SER
3	F	302	LEU
3	F	305	SER
3	F	313	THR
3	F	316	GLU
3	F	329	LEU
3	F	332	CYS
3	F	338	LEU
3	F	344	ASP
3	F	346	LEU
3	F	363	GLU
3	F	387	CYS
3	F	393	ASN
3	F	415	LEU
3	F	419	LEU
3	F	431	GLU
3	F	432	ASP
3	F	434	ASP
3	F	438	LEU
3	F	442	LYS
3	F	445	LEU
3	F	455	ASP
3	F	460	LEU
3	F	467	THR
3	F	468	LEU
3	F	471	LEU
3	F	474	GLN
3	F	478	LEU
3	F	479	SER
3	F	481	GLU
3	F	485	LEU
3	F	496	LEU
3	F	536	LYS
3	F	553	HIS
3	F	564	SER
3	F	585	ASN
3	F	590	VAL
3	F	605	GLN
3	F	625	VAL

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Mol	Chain	Res	Type
3	F	628	LEU
3	F	629	PHE
3	F	649	LEU
3	F	650	LEU
3	F	652	ASP
3	F	666	THR
3	F	667	THR
3	F	669	LEU
3	F	678	VAL
3	F	682	VAL
3	F	686	LEU
3	F	692	PHE
3	F	706	GLN
3	F	714	ARG
3	F	719	LEU
3	F	723	VAL
3	F	730	VAL
3	F	751	CYS
3	F	753	PHE
3	F	754	SER
3	F	774	GLN
3	F	775	LEU
3	F	793	GLU
3	F	797	ASP
3	F	811	VAL
3	F	812	LEU
3	F	820	CYS
3	F	840	ASP
3	F	846	MET
3	F	848	ASP
3	F	849	CYS
3	F	851	ASP
3	F	852	VAL
3	F	853	LEU
3	F	854	THR
3	F	855	ARG
3	F	860	ASP
3	F	861	VAL
3	F	863	ILE
3	F	864	MET
3	F	872	ASP
3	F	875	PRO

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Mol	Chain	Res	Type
3	F	888	VAL
3	F	889	LYS
3	F	896	LEU
3	F	902	ARG
3	F	912	LEU
3	F	916	LEU
3	F	932	LEU
3	F	943	LEU
3	F	944	GLU
3	F	959	LYS
3	F	982	LEU
3	F	990	LEU
3	F	1010	ARG
3	F	1026	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (35) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	11	GLN
2	B	51	HIS
2	B	76	HIS
2	B	85	HIS
3	C	29	GLN
3	C	81	HIS
3	C	140	HIS
3	C	146	GLN
3	C	180	GLN
3	C	401	GLN
3	C	461	GLN
3	C	489	HIS
3	C	566	HIS
3	C	734	GLN
3	C	736	ASN
3	C	745	GLN
3	C	769	GLN
3	C	774	GLN
3	C	873	ASN
3	C	901	ASN
1	D	11	GLN
2	E	11	ASN
2	E	51	HIS
3	F	79	GLN

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Mol	Chain	Res	Type
3	F	81	HIS
3	F	140	HIS
3	F	180	GLN
3	F	401	GLN
3	F	461	GLN
3	F	489	HIS
3	F	566	HIS
3	F	749	HIS
3	F	769	GLN
3	F	873	ASN
3	F	901	ASN

5.3.3 RNA

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates

There are no monosaccharides in this entry.

5.6 Ligand geometry

There are no ligands in this entry.

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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	336/338 (99%)	-0.07	11 (3%) 46 31	148, 195, 264, 303	0
1	D	336/338 (99%)	1.30	91 (27%) 0 0	314, 381, 426, 449	0
2	B	154/159 (96%)	-0.17	7 (4%) 33 21	164, 192, 281, 306	0
2	E	154/159 (96%)	0.02	10 (6%) 18 11	220, 249, 307, 323	0
3	C	994/1035 (96%)	-0.42	21 (2%) 63 48	118, 184, 263, 377	0
3	F	989/1035 (95%)	-0.46	15 (1%) 73 60	111, 167, 234, 375	0
All	All	2963/3064 (96%)	-0.16	155 (5%) 27 17	111, 189, 385, 449	0

All (155) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	31	SER	8.4
1	D	28	VAL	8.1
1	D	223	ALA	7.5
1	D	90	SER	6.8
1	D	91	GLY	6.7
1	D	226	PRO	6.5
1	D	136	ASP	6.3
3	F	30	GLU	6.1
3	F	31	GLY	6.1
1	D	277	ARG	5.9
1	D	229	THR	5.8
1	D	27	ASN	5.3
1	D	193	HIS	5.3
1	D	248	SER	5.2
3	F	591	THR	5.2
1	D	108	SER	5.1
1	D	135	ASP	5.0
1	D	92	GLU	4.9
1	D	176	ALA	4.7

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Mol	Chain	Res	Type	RSRZ
1	D	204	ALA	4.7
1	D	268	ALA	4.5
1	D	227	GLY	4.5
1	D	192	SER	4.3
1	D	238	GLN	4.1
1	D	326	GLY	4.1
1	D	283	SER	4.0
1	D	69	PRO	3.9
1	D	275	GLY	3.9
1	D	142	ALA	3.9
2	B	155	LYS	3.9
1	A	321	SER	3.9
2	E	11	ASN	3.9
1	D	228	ASN	3.8
1	D	269	THR	3.8
1	D	89	SER	3.8
1	D	314	VAL	3.7
1	D	239	THR	3.7
1	A	59	LYS	3.6
3	F	498	GLU	3.6
2	B	85	HIS	3.6
2	B	13	TYR	3.6
1	D	205	ASP	3.6
1	D	30	ALA	3.6
1	D	264	THR	3.6
1	D	211	SER	3.5
3	F	235	TYR	3.5
1	D	11	GLN	3.5
1	D	191	THR	3.4
3	C	638	PRO	3.4
1	D	110	SER	3.4
3	C	703	GLN	3.4
1	D	250	GLN	3.3
3	C	432	ASP	3.3
1	D	46	ASN	3.3
3	C	591	THR	3.3
1	D	88	LYS	3.2
1	D	225	HIS	3.2
3	F	586	LYS	3.2
3	F	749	HIS	3.2
3	C	433	ARG	3.1
2	E	85	HIS	3.1

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Mol	Chain	Res	Type	RSRZ
1	D	180	ILE	3.1
1	D	141	ALA	3.0
3	F	434	ASP	3.0
3	C	15	GLY	3.0
1	D	21	ALA	2.9
1	D	199	GLY	2.9
1	D	243	CYS	2.9
1	D	144	LEU	2.8
1	D	75	ALA	2.8
1	D	39	ARG	2.8
1	D	322	CYS	2.8
1	A	326	GLY	2.7
2	E	12	VAL	2.7
3	C	340	ALA	2.7
3	C	696	ASN	2.7
1	D	119	ALA	2.7
1	D	323	SER	2.7
3	F	748	GLY	2.7
1	D	327	THR	2.7
2	E	84	PRO	2.7
3	F	234	PRO	2.7
1	D	57	GLY	2.7
1	D	1	ARG	2.7
1	D	262	LYS	2.7
1	D	236	ASP	2.7
1	D	256	TYR	2.6
1	D	184	TRP	2.6
1	D	251	HIS	2.6
1	A	269	THR	2.6
1	D	173	LYS	2.5
3	C	336	SER	2.5
2	B	84	PRO	2.5
1	A	231	GLY	2.5
1	A	133	ALA	2.5
1	D	261	CYS	2.5
1	D	126	SER	2.5
2	E	18	GLU	2.5
2	B	119	HIS	2.5
1	D	100	GLU	2.5
1	D	3	ARG	2.5
1	D	113	ARG	2.5
3	C	341	ASP	2.5

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Mol	Chain	Res	Type	RSRZ
3	F	60	ASN	2.5
2	E	14	ASP	2.4
1	D	158	PRO	2.4
1	D	155	VAL	2.4
3	F	750	SER	2.4
3	C	434	ASP	2.4
1	D	121	CYS	2.4
3	F	967	TYR	2.4
3	C	699	PRO	2.4
3	C	498	GLU	2.3
1	D	26	GLY	2.3
1	D	98	THR	2.3
2	E	155	LYS	2.3
3	C	750	SER	2.3
3	C	550	CYS	2.3
2	E	17	LYS	2.3
1	D	59	LYS	2.2
1	D	70	CYS	2.2
3	C	586	LYS	2.2
1	D	143	VAL	2.2
3	C	235	TYR	2.2
1	A	0	GLY	2.2
1	D	56	ASP	2.2
2	B	15	ARG	2.2
1	D	222	ARG	2.2
1	D	64	GLU	2.2
1	A	43	LEU	2.1
3	F	436	ARG	2.1
1	D	145	ASN	2.1
1	A	277	ARG	2.1
1	D	179	PRO	2.1
2	E	2	PRO	2.1
1	D	219	LYS	2.1
1	D	252	SER	2.1
3	C	588	ASN	2.1
1	D	286	LYS	2.1
1	D	297	ALA	2.1
1	D	175	PHE	2.1
3	C	102	ASP	2.1
1	D	198	TRP	2.1
1	D	20	VAL	2.1
1	D	177	GLU	2.1

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Mol	Chain	Res	Type	RSRZ
1	A	76	SER	2.1
3	C	749	HIS	2.1
1	D	318	GLN	2.1
1	D	259	SER	2.0
1	A	327	THR	2.0
2	B	14	ASP	2.0
3	F	502	SER	2.0
2	E	108	PHE	2.0
1	D	0	GLY	2.0
3	C	587	GLY	2.0

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

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

6.3 Carbohydrates (i)

There are no monosaccharides in this entry.

6.4 Ligands (i)

There are no ligands in this entry.

6.5 Other polymers (i)

There are no such residues in this entry.