Full wwPDB X-ray Structure Validation Report (i)

Sep 10, 2023 – 07:46 AM EDT

PDB ID	:	4IOF
Title	:	Crystal structure analysis of Fab-bound human Insulin Degrading Enzyme (IDE)
Authors	:	McCord, L.A.; Liang, W.G.; Hoey, R.; Dowdell, E.; Koide, A.; Koide, S.; Tang, W.J.
Deposited on	:	2013-01-07
Resolution	:	3.35 Å(reported)

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

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

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

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

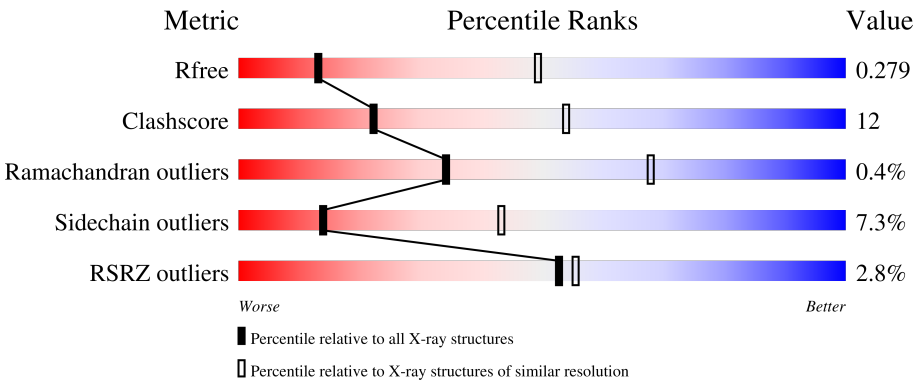
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.35.1
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35.1

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 3.35 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	1558 (3.42-3.30)
Clashscore	141614	1627 (3.42-3.30)
Ramachandran outliers	138981	1599 (3.42-3.30)
Sidechain outliers	138945	1598 (3.42-3.30)
RSRZ outliers	127900	1507 (3.42-3.30)

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	990	% 75% 18% • 6%
1	B	990	2% 63% 22% • 13%
2	C	263	50% 30% • 18%
2	E	263	3% 43% 33% • 20%
3	D	239	6% 49% 29% 5% 17%

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Mol	Chain	Length	Quality of chain
3	F	239	7% 45% 33% • • 18%

2 Entry composition (i)

There are 5 unique types of molecules in this entry. The entry contains 20939 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 Insulin-degrading enzyme.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	932	7622	4911	1274	1415	22	0	0	0
1	B	861	7040	4550	1173	1296	21	0	0	0

There are 50 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	30	MET	-	expression tag	UNP P14735
A	31	HIS	-	expression tag	UNP P14735
A	32	HIS	-	expression tag	UNP P14735
A	33	HIS	-	expression tag	UNP P14735
A	34	HIS	-	expression tag	UNP P14735
A	35	HIS	-	expression tag	UNP P14735
A	36	HIS	-	expression tag	UNP P14735
A	37	ALA	-	expression tag	UNP P14735
A	38	ALA	-	expression tag	UNP P14735
A	39	GLY	-	expression tag	UNP P14735
A	40	ILE	-	expression tag	UNP P14735
A	41	PRO	-	expression tag	UNP P14735
A	110	LEU	CYS	conflict	UNP P14735
A	171	SER	CYS	conflict	UNP P14735
A	178	ALA	CYS	conflict	UNP P14735
A	257	VAL	CYS	conflict	UNP P14735
A	414	LEU	CYS	conflict	UNP P14735
A	573	ASN	CYS	conflict	UNP P14735
A	590	SER	CYS	conflict	UNP P14735
A	789	SER	CYS	conflict	UNP P14735
A	812	ALA	CYS	conflict	UNP P14735
A	819	ALA	CYS	conflict	UNP P14735
A	904	SER	CYS	conflict	UNP P14735
A	966	ASN	CYS	conflict	UNP P14735
A	974	ALA	CYS	conflict	UNP P14735

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Chain	Residue	Modelled	Actual	Comment	Reference
B	30	MET	-	expression tag	UNP P14735
B	31	HIS	-	expression tag	UNP P14735
B	32	HIS	-	expression tag	UNP P14735
B	33	HIS	-	expression tag	UNP P14735
B	34	HIS	-	expression tag	UNP P14735
B	35	HIS	-	expression tag	UNP P14735
B	36	HIS	-	expression tag	UNP P14735
B	37	ALA	-	expression tag	UNP P14735
B	38	ALA	-	expression tag	UNP P14735
B	39	GLY	-	expression tag	UNP P14735
B	40	ILE	-	expression tag	UNP P14735
B	41	PRO	-	expression tag	UNP P14735
B	110	LEU	CYS	conflict	UNP P14735
B	171	SER	CYS	conflict	UNP P14735
B	178	ALA	CYS	conflict	UNP P14735
B	257	VAL	CYS	conflict	UNP P14735
B	414	LEU	CYS	conflict	UNP P14735
B	573	ASN	CYS	conflict	UNP P14735
B	590	SER	CYS	conflict	UNP P14735
B	789	SER	CYS	conflict	UNP P14735
B	812	ALA	CYS	conflict	UNP P14735
B	819	ALA	CYS	conflict	UNP P14735
B	904	SER	CYS	conflict	UNP P14735
B	966	ASN	CYS	conflict	UNP P14735
B	974	ALA	CYS	conflict	UNP P14735

- Molecule 2 is a protein called Fab-bound IDE, heavy chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	C	216	1637	1043	268	319	7	0	0	0
			Total	C	N	O	S			
2	E	211	1602	1023	263	309	7	0	0	0

- Molecule 3 is a protein called Fab-bound IDE, light chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
3	D	199	1528	962	255	306	5	0	0	0
			Total	C	N	O	S			
3	F	197	1508	947	250	306	5	0	0	0

- Molecule 4 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Zn		
4	A	1	1	1	0	0

- Molecule 5 is water.

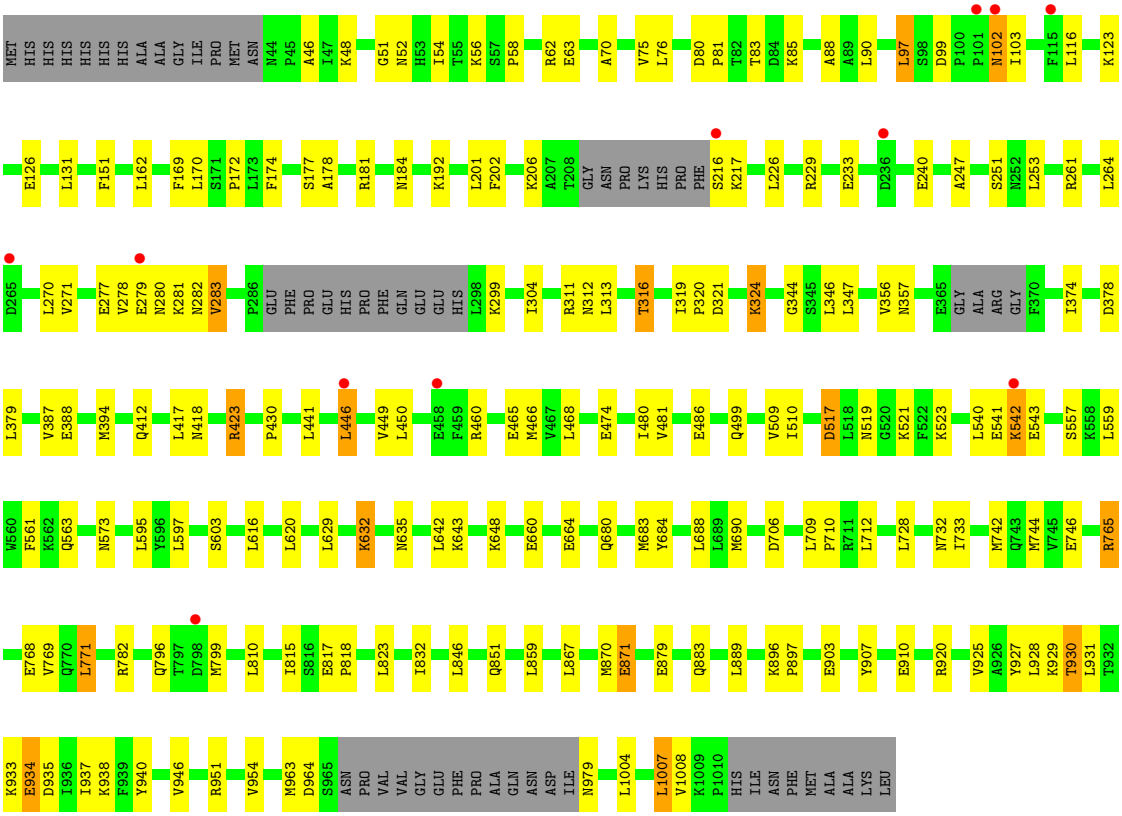
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
5	B	1	1	1	0	0

3 Residue-property plots (i)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry 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.

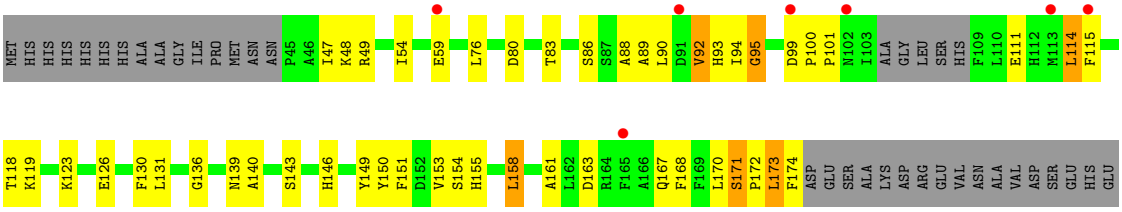
• Molecule 1: Insulin-degrading enzyme

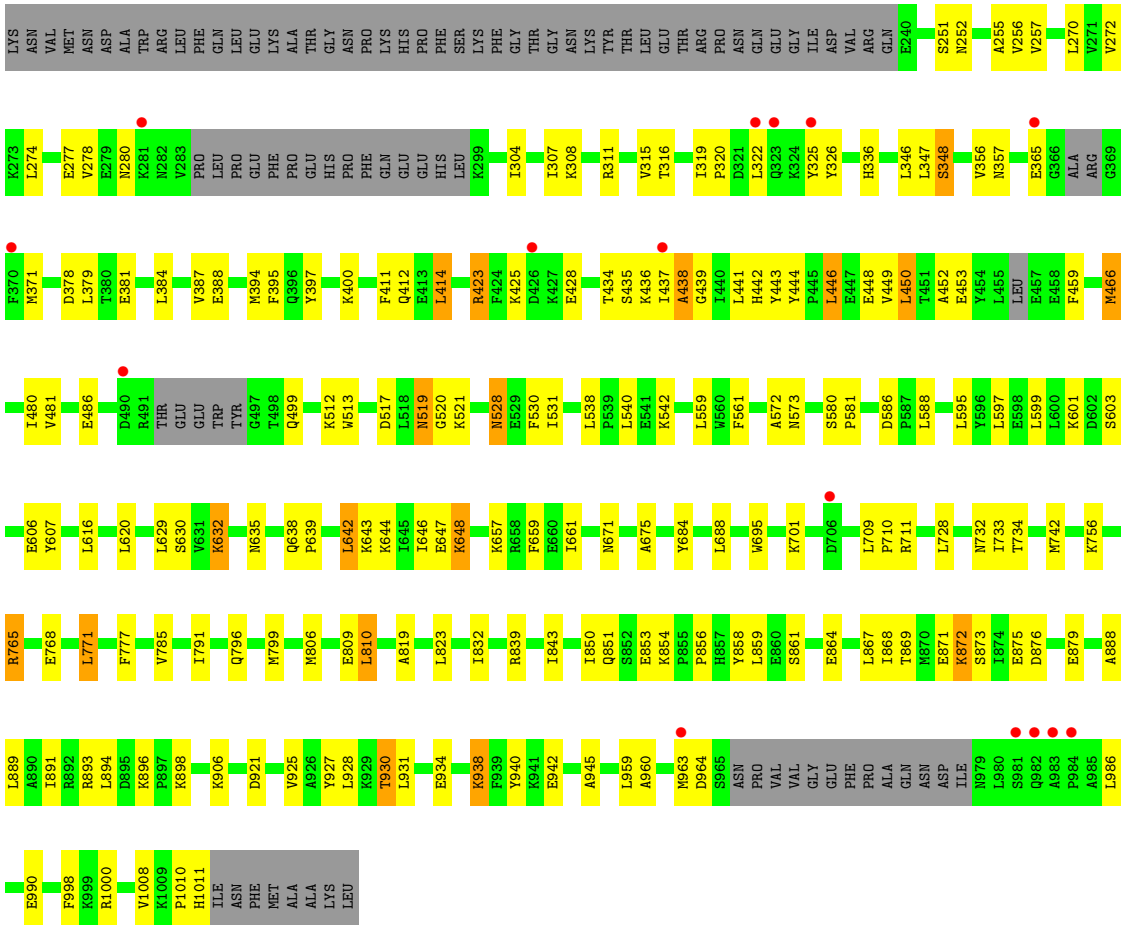
Chain A:



• Molecule 1: Insulin-degrading enzyme

Chain B:



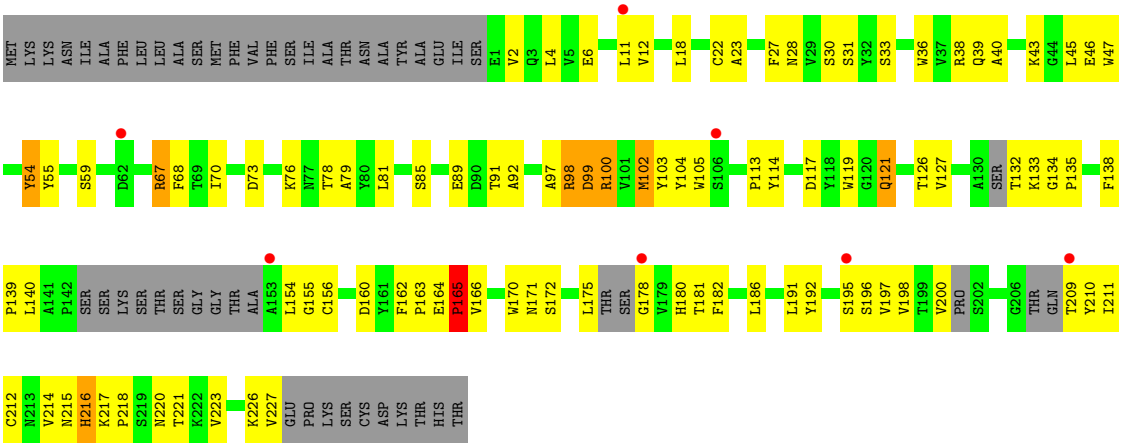


- Molecule 2: Fab-bound IDE, heavy chain

Chain C:

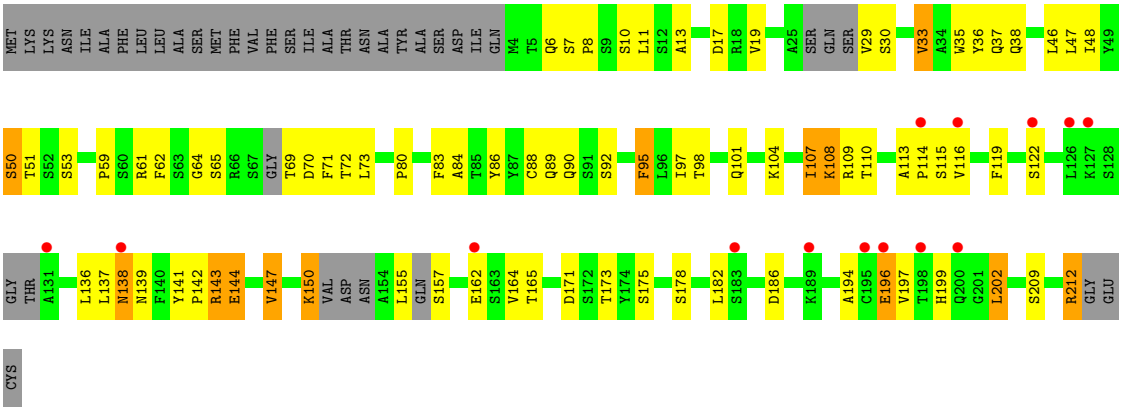
- Molecule 2: Fab-bound IDE, heavy chain

Chain E:



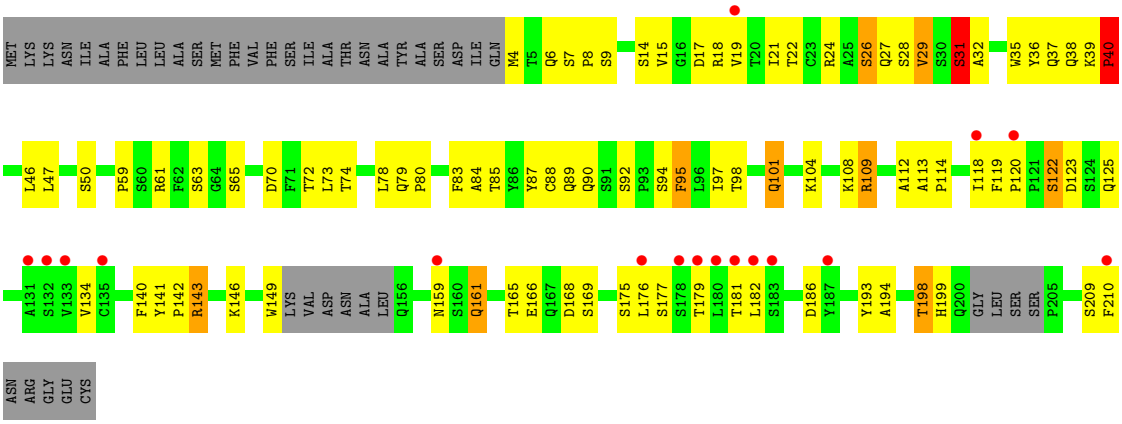
• Molecule 3: Fab-bound IDE, light chain

Chain D:



• Molecule 3: Fab-bound IDE, light chain

Chain F:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	56.95Å 131.66Å 377.04Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.85 – 3.35 49.85 – 3.35	Depositor EDS
% Data completeness (in resolution range)	99.9 (49.85-3.35) 95.1 (49.85-3.35)	Depositor EDS
R_{merge}	0.12	Depositor
R_{sym}	0.12	Depositor
$< I/\sigma(I) >$ [1]	5.65 (at 3.33Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.8.1_1168)	Depositor
R, R_{free}	0.232 , 0.280 0.235 , 0.279	Depositor DCC
R_{free} test set	2012 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å^2)	46.0	Xtriage
Anisotropy	0.255	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.23 , 10.1	EDS
L-test for twinning[2]	$< \|L\| > = 0.44$, $< L^2 > = 0.27$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.82	EDS
Total number of atoms	20939	wwPDB-VP
Average B, all atoms (Å^2)	50.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.84% 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 (i)

5.1 Standard geometry (i)

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

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	0.32	0/7803	0.68	4/10549 (0.0%)
1	B	0.34	0/7206	0.72	6/9733 (0.1%)
2	C	0.34	0/1679	0.88	1/2285 (0.0%)
2	E	0.50	0/1641	0.85	2/2229 (0.1%)
3	D	0.33	0/1557	0.83	3/2106 (0.1%)
3	F	0.40	0/1540	0.90	5/2088 (0.2%)
All	All	0.35	0/21426	0.75	21/28990 (0.1%)

There are no bond length outliers.

All (21) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	280	ASN	CB-CA-C	-15.27	79.86	110.40
1	B	171	SER	C-N-CD	-13.15	91.66	120.60
3	F	29	VAL	CB-CA-C	-11.61	89.35	111.40
2	E	220	ASN	CB-CA-C	-9.30	91.81	110.40
1	A	51	GLY	N-CA-C	-8.68	91.40	113.10
1	B	92	VAL	CB-CA-C	-7.74	96.69	111.40
1	A	97	LEU	CA-CB-CG	6.74	130.80	115.30
1	B	438	ALA	CB-CA-C	-6.40	100.50	110.10
3	F	31	SER	N-CA-C	-6.24	94.17	111.00
1	B	114	LEU	CB-CA-C	-6.11	98.59	110.20
3	D	64	GLY	N-CA-C	-6.09	97.86	113.10
3	D	50	SER	N-CA-C	-5.98	94.84	111.00
3	F	101	GLN	N-CA-C	-5.96	94.90	111.00
1	A	279	GLU	CB-CA-C	-5.92	98.56	110.40
3	F	50	SER	N-CA-C	-5.85	95.21	111.00
2	E	114	TYR	N-CA-C	-5.72	95.56	111.00
2	C	120	GLY	N-CA-C	-5.43	99.52	113.10
3	F	182	LEU	CA-CB-CG	5.39	127.70	115.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	439	GLY	N-CA-C	-5.34	99.75	113.10
1	B	95	GLY	N-CA-C	5.21	126.13	113.10
3	D	92	SER	CB-CA-C	5.15	119.89	110.10

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	7622	0	7588	104	0
1	B	7040	0	7032	158	0
2	C	1637	0	1577	55	0
2	E	1602	0	1548	77	0
3	D	1528	0	1501	54	0
3	F	1508	0	1472	60	0
4	A	1	0	0	0	0
5	B	1	0	0	0	0
All	All	20939	0	20718	488	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 12.

All (488) 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)
2:E:216:HIS:ND1	2:E:218:PRO:HD2	1.68	1.09
3:F:27:GLN:HG3	3:F:28:SER:H	1.17	1.08
1:B:118:THR:HG21	1:B:167:GLN:CB	1.87	1.04
1:B:118:THR:HG21	1:B:167:GLN:HB3	1.03	1.00
1:B:118:THR:CG2	1:B:167:GLN:HB3	1.97	0.94
3:D:115:SER:HB2	3:D:138:ASN:CB	1.99	0.93
1:B:173:LEU:HD13	1:B:174:PHE:C	1.91	0.90
1:B:114:LEU:O	1:B:114:LEU:HG	1.71	0.87
3:D:115:SER:HB2	3:D:138:ASN:HB2	1.56	0.85

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:765:ARG:HH11	1:A:765:ARG:HG2	1.40	0.84
2:C:40:ALA:HB3	2:C:43:LYS:HB2	1.59	0.83
3:D:137:LEU:HD21	3:D:197:VAL:HG11	1.62	0.82
2:E:67:ARG:HG3	2:E:85:SER:HB2	1.60	0.82
1:B:768:GLU:HB3	1:B:843:ILE:HD13	1.62	0.82
1:B:519:ASN:ND2	1:B:521:LYS:H	1.79	0.81
2:E:40:ALA:HB3	2:E:43:LYS:HB2	1.61	0.80
2:E:216:HIS:CE1	2:E:218:PRO:HD2	2.17	0.80
3:F:143:ARG:HH11	3:F:143:ARG:HB3	1.47	0.79
1:B:528:ASN:HD21	1:B:530:PHE:HB2	1.48	0.78
1:A:771:LEU:H	1:A:796:GLN:HE22	1.32	0.77
3:F:27:GLN:HG3	3:F:28:SER:N	1.93	0.76
1:B:423:ARG:HG3	1:B:423:ARG:HH11	1.50	0.76
1:A:573:ASN:ND2	1:A:632:LYS:HB3	2.01	0.75
1:B:573:ASN:ND2	1:B:632:LYS:HB3	2.02	0.75
2:E:99:ASP:N	2:E:99:ASP:OD1	2.19	0.75
1:A:423:ARG:HH11	1:A:423:ARG:CG	1.99	0.75
1:B:519:ASN:HD22	1:B:519:ASN:C	1.90	0.74
1:B:519:ASN:HD22	1:B:520:GLY:N	1.86	0.74
1:A:460:ARG:NH2	2:C:102:MET:O	2.20	0.74
1:B:118:THR:HG23	1:B:171:SER:O	1.88	0.74
1:A:620:LEU:HD13	1:A:629:LEU:HD13	1.71	0.73
3:F:165:THR:HG22	3:F:175:SER:H	1.53	0.73
1:B:92:VAL:HG12	1:B:92:VAL:O	1.88	0.73
1:B:123:LYS:HE2	1:B:126:GLU:HB2	1.71	0.73
2:E:23:ALA:HA	2:E:78:THR:HG23	1.69	0.73
1:B:115:PHE:CD1	1:B:168:PHE:CE2	2.76	0.73
2:E:39:GLN:O	2:E:92:ALA:HB1	1.90	0.72
1:B:118:THR:HG22	1:B:119:LYS:H	1.55	0.72
3:F:4:MET:HG3	3:F:26:SER:OG	1.89	0.71
3:D:13:ALA:HA	3:D:108:LYS:HZ2	1.55	0.71
1:B:572:ALA:HB3	1:B:638:GLN:HE22	1.55	0.71
1:B:388:GLU:OE2	1:B:512:LYS:HE2	1.91	0.71
1:B:893:ARG:NH2	1:B:921:ASP:OD1	2.25	0.70
1:B:255:ALA:HB1	1:B:441:LEU:HD12	1.74	0.70
1:B:809:GLU:OE2	1:B:839:ARG:NH2	2.23	0.70
3:D:89:GLN:HG2	3:D:90:GLN:N	2.07	0.70
2:E:135:PRO:HD3	2:E:216:HIS:HD2	1.57	0.69
2:C:39:GLN:O	2:C:92:ALA:HB1	1.92	0.69
3:F:89:GLN:HG2	3:F:90:GLN:N	2.06	0.69
1:A:229:ARG:NE	1:A:233:GLU:OE2	2.25	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:765:ARG:HG2	1:A:765:ARG:NH1	2.05	0.69
1:B:173:LEU:O	1:B:173:LEU:HD22	1.92	0.69
1:B:48:LYS:HG2	1:B:49:ARG:H	1.57	0.69
3:F:59:PRO:HB3	3:F:61:ARG:NH1	2.08	0.69
1:B:528:ASN:ND2	1:B:530:PHE:H	1.91	0.68
1:B:960:ALA:HB3	1:B:963:MET:HG3	1.75	0.68
1:A:935:ASP:HA	1:A:938:LYS:HE2	1.74	0.68
2:C:23:ALA:HA	2:C:78:THR:HG23	1.74	0.68
3:F:39:LYS:HD3	3:F:84:ALA:HB2	1.75	0.68
2:E:216:HIS:ND1	2:E:218:PRO:CD	2.54	0.68
1:A:465:GLU:HG2	2:C:105:TRP:HZ3	1.58	0.68
1:B:519:ASN:HD22	1:B:521:LYS:H	1.39	0.67
3:F:134:VAL:HG22	3:F:179:THR:HG23	1.77	0.67
3:F:159:ASN:ND2	3:F:181:THR:O	2.26	0.67
1:B:118:THR:HG22	1:B:119:LYS:N	2.09	0.67
2:E:67:ARG:HB3	2:E:68:PHE:HD1	1.60	0.67
3:D:115:SER:HB2	3:D:138:ASN:HB3	1.75	0.66
2:E:216:HIS:HE1	2:E:218:PRO:HG2	1.59	0.66
1:A:253:LEU:HD11	1:A:283:VAL:HG12	1.76	0.66
2:E:135:PRO:HD3	2:E:216:HIS:CD2	2.31	0.66
1:A:58:PRO:HG2	1:A:423:ARG:NH1	2.11	0.66
1:A:281:LYS:HD2	1:A:281:LYS:O	1.96	0.66
3:D:33:VAL:HG12	3:D:51:THR:HG23	1.78	0.65
2:E:22:CYS:HB3	2:E:79:ALA:HB3	1.78	0.65
2:E:154:LEU:HD21	2:E:210:TYR:HD2	1.60	0.65
1:B:387:VAL:HG21	1:B:480:ILE:HD13	1.78	0.65
2:C:14:PRO:HD2	2:C:129:SER:HB3	1.79	0.65
2:C:172:SER:H	2:C:213:ASN:HD21	1.44	0.65
2:E:55:TYR:HE2	2:E:105:TRP:HA	1.61	0.64
1:A:387:VAL:HG21	1:A:480:ILE:HD13	1.78	0.64
3:D:165:THR:HG22	3:D:175:SER:H	1.63	0.64
1:B:170:LEU:HD22	1:B:277:GLU:HG3	1.80	0.64
1:B:118:THR:CG2	1:B:171:SER:O	2.46	0.63
3:D:143:ARG:NH1	3:D:164:VAL:HG21	2.13	0.63
1:A:573:ASN:HD22	1:A:632:LYS:HB3	1.63	0.63
1:B:173:LEU:HD22	1:B:173:LEU:C	2.18	0.63
2:C:67:ARG:O	2:C:68:PHE:CD1	2.50	0.63
3:F:29:VAL:HG12	3:F:29:VAL:O	1.98	0.63
1:A:423:ARG:HH11	1:A:423:ARG:HG3	1.63	0.63
1:A:441:LEU:HD23	1:A:449:VAL:HG11	1.81	0.63
1:B:114:LEU:O	1:B:114:LEU:CG	2.47	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:6:GLU:OE2	2:C:120:GLY:HA3	1.98	0.63
3:D:116:VAL:HG22	3:D:137:LEU:HD22	1.82	0.62
2:C:67:ARG:C	2:C:68:PHE:HD1	2.01	0.62
1:B:864:GLU:HG3	1:B:986:LEU:HD21	1.81	0.62
2:C:55:TYR:CE2	2:C:105:TRP:HA	2.35	0.62
2:C:12:VAL:HG11	2:C:18:LEU:HG	1.82	0.61
1:A:817:GLU:HG3	1:A:818:PRO:HD3	1.81	0.61
1:B:423:ARG:HH11	1:B:423:ARG:CG	2.13	0.61
1:B:311:ARG:HB3	1:B:379:LEU:HB2	1.82	0.61
1:A:99:ASP:O	1:A:217:LYS:NZ	2.32	0.61
2:E:209:THR:O	2:E:209:THR:HG23	2.00	0.60
1:B:47:ILE:HD11	1:B:272:VAL:HG22	1.83	0.60
1:A:388:GLU:OE2	1:A:509:VAL:HG22	2.02	0.60
1:A:559:LEU:HD22	1:A:742:MET:HB2	1.84	0.60
2:C:55:TYR:HE2	2:C:105:TRP:HA	1.66	0.60
3:F:142:PRO:HD2	3:F:199:HIS:NE2	2.17	0.59
1:A:910:GLU:OE1	1:A:920:ARG:NH1	2.35	0.59
1:B:119:LYS:O	1:B:119:LYS:HG2	2.02	0.59
1:B:832:ILE:HB	1:B:851:GLN:HB3	1.84	0.59
1:B:635:ASN:HA	1:B:638:GLN:HB2	1.84	0.59
2:E:180:HIS:HB2	2:E:197:VAL:HG12	1.83	0.59
1:B:657:LYS:HE3	1:B:661:ILE:HD11	1.84	0.59
1:A:202:PHE:CZ	1:A:206:LYS:HE3	2.38	0.59
1:B:115:PHE:CD1	1:B:168:PHE:HE2	2.17	0.59
3:D:6:GLN:HB3	3:D:101:GLN:HE22	1.68	0.59
1:B:635:ASN:ND2	1:B:732:ASN:O	2.36	0.59
1:B:528:ASN:C	1:B:528:ASN:HD22	2.04	0.59
1:A:304:ILE:HB	1:A:481:VAL:HG22	1.84	0.58
2:E:216:HIS:CE1	2:E:218:PRO:CD	2.86	0.58
2:C:170:TRP:CZ3	2:C:212:CYS:HB3	2.38	0.58
1:B:251:SER:OG	1:B:280:ASN:HB2	2.03	0.58
2:C:135:PRO:HD2	2:C:221:THR:HG21	1.86	0.58
3:F:143:ARG:HB3	3:F:143:ARG:NH1	2.17	0.58
1:B:76:LEU:HB3	1:B:257:VAL:HG23	1.86	0.58
2:C:142:PRO:HD2	2:C:229:PRO:HA	1.85	0.58
3:F:146:LYS:HB3	3:F:198:THR:HG23	1.85	0.58
1:A:357:ASN:HB2	1:A:378:ASP:OD2	2.04	0.58
1:A:782:ARG:NH1	1:A:963:MET:O	2.36	0.57
2:E:38:ARG:NE	2:E:46:GLU:OE1	2.33	0.57
3:F:140:PHE:HE1	3:F:143:ARG:HA	1.69	0.57
1:B:894:LEU:HG	1:B:925:VAL:HG21	1.86	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:F:79:GLN:HB3	3:F:80:PRO:HD2	1.86	0.57
1:B:573:ASN:HD22	1:B:632:LYS:HB3	1.67	0.57
3:F:18:ARG:NH2	3:F:74:THR:HG21	2.19	0.57
3:F:38:GLN:O	3:F:84:ALA:HB1	2.05	0.56
1:B:528:ASN:HD22	1:B:530:PHE:H	1.53	0.56
3:D:50:SER:HG	3:D:53:SER:HG	1.53	0.56
3:F:6:GLN:NE2	3:F:88:CYS:SG	2.78	0.56
1:B:99:ASP:OD1	1:B:99:ASP:N	2.38	0.56
1:B:326:TYR:CE2	1:B:443:TYR:HB3	2.40	0.56
2:E:55:TYR:CE2	2:E:105:TRP:HA	2.39	0.56
1:B:765:ARG:HG3	1:B:765:ARG:HH11	1.69	0.56
1:B:771:LEU:H	1:B:796:GLN:HE22	1.54	0.56
2:E:91:THR:HG1	2:E:127:VAL:H	1.52	0.56
3:F:35:TRP:CH2	3:F:88:CYS:HB3	2.41	0.55
1:A:541:GLU:OE2	1:A:542:LYS:HE3	2.06	0.55
3:D:165:THR:CG2	3:D:175:SER:H	2.19	0.55
1:A:312:ASN:HD22	1:A:378:ASP:HA	1.71	0.55
1:A:321:ASP:O	1:A:324:LYS:NZ	2.39	0.55
1:B:153:VAL:HG22	1:B:154:SER:H	1.72	0.55
1:B:251:SER:HB3	1:B:278:VAL:HG12	1.87	0.55
3:D:38:GLN:O	3:D:84:ALA:HB1	2.07	0.55
1:A:75:VAL:HG11	1:A:271:VAL:HG11	1.89	0.55
1:B:348:SER:HB2	1:B:606:GLU:OE2	2.06	0.55
1:B:365:GLU:HG2	1:B:371:MET:HG2	1.89	0.55
2:E:2:VAL:HG22	2:E:27:PHE:HD1	1.72	0.55
2:C:83:MET:HB3	2:C:86:LEU:HD21	1.89	0.55
3:D:194:ALA:HA	3:D:209:SER:HA	1.88	0.55
1:B:888:ALA:O	1:B:891:ILE:HG13	2.07	0.54
3:D:143:ARG:O	3:D:143:ARG:NE	2.38	0.54
2:E:11:LEU:HD12	2:E:163:PRO:HD3	1.89	0.54
1:B:538:LEU:HD22	1:B:734:THR:HG23	1.90	0.54
1:B:88:ALA:HB3	1:B:151:PHE:CZ	2.42	0.54
1:B:765:ARG:HH11	1:B:765:ARG:CG	2.21	0.54
1:A:517:ASP:OD1	1:A:517:ASP:N	2.25	0.54
3:D:50:SER:OG	3:D:53:SER:OG	2.24	0.54
2:E:135:PRO:HD2	2:E:221:THR:OG1	2.05	0.54
2:E:138:PHE:CG	3:F:125:GLN:HG3	2.42	0.54
1:B:47:ILE:HG22	1:B:48:LYS:O	2.07	0.54
2:E:216:HIS:CE1	2:E:218:PRO:HG2	2.40	0.54
3:F:109:ARG:HH11	3:F:109:ARG:HB2	1.71	0.54
3:F:40:PRO:HG2	3:F:166:GLU:HG2	1.89	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:59:SER:HB2	3:F:95:PHE:HB3	1.89	0.54
1:A:635:ASN:ND2	1:A:732:ASN:O	2.41	0.54
2:C:67:ARG:C	2:C:68:PHE:CD1	2.81	0.54
3:D:6:GLN:HB3	3:D:101:GLN:NE2	2.23	0.54
2:C:197:VAL:HG11	3:D:136:LEU:HD13	1.89	0.53
2:E:4:LEU:HD21	2:E:27:PHE:HZ	1.72	0.53
2:C:4:LEU:HD21	2:C:27:PHE:CZ	2.44	0.53
2:C:32:TYR:CZ	2:C:102:MET:HG2	2.43	0.53
1:A:561:PHE:HE1	1:A:733:ILE:HD12	1.74	0.53
2:C:4:LEU:HD21	2:C:27:PHE:HZ	1.74	0.53
1:B:436:LYS:HE3	1:B:453:GLU:OE2	2.09	0.53
1:B:322:LEU:HA	1:B:325:TYR:CD2	2.44	0.52
2:C:11:LEU:HD11	2:C:162:PHE:HE1	1.74	0.52
1:A:896:LYS:HD2	1:A:897:PRO:HD2	1.91	0.52
1:A:519:ASN:OD1	1:A:521:LYS:HG2	2.09	0.52
1:B:434:THR:O	1:B:437:ILE:O	2.28	0.52
1:B:173:LEU:O	1:B:174:PHE:HD1	1.92	0.52
1:B:938:LYS:O	1:B:942:GLU:HG2	2.10	0.52
3:D:37:GLN:HB2	3:D:47:LEU:HD11	1.91	0.52
2:E:186:LEU:HG	2:E:192:TYR:CE1	2.45	0.52
1:B:139:ASN:HB3	1:B:150:TYR:CZ	2.45	0.51
1:A:706:ASP:OD1	1:B:756:LYS:NZ	2.38	0.51
1:A:963:MET:SD	1:A:964:ASP:N	2.84	0.51
2:C:64:VAL:HG12	2:C:67:ARG:NH2	2.25	0.51
1:B:561:PHE:HE1	1:B:733:ILE:HD12	1.76	0.51
1:B:799:MET:HE3	1:B:1008:VAL:HG22	1.92	0.51
2:C:157:LEU:HD13	2:C:195:SER:HB3	1.92	0.51
1:A:316:THR:HB	1:A:374:ILE:HG22	1.92	0.51
1:B:346:LEU:HD21	1:B:394:MET:HG2	1.91	0.51
2:E:211:ILE:HG22	2:E:226:LYS:HA	1.92	0.51
1:A:557:SER:OG	1:A:746:GLU:OE2	2.20	0.51
1:B:423:ARG:CG	1:B:423:ARG:NH1	2.73	0.51
1:B:607:TYR:CZ	1:B:644:LYS:HD2	2.46	0.51
3:D:212:ARG:HB3	3:D:212:ARG:CZ	2.40	0.51
2:E:100:ARG:HB3	2:E:117:ASP:HB3	1.92	0.51
2:C:59:SER:HB2	3:D:95:PHE:HB3	1.92	0.51
3:F:161:GLN:HG3	3:F:179:THR:HB	1.91	0.51
1:A:465:GLU:HG2	2:C:105:TRP:CZ3	2.43	0.50
3:D:51:THR:HG21	3:D:71:PHE:HD2	1.76	0.50
1:A:162:LEU:HD23	1:A:270:LEU:HG	1.92	0.50
1:A:311:ARG:HB3	1:A:379:LEU:HB2	1.92	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:11:LEU:HD13	3:D:19:VAL:HG13	1.92	0.50
3:D:35:TRP:CH2	3:D:88:CYS:HB3	2.47	0.50
1:A:52:ASN:O	1:A:54:ILE:HG12	2.11	0.50
1:A:643:LYS:HE2	1:A:744:MET:SD	2.52	0.50
1:B:311:ARG:HD3	1:B:384:LEU:HB2	1.94	0.50
2:E:154:LEU:HD21	2:E:210:TYR:CD2	2.45	0.50
1:B:311:ARG:NH2	1:B:381:GLU:OE1	2.45	0.50
1:A:446:LEU:O	1:A:449:VAL:HG22	2.12	0.49
2:C:158:VAL:HB	2:C:194:LEU:HD23	1.94	0.49
1:B:173:LEU:O	1:B:174:PHE:HB2	2.12	0.49
1:A:123:LYS:HB2	1:A:126:GLU:HB2	1.95	0.49
1:B:896:LYS:O	1:B:898:LYS:NZ	2.41	0.49
1:B:143:SER:OG	1:B:146:HIS:HB2	2.12	0.49
2:C:162:PHE:HB2	2:C:191:LEU:HD22	1.93	0.49
2:E:113:PRO:HG2	3:F:32:ALA:O	2.12	0.49
2:C:132:THR:HG23	2:C:162:PHE:O	2.12	0.49
1:B:395:PHE:CD2	1:B:513:TRP:HB3	2.48	0.49
1:B:643:LYS:HE3	1:B:647:GLU:CD	2.33	0.49
3:D:116:VAL:HG21	3:D:197:VAL:HG21	1.93	0.49
3:F:35:TRP:CD2	3:F:73:LEU:HB2	2.47	0.49
1:B:519:ASN:ND2	1:B:519:ASN:C	2.64	0.49
3:D:115:SER:O	3:D:138:ASN:HB2	2.12	0.49
2:E:104:TYR:CD1	2:E:104:TYR:C	2.85	0.49
1:B:86:SER:HB3	1:B:158:LEU:HG	1.94	0.49
3:D:150:LYS:HB2	3:D:194:ALA:HB3	1.95	0.49
2:E:54:TYR:HD2	2:E:103:TYR:CD1	2.30	0.49
1:B:48:LYS:HG2	1:B:49:ARG:N	2.25	0.48
1:B:90:LEU:HD12	1:B:256:VAL:HG22	1.94	0.48
1:B:315:VAL:HG21	1:B:394:MET:HE1	1.94	0.48
3:F:122:SER:OG	3:F:125:GLN:HB2	2.13	0.48
1:A:799:MET:HE3	1:A:1008:VAL:HG22	1.95	0.48
1:B:601:LYS:HD3	1:B:620:LEU:O	2.13	0.48
2:E:45:LEU:HD12	3:F:87:TYR:CD2	2.48	0.48
1:A:177:SER:OG	1:A:181:ARG:NH1	2.45	0.48
1:A:344:GLY:HA3	1:A:523:LYS:HG2	1.94	0.48
1:B:588:LEU:HD22	1:B:711:ARG:HH11	1.78	0.48
1:A:81:PRO:HA	1:A:261:ARG:HD3	1.95	0.48
3:D:7:SER:HA	3:D:8:PRO:HA	1.58	0.48
1:A:423:ARG:HH11	1:A:423:ARG:HG2	1.77	0.48
2:E:170:TRP:CZ3	2:E:212:CYS:HB3	2.49	0.48
2:C:32:TYR:CZ	2:C:98:ARG:NH2	2.82	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:10:SER:HB2	3:D:104:LYS:O	2.14	0.48
3:D:115:SER:CB	3:D:138:ASN:HB2	2.36	0.48
1:B:893:ARG:HA	1:B:893:ARG:HH11	1.79	0.47
3:F:108:LYS:HA	3:F:141:TYR:OH	2.14	0.47
1:A:311:ARG:NH2	1:A:664:GLU:OE2	2.39	0.47
1:B:599:LEU:HD21	1:B:659:PHE:HA	1.96	0.47
2:E:216:HIS:CE1	2:E:218:PRO:CG	2.97	0.47
1:B:927:TYR:O	1:B:930:THR:HB	2.13	0.47
3:D:147:VAL:HA	3:D:196:GLU:O	2.14	0.47
2:E:73:ASP:OD2	2:E:76:LYS:HG3	2.14	0.47
1:B:437:ILE:O	1:B:438:ALA:HB3	2.15	0.47
2:C:54:TYR:HD2	2:C:103:TYR:HD1	1.63	0.47
2:E:135:PRO:HA	2:E:160:ASP:O	2.14	0.47
3:F:22:THR:HG22	3:F:72:THR:OG1	2.14	0.47
2:E:22:CYS:HB2	2:E:36:TRP:CZ2	2.49	0.47
3:D:80:PRO:HA	3:D:83:PHE:HE2	1.80	0.47
1:A:815:ILE:HG22	1:A:870:MET:HG3	1.97	0.46
1:B:438:ALA:HA	1:B:441:LEU:HG	1.96	0.46
1:B:777:PHE:HD1	1:B:990:GLU:HB3	1.79	0.46
1:A:879:GLU:OE2	1:A:883:GLN:HG2	2.15	0.46
2:E:139:PRO:HB2	2:E:227:VAL:HG22	1.97	0.46
2:E:200:VAL:HG11	2:E:210:TYR:CE2	2.49	0.46
1:B:93:HIS:O	1:B:94:ILE:HG12	2.16	0.46
1:B:336:HIS:CD2	1:B:414:LEU:HD11	2.50	0.46
1:B:444:TYR:CD2	1:B:452:ALA:HB1	2.51	0.46
1:B:638:GLN:N	1:B:639:PRO:HD2	2.30	0.46
2:C:137:VAL:HG22	2:C:214:VAL:HG21	1.98	0.46
1:B:59:GLU:CD	1:B:59:GLU:O	2.53	0.46
1:B:528:ASN:ND2	1:B:528:ASN:C	2.69	0.46
3:F:118:ILE:HG13	3:F:119:PHE:N	2.31	0.46
1:B:304:ILE:HB	1:B:481:VAL:HG22	1.98	0.46
2:E:12:VAL:HG11	2:E:18:LEU:HG	1.98	0.46
1:B:671:ASN:HA	1:B:701:LYS:HZ1	1.81	0.46
1:B:684:TYR:CZ	1:B:688:LEU:HD11	2.51	0.46
3:D:36:TYR:CE2	3:D:46:LEU:HD13	2.51	0.46
3:D:199:HIS:HB3	3:D:202:LEU:HD22	1.97	0.46
2:E:4:LEU:HD13	2:E:22:CYS:SG	2.55	0.46
1:B:54:ILE:HG22	1:B:450:LEU:HD22	1.98	0.46
2:C:38:ARG:NE	2:C:46:GLU:OE1	2.41	0.46
1:A:460:ARG:NH2	2:C:101:VAL:HB	2.30	0.46
1:A:541:GLU:HG2	1:A:563:GLN:OE1	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:85:LYS:HG3	1:A:430:PRO:HG2	1.97	0.45
3:F:29:VAL:C	3:F:31:SER:H	2.19	0.45
3:F:149:TRP:HA	3:F:194:ALA:O	2.16	0.45
1:A:170:LEU:HD21	1:A:277:GLU:HG2	1.97	0.45
1:A:251:SER:HB3	1:A:278:VAL:HG12	1.98	0.45
1:A:299:LYS:HD2	1:A:510:ILE:HD13	1.98	0.45
1:A:346:LEU:HD21	1:A:394:MET:HG2	1.97	0.45
1:B:115:PHE:CD1	1:B:168:PHE:CD2	3.04	0.45
1:B:709:LEU:HB3	1:B:710:PRO:CD	2.47	0.45
1:A:253:LEU:HD11	1:A:283:VAL:CG1	2.44	0.45
2:C:178:GLY:O	2:C:198:VAL:HA	2.16	0.45
3:F:65:SER:OG	3:F:72:THR:HB	2.16	0.45
2:C:4:LEU:HD13	2:C:22:CYS:SG	2.57	0.45
3:F:176:LEU:HD12	3:F:177:SER:H	1.81	0.45
1:A:319:ILE:HB	1:A:320:PRO:HD2	1.98	0.45
1:A:680:GLN:HA	1:A:683:MET:HE3	1.99	0.45
2:E:121:GLN:H	2:E:121:GLN:CD	2.19	0.45
1:B:856:PRO:HG2	1:B:959:LEU:HD23	1.98	0.45
2:E:47:TRP:CD2	3:F:97:ILE:HB	2.51	0.45
1:A:771:LEU:HB2	1:A:796:GLN:NE2	2.31	0.45
1:B:586:ASP:HA	1:B:695:TRP:CZ2	2.52	0.45
1:A:116:LEU:HD13	1:A:178:ALA:HB1	1.99	0.45
1:B:325:TYR:HE1	2:E:103:TYR:CB	2.30	0.45
1:B:648:LYS:HA	1:B:648:LYS:HD3	1.72	0.45
2:E:214:VAL:HB	2:E:223:VAL:HG13	1.99	0.45
2:E:23:ALA:CA	2:E:78:THR:HG23	2.44	0.45
1:A:769:VAL:HA	1:A:1004:LEU:HD23	1.98	0.45
1:A:927:TYR:O	1:A:930:THR:HB	2.16	0.45
1:B:896:LYS:HB2	1:B:896:LYS:HE2	1.50	0.45
1:A:466:MET:HB2	2:C:105:TRP:CD2	2.53	0.44
2:E:155:GLY:HA2	2:E:170:TRP:CH2	2.52	0.44
2:E:200:VAL:HG21	2:E:210:TYR:HE2	1.83	0.44
1:B:93:HIS:CE1	1:B:442:HIS:HB3	2.52	0.44
2:C:54:TYR:HD1	2:C:54:TYR:O	2.00	0.44
3:D:59:PRO:HG2	3:D:62:PHE:CE2	2.52	0.44
3:F:37:GLN:HB2	3:F:47:LEU:HD11	1.98	0.44
2:C:140:LEU:HB3	3:D:119:PHE:CD1	2.52	0.44
1:B:425:LYS:HD2	1:B:428:GLU:OE2	2.16	0.44
1:B:854:LYS:HE3	1:B:858:TYR:CE2	2.52	0.44
3:D:35:TRP:CZ3	3:D:88:CYS:HB3	2.53	0.44
2:C:159:LYS:NZ	2:C:159:LYS:HB3	2.32	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:217:LYS:N	2:E:218:PRO:CD	2.81	0.44
3:F:35:TRP:CZ3	3:F:88:CYS:HB3	2.53	0.44
3:F:119:PHE:HA	3:F:120:PRO:HD3	1.82	0.44
3:D:35:TRP:HB2	3:D:48:ILE:HB	1.98	0.44
3:F:14:SER:O	3:F:17:ASP:HB2	2.18	0.44
3:F:36:TYR:CE2	3:F:46:LEU:HD13	2.52	0.44
1:A:206:LYS:O	1:A:216:SER:HA	2.17	0.44
1:B:411:PHE:CE2	1:B:459:PHE:HB2	2.53	0.44
2:E:6:GLU:N	2:E:6:GLU:OE1	2.51	0.44
2:E:31:SER:O	2:E:102:MET:O	2.36	0.44
1:B:100:PRO:HA	1:B:101:PRO:HD3	1.68	0.44
1:B:448:GLU:O	1:B:452:ALA:N	2.50	0.44
1:B:777:PHE:CD2	1:B:998:PHE:HE1	2.34	0.44
1:A:62:ARG:HG2	1:A:80:ASP:HB2	2.00	0.43
1:B:140:ALA:HB2	1:B:149:TYR:HA	2.00	0.43
1:B:872:LYS:HD2	1:B:876:ASP:OD2	2.18	0.43
1:A:684:TYR:CZ	1:A:688:LEU:HD11	2.53	0.43
1:A:771:LEU:H	1:A:796:GLN:NE2	2.09	0.43
1:B:559:LEU:HD22	1:B:742:MET:HB2	2.00	0.43
3:D:59:PRO:HG2	3:D:62:PHE:HE2	1.84	0.43
2:E:182:PHE:CZ	3:F:177:SER:HB2	2.53	0.43
1:B:131:LEU:O	1:B:136:GLY:N	2.43	0.43
2:C:167:THR:OG1	2:C:215:ASN:HB3	2.19	0.43
3:D:107:ILE:O	3:D:107:ILE:HG13	2.19	0.43
1:B:630:SER:OG	1:B:632:LYS:HE3	2.19	0.43
2:E:47:TRP:CE2	3:F:97:ILE:HB	2.53	0.43
1:B:446:LEU:O	1:B:449:VAL:HG12	2.19	0.43
3:F:113:ALA:HA	3:F:114:PRO:HD3	1.82	0.43
3:F:168:ASP:OD1	3:F:169:SER:N	2.52	0.43
1:A:90:LEU:HD13	1:A:169:PHE:CE2	2.54	0.43
1:A:181:ARG:O	1:A:184:ASN:HB3	2.18	0.43
1:B:308:LYS:HG2	1:B:675:ALA:HB3	2.01	0.43
1:B:466:MET:HB2	2:E:105:TRP:CD2	2.52	0.43
1:B:806:MET:O	1:B:810:LEU:HB2	2.19	0.43
2:E:31:SER:HB2	2:E:103:TYR:CE1	2.54	0.43
2:E:54:TYR:HD1	2:E:54:TYR:O	2.01	0.43
1:B:86:SER:OG	1:B:155:HIS:HA	2.18	0.43
1:B:115:PHE:CE1	1:B:168:PHE:CE2	3.07	0.43
2:C:141:ALA:HA	2:C:142:PRO:HD3	1.82	0.43
2:C:164:GLU:HA	2:C:165:PRO:HA	1.73	0.43
2:C:215:ASN:OD1	2:C:222:LYS:HG2	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:313:LEU:HD22	1:A:387:VAL:HG13	2.01	0.43
1:B:130:PHE:HE1	1:B:161:ALA:HB2	1.83	0.43
1:B:252:ASN:HB3	1:B:280:ASN:ND2	2.34	0.43
3:F:7:SER:HA	3:F:8:PRO:HA	1.56	0.43
1:A:48:LYS:HB2	1:A:48:LYS:HE3	1.75	0.42
1:B:173:LEU:O	1:B:174:PHE:CD1	2.70	0.42
3:D:155:LEU:HB3	3:D:157:SER:HB2	2.00	0.42
3:F:35:TRP:HA	3:F:87:TYR:O	2.19	0.42
1:A:709:LEU:HB3	1:A:710:PRO:CD	2.48	0.42
1:B:92:VAL:O	1:B:92:VAL:CG1	2.59	0.42
3:D:59:PRO:HB3	3:D:61:ARG:NH1	2.34	0.42
1:A:690:MET:O	1:A:768:GLU:HG3	2.19	0.42
1:B:307:ILE:HD11	1:B:785:VAL:HG13	2.00	0.42
2:E:55:TYR:CE2	2:E:105:TRP:HD1	2.37	0.42
3:F:19:VAL:HG21	3:F:78:LEU:HD22	2.01	0.42
3:F:193:TYR:HB2	3:F:210:PHE:CZ	2.53	0.42
1:A:903:GLU:OE1	1:A:907:TYR:OH	2.29	0.42
1:B:130:PHE:CE1	1:B:161:ALA:HB2	2.55	0.42
2:E:33:SER:HB2	2:E:99:ASP:OD2	2.19	0.42
2:E:164:GLU:HG3	2:E:192:TYR:CE2	2.55	0.42
1:A:946:VAL:HA	1:A:951:ARG:CZ	2.50	0.42
1:A:46:ALA:O	1:A:70:ALA:N	2.47	0.42
3:D:212:ARG:HB3	3:D:212:ARG:NH1	2.35	0.42
2:E:98:ARG:HD2	2:E:99:ASP:O	2.19	0.42
1:A:102:ASN:O	1:A:102:ASN:ND2	2.45	0.42
1:A:247:ALA:O	1:A:283:VAL:HG21	2.20	0.42
1:B:642:LEU:O	1:B:646:ILE:HG12	2.19	0.42
1:B:528:ASN:O	1:B:531:ILE:HG12	2.19	0.42
2:C:36:TRP:CE2	2:C:81:LEU:HB2	2.55	0.42
3:D:47:LEU:HD11	3:D:86:TYR:HE1	1.85	0.42
3:D:141:TYR:CD1	3:D:142:PRO:HA	2.55	0.42
1:A:270:LEU:HD12	1:A:270:LEU:HA	1.83	0.42
2:C:2:VAL:HG22	2:C:27:PHE:HD1	1.84	0.42
2:E:139:PRO:CB	2:E:227:VAL:HG22	2.49	0.42
3:D:162:GLU:HG2	3:D:178:SER:HA	2.02	0.42
2:E:162:PHE:HB2	2:E:191:LEU:HD22	2.02	0.42
3:F:21:ILE:O	3:F:72:THR:HG23	2.19	0.42
1:A:56:LYS:NZ	1:A:62:ARG:O	2.47	0.41
1:A:80:ASP:O	1:A:83:THR:HG22	2.20	0.41
1:B:580:SER:HA	1:B:581:PRO:HD2	1.85	0.41
2:E:36:TRP:HD1	2:E:70:ILE:HD11	1.85	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:131:LEU:HD23	1:A:131:LEU:HA	1.91	0.41
1:A:540:LEU:HD12	1:A:540:LEU:HA	1.87	0.41
2:C:100:ARG:HG3	2:C:117:ASP:HB3	2.02	0.41
2:E:12:VAL:HG23	2:E:127:VAL:HG22	2.01	0.41
2:E:166:VAL:HG12	2:E:216:HIS:HA	2.02	0.41
1:A:871:GLU:HB2	1:A:940:TYR:CE2	2.56	0.41
2:C:33:SER:HB2	2:C:99:ASP:OD2	2.20	0.41
2:E:67:ARG:HB3	2:E:68:PHE:CD1	2.48	0.41
2:E:97:ALA:HB2	2:E:119:TRP:CG	2.56	0.41
2:E:164:GLU:HA	2:E:165:PRO:HA	1.90	0.41
3:F:29:VAL:C	3:F:31:SER:N	2.72	0.41
3:D:69:THR:HB	3:D:70:ASP:H	1.57	0.41
1:A:63:GLU:HB3	1:A:264:LEU:HD11	2.02	0.41
1:A:88:ALA:HB3	1:A:151:PHE:CE2	2.56	0.41
1:A:468:LEU:HD12	1:A:468:LEU:HA	1.89	0.41
1:A:765:ARG:HH11	1:A:765:ARG:CG	2.20	0.41
1:B:80:ASP:O	1:B:83:THR:HG22	2.21	0.41
1:B:437:ILE:O	1:B:438:ALA:CB	2.69	0.41
3:F:85:THR:HG23	3:F:104:LYS:HD2	2.01	0.41
1:B:940:TYR:CE2	1:B:945:ALA:HB2	2.55	0.41
3:F:24:ARG:HD2	3:F:70:ASP:OD1	2.21	0.41
3:F:112:ALA:HB3	3:F:140:PHE:HA	2.03	0.41
3:F:159:ASN:ND2	3:F:181:THR:OG1	2.53	0.41
3:F:194:ALA:CB	3:F:209:SER:HB3	2.50	0.41
1:A:172:PRO:HG2	1:A:174:PHE:CE2	2.55	0.41
1:A:925:VAL:O	1:A:929:LYS:HG3	2.21	0.41
1:B:89:ALA:HA	1:B:149:TYR:O	2.20	0.41
1:B:153:VAL:HG22	1:B:154:SER:N	2.35	0.41
1:B:397:TYR:O	1:B:400:LYS:HB3	2.21	0.41
1:B:540:LEU:HA	1:B:540:LEU:HD12	1.86	0.41
3:D:35:TRP:CE2	3:D:73:LEU:HB2	2.55	0.41
3:D:138:ASN:HB3	3:D:139:ASN:H	1.73	0.41
1:A:799:MET:HE3	1:A:799:MET:HB3	1.74	0.41
1:A:933:LYS:O	1:A:937:ILE:HG13	2.21	0.41
1:B:357:ASN:HB2	1:B:378:ASP:OD2	2.21	0.41
1:B:765:ARG:CG	1:B:765:ARG:NH1	2.80	0.41
1:B:791:ILE:HG22	1:B:850:ILE:HB	2.02	0.41
1:B:906:LYS:HB3	1:B:906:LYS:HE3	1.83	0.41
2:C:3:GLN:HG3	2:C:25:SER:OG	2.20	0.41
3:D:29:VAL:HB	3:D:30:SER:H	1.72	0.41
2:E:133:LYS:HG3	2:E:134:GLY:N	2.36	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:F:83:PHE:O	3:F:83:PHE:CG	2.73	0.41
1:A:474:GLU:H	1:A:474:GLU:HG2	1.62	0.41
1:A:616:LEU:HA	1:A:616:LEU:HD12	1.77	0.41
2:C:51:ILE:HB	2:C:70:ILE:HD13	2.02	0.41
2:C:170:TRP:CE3	2:C:212:CYS:HB3	2.55	0.41
2:E:28:ASN:C	2:E:30:SER:H	2.24	0.41
2:C:23:ALA:CA	2:C:78:THR:HG23	2.47	0.40
2:E:138:PHE:HB3	3:F:122:SER:OG	2.21	0.40
2:E:178:GLY:O	2:E:198:VAL:HA	2.20	0.40
1:A:103:ILE:HD11	1:A:240:GLU:HG3	2.03	0.40
1:A:934:GLU:H	1:A:934:GLU:HG2	1.38	0.40
1:B:93:HIS:C	1:B:94:ILE:HG12	2.40	0.40
1:B:163:ASP:HA	1:B:274:LEU:HD13	2.03	0.40
1:B:319:ILE:HB	1:B:320:PRO:HD2	2.02	0.40
2:E:181:THR:HG22	2:E:196:SER:OG	2.21	0.40
1:A:832:ILE:HB	1:A:851:GLN:HB3	2.03	0.40
1:B:436:LYS:HE3	1:B:453:GLU:CD	2.42	0.40
1:B:819:ALA:O	1:B:823:LEU:HB2	2.22	0.40
1:B:868:ILE:HG13	1:B:869:THR:N	2.37	0.40
1:B:872:LYS:HG3	1:B:873:SER:N	2.36	0.40
3:D:142:PRO:HB2	3:D:144:GLU:HG2	2.03	0.40
3:F:109:ARG:HG2	3:F:141:TYR:CD1	2.56	0.40
1:A:1007:LEU:HD23	1:B:1000:ARG:HG2	2.03	0.40
1:B:709:LEU:HD12	1:B:709:LEU:HA	1.88	0.40
2:C:211:ILE:HD13	2:C:226:LYS:HB3	2.03	0.40
2:C:135:PRO:HA	2:C:160:ASP:O	2.21	0.40
3:D:83:PHE:CD1	3:D:107:ILE:HG22	2.57	0.40
3:D:113:ALA:HA	3:D:114:PRO:HD3	1.84	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	922/990 (93%)	886 (96%)	35 (4%)	1 (0%)	51	82
1	B	845/990 (85%)	804 (95%)	38 (4%)	3 (0%)	34	68
2	C	206/263 (78%)	188 (91%)	15 (7%)	3 (2%)	10	39
2	E	199/263 (76%)	178 (89%)	19 (10%)	2 (1%)	15	49
3	D	187/239 (78%)	165 (88%)	21 (11%)	1 (0%)	29	63
3	F	191/239 (80%)	162 (85%)	28 (15%)	1 (0%)	29	63
All	All	2550/2984 (86%)	2383 (94%)	156 (6%)	11 (0%)	34	68

All (11) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	D	138	ASN
1	A	282	ASN
1	B	95	GLY
1	B	172	PRO
1	B	1010	PRO
2	C	122	GLY
3	F	40	PRO
2	C	165	PRO
2	E	165	PRO
2	E	171	ASN
2	C	85	SER

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	832/879 (95%)	785 (94%)	47 (6%)	21	53
1	B	768/879 (87%)	719 (94%)	49 (6%)	17	48
2	C	181/220 (82%)	169 (93%)	12 (7%)	16	47
2	E	176/220 (80%)	157 (89%)	19 (11%)	6	25
3	D	178/210 (85%)	155 (87%)	23 (13%)	4	17
3	F	176/210 (84%)	158 (90%)	18 (10%)	7	28

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
All	All	2311/2618 (88%)	2143 (93%)	168 (7%)	14 43

All (168) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	76	LEU
1	A	97	LEU
1	A	102	ASN
1	A	192	LYS
1	A	201	LEU
1	A	226	LEU
1	A	283	VAL
1	A	316	THR
1	A	324	LYS
1	A	347	LEU
1	A	356	VAL
1	A	412	GLN
1	A	417	LEU
1	A	418	ASN
1	A	423	ARG
1	A	446	LEU
1	A	450	LEU
1	A	486	GLU
1	A	499	GLN
1	A	517	ASP
1	A	542	LYS
1	A	543	GLU
1	A	595	LEU
1	A	597	LEU
1	A	603	SER
1	A	632	LYS
1	A	642	LEU
1	A	648	LYS
1	A	660	GLU
1	A	712	LEU
1	A	728	LEU
1	A	765	ARG
1	A	771	LEU
1	A	810	LEU
1	A	823	LEU
1	A	846	LEU
1	A	859	LEU

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Mol	Chain	Res	Type
1	A	867	LEU
1	A	871	GLU
1	A	889	LEU
1	A	928	LEU
1	A	930	THR
1	A	931	LEU
1	A	934	GLU
1	A	954	VAL
1	A	979	ASN
1	A	1007	LEU
1	B	111	GLU
1	B	158	LEU
1	B	173	LEU
1	B	270	LEU
1	B	316	THR
1	B	347	LEU
1	B	348	SER
1	B	356	VAL
1	B	412	GLN
1	B	414	LEU
1	B	423	ARG
1	B	435	SER
1	B	446	LEU
1	B	450	LEU
1	B	466	MET
1	B	486	GLU
1	B	499	GLN
1	B	517	ASP
1	B	519	ASN
1	B	528	ASN
1	B	542	LYS
1	B	595	LEU
1	B	597	LEU
1	B	603	SER
1	B	616	LEU
1	B	629	LEU
1	B	632	LYS
1	B	642	LEU
1	B	648	LYS
1	B	728	LEU
1	B	765	ARG
1	B	771	LEU

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Mol	Chain	Res	Type
1	B	810	LEU
1	B	853	GLU
1	B	859	LEU
1	B	861	SER
1	B	867	LEU
1	B	871	GLU
1	B	872	LYS
1	B	875	GLU
1	B	879	GLU
1	B	889	LEU
1	B	928	LEU
1	B	930	THR
1	B	931	LEU
1	B	934	GLU
1	B	938	LYS
1	B	964	ASP
1	B	1011	HIS
2	C	54	TYR
2	C	81	LEU
2	C	94	TYR
2	C	110	TYR
2	C	123	THR
2	C	125	VAL
2	C	126	THR
2	C	175	LEU
2	C	185	VAL
2	C	187	GLN
2	C	195	SER
2	C	213	ASN
3	D	17	ASP
3	D	33	VAL
3	D	65	SER
3	D	72	THR
3	D	95	PHE
3	D	97	ILE
3	D	98	THR
3	D	107	ILE
3	D	108	LYS
3	D	109	ARG
3	D	110	THR
3	D	122	SER
3	D	143	ARG

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Mol	Chain	Res	Type
3	D	144	GLU
3	D	147	VAL
3	D	150	LYS
3	D	171	ASP
3	D	173	THR
3	D	182	LEU
3	D	186	ASP
3	D	196	GLU
3	D	202	LEU
3	D	212	ARG
2	E	54	TYR
2	E	67	ARG
2	E	81	LEU
2	E	89	GLU
2	E	98	ARG
2	E	99	ASP
2	E	100	ARG
2	E	102	MET
2	E	121	GLN
2	E	126	THR
2	E	132	THR
2	E	140	LEU
2	E	156	CYS
2	E	165	PRO
2	E	172	SER
2	E	175	LEU
2	E	195	SER
2	E	215	ASN
2	E	216	HIS
3	F	9	SER
3	F	15	VAL
3	F	26	SER
3	F	31	SER
3	F	40	PRO
3	F	63	SER
3	F	92	SER
3	F	94	SER
3	F	95	PHE
3	F	98	THR
3	F	101	GLN
3	F	109	ARG
3	F	122	SER

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Mol	Chain	Res	Type
3	F	123	ASP
3	F	143	ARG
3	F	161	GLN
3	F	186	ASP
3	F	198	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (20) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	312	ASN
1	A	418	ASN
1	A	573	ASN
1	A	743	GLN
1	A	781	GLN
1	A	796	GLN
1	B	519	ASN
1	B	528	ASN
1	B	573	ASN
1	B	638	GLN
1	B	743	GLN
1	B	781	GLN
1	B	796	GLN
2	C	39	GLN
2	C	213	ASN
3	D	167	GLN
2	E	39	GLN
2	E	215	ASN
3	F	148	GLN
3	F	167	GLN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 1 ligands modelled in this entry, 1 is monoatomic - leaving 0 for Mogul analysis.

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.

No monomer is involved in short contacts.

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data (i)

6.1 Protein, DNA and RNA chains (i)

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
1	A	932/990 (94%)	0.00	11 (1%)	79	82	12, 39, 101, 152	0
1	B	861/990 (86%)	0.05	22 (2%)	56	58	11, 41, 100, 151	0
2	C	216/263 (82%)	0.25	1 (0%)	91	93	19, 56, 97, 112	0
2	E	211/263 (80%)	0.19	7 (3%)	46	48	18, 55, 98, 144	0
3	D	199/239 (83%)	0.46	14 (7%)	16	18	22, 55, 102, 138	0
3	F	197/239 (82%)	0.55	17 (8%)	10	12	20, 69, 116, 147	0
All	All	2616/2984 (87%)	0.13	72 (2%)	53	55	11, 46, 103, 152	0

All (72) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	F	179	THR	6.7
3	F	135	CYS	5.6
1	B	102	ASN	5.0
3	F	181	THR	3.9
1	B	370	PHE	3.8
3	F	120	PRO	3.7
1	B	115	PHE	3.7
1	B	99	ASP	3.6
3	F	178	SER	3.6
3	F	133	VAL	3.1
1	B	706	ASP	3.1
3	F	187	TYR	3.1
1	B	325	TYR	3.0
3	F	132	SER	3.0
1	B	323	GLN	3.0
3	F	210	PHE	2.9
3	D	138	ASN	2.9
1	B	322	LEU	2.9
3	F	180	LEU	2.9

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Mol	Chain	Res	Type	RSRZ
1	A	279	GLU	2.9
2	C	139	PRO	2.8
1	A	102	ASN	2.7
3	D	131	ALA	2.7
3	D	196	GLU	2.6
3	D	114	PRO	2.6
1	A	458	GLU	2.6
1	B	59	GLU	2.6
3	D	183	SER	2.5
1	B	437	ILE	2.5
3	D	122	SER	2.5
3	D	162	GLU	2.5
1	B	984	PRO	2.5
2	E	153	ALA	2.4
2	E	178	GLY	2.4
1	B	983	ALA	2.4
1	A	101	PRO	2.4
1	A	446	LEU	2.4
2	E	195	SER	2.4
1	A	115	PHE	2.4
3	F	183	SER	2.4
1	B	365	GLU	2.4
1	B	982	GLN	2.3
1	A	542	LYS	2.3
3	D	126	LEU	2.3
3	F	19	VAL	2.3
1	B	963	MET	2.3
3	D	116	VAL	2.3
1	B	165	PHE	2.2
1	B	426	ASP	2.2
1	B	113	MET	2.2
2	E	209	THR	2.2
3	F	182	LEU	2.2
3	F	176	LEU	2.1
2	E	11	LEU	2.1
1	A	265	ASP	2.1
1	A	798	ASP	2.1
3	F	131	ALA	2.1
1	B	981	SER	2.1
3	D	200	GLN	2.1
3	F	159	ASN	2.1
1	A	216	SER	2.1

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Mol	Chain	Res	Type	RSRZ
1	B	490	ASP	2.1
1	A	236	ASP	2.1
2	E	106	SER	2.1
3	D	195	CYS	2.0
3	D	198	THR	2.0
1	B	281	LYS	2.0
3	F	118	ILE	2.0
1	B	91	ASP	2.0
2	E	62	ASP	2.0
3	D	189	LYS	2.0
3	D	127	LYS	2.0

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

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

6.3 Carbohydrates (i)

There are no monosaccharides in this entry.

6.4 Ligands (i)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
4	ZN	A	1101	1/1	0.96	0.05	75,75,75,75	0

6.5 Other polymers (i)

There are no such residues in this entry.