Full wwPDB X-ray Structure Validation Report (i)

Nov 15, 2016 – 11:13 AM EST

PDB ID	:	5J3D
Title	:	Crystal structure of human Fab 14N4 in complex with post-fusion RSV F
Authors	:	Mousa, J.J.; Crowe, J.E.
Deposited on	:	2016-03-30
Resolution	:	4.08 Å(reported)

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

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
http://wwpdb.org/validation/2016/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

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

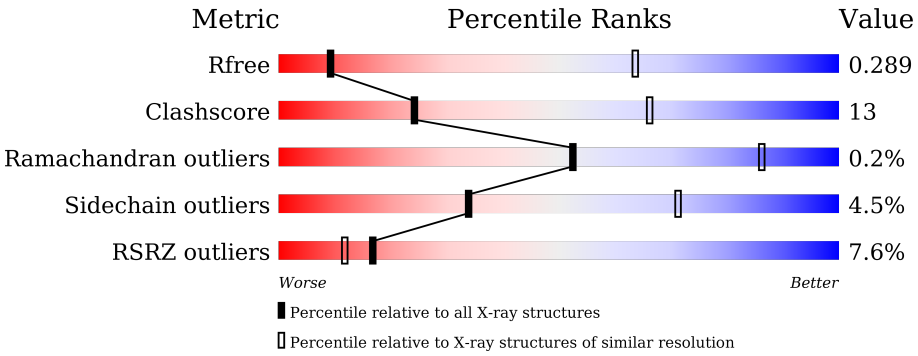
MolProbity	:	4.02b-467
Mogul	:	unknown
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20028320
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	rb-20028320

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 4.08 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	91344	1009 (4.52-3.60)
Clashscore	102246	1107 (4.52-3.60)
Ramachandran outliers	100387	1053 (4.52-3.60)
Sidechain outliers	100360	1039 (4.52-3.60)
RSRZ outliers	91569	1012 (4.52-3.60)

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

Mol	Chain	Length	Quality of chain
1	A	224	7% 72% 25% ·
1	C	224	2% 72% 24% · ·
1	H	224	29% 73% 25% ·
2	B	218	5% 69% 28% ··
2	D	218	2% 71% 26% ··
2	L	218	40% 79% 19% ·

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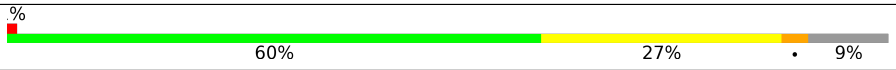
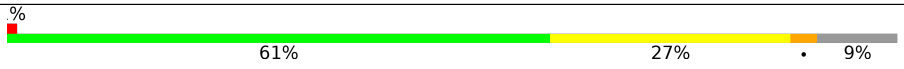
Mol	Chain	Length	Quality of chain
3	E	73	
3	G	73	
3	J	73	
4	F	394	
4	I	394	
4	K	394	

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 19902 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 14N4 heavy chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	220	Total	C	N	O	S	0	0	0
			1624	1020	275	322	7			
1	C	220	Total	C	N	O	S	0	0	0
			1624	1020	275	322	7			
1	H	220	Total	C	N	O	S	0	0	0
			1624	1020	275	322	7			

- Molecule 2 is a protein called 14N4 light chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	215	Total	C	N	O	S	0	0	0
			1665	1044	276	339	6			
2	D	215	Total	C	N	O	S	0	0	0
			1665	1044	276	339	6			
2	L	215	Total	C	N	O	S	0	0	0
			1665	1044	276	339	6			

- Molecule 3 is a protein called Fusion glycoprotein F0.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	E	73	Total	C	N	O	S	0	0	0
			580	366	95	116	3			
3	G	73	Total	C	N	O	S	0	0	0
			580	366	95	116	3			
3	J	73	Total	C	N	O	S	0	0	0
			580	366	95	116	3			

- Molecule 4 is a protein called Fusion glycoprotein F0.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	F	358	Total	C	N	O	S	0	0	0
			2765	1744	458	545	18			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	I	358	Total	C	N	O	S	0	0	0
			2765	1744	458	545	18			
4	K	358	Total	C	N	O	S	0	0	0
			2765	1744	458	545	18			

There are 87 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
F	379	VAL	ILE	conflict	UNP P03420
F	447	VAL	MET	conflict	UNP P03420
F	514	GLY	-	expression tag	UNP P03420
F	515	LEU	-	expression tag	UNP P03420
F	516	GLU	-	expression tag	UNP P03420
F	517	VAL	-	expression tag	UNP P03420
F	518	LEU	-	expression tag	UNP P03420
F	519	PHE	-	expression tag	UNP P03420
F	520	GLN	-	expression tag	UNP P03420
F	521	GLY	-	expression tag	UNP P03420
F	522	PRO	-	expression tag	UNP P03420
F	523	HIS	-	expression tag	UNP P03420
F	524	HIS	-	expression tag	UNP P03420
F	525	HIS	-	expression tag	UNP P03420
F	526	HIS	-	expression tag	UNP P03420
F	527	HIS	-	expression tag	UNP P03420
F	528	HIS	-	expression tag	UNP P03420
F	529	HIS	-	expression tag	UNP P03420
F	530	HIS	-	expression tag	UNP P03420
F	531	SER	-	expression tag	UNP P03420
F	532	ALA	-	expression tag	UNP P03420
F	533	TRP	-	expression tag	UNP P03420
F	534	SER	-	expression tag	UNP P03420
F	535	HIS	-	expression tag	UNP P03420
F	536	PRO	-	expression tag	UNP P03420
F	537	GLN	-	expression tag	UNP P03420
F	538	PHE	-	expression tag	UNP P03420
F	539	GLU	-	expression tag	UNP P03420
F	540	LYS	-	expression tag	UNP P03420
I	379	VAL	ILE	conflict	UNP P03420
I	447	VAL	MET	conflict	UNP P03420
I	514	GLY	-	expression tag	UNP P03420
I	515	LEU	-	expression tag	UNP P03420
I	516	GLU	-	expression tag	UNP P03420

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Chain	Residue	Modelled	Actual	Comment	Reference
I	517	VAL	-	expression tag	UNP P03420
I	518	LEU	-	expression tag	UNP P03420
I	519	PHE	-	expression tag	UNP P03420
I	520	GLN	-	expression tag	UNP P03420
I	521	GLY	-	expression tag	UNP P03420
I	522	PRO	-	expression tag	UNP P03420
I	523	HIS	-	expression tag	UNP P03420
I	524	HIS	-	expression tag	UNP P03420
I	525	HIS	-	expression tag	UNP P03420
I	526	HIS	-	expression tag	UNP P03420
I	527	HIS	-	expression tag	UNP P03420
I	528	HIS	-	expression tag	UNP P03420
I	529	HIS	-	expression tag	UNP P03420
I	530	HIS	-	expression tag	UNP P03420
I	531	SER	-	expression tag	UNP P03420
I	532	ALA	-	expression tag	UNP P03420
I	533	TRP	-	expression tag	UNP P03420
I	534	SER	-	expression tag	UNP P03420
I	535	HIS	-	expression tag	UNP P03420
I	536	PRO	-	expression tag	UNP P03420
I	537	GLN	-	expression tag	UNP P03420
I	538	PHE	-	expression tag	UNP P03420
I	539	GLU	-	expression tag	UNP P03420
I	540	LYS	-	expression tag	UNP P03420
K	379	VAL	ILE	conflict	UNP P03420
K	447	VAL	MET	conflict	UNP P03420
K	514	GLY	-	expression tag	UNP P03420
K	515	LEU	-	expression tag	UNP P03420
K	516	GLU	-	expression tag	UNP P03420
K	517	VAL	-	expression tag	UNP P03420
K	518	LEU	-	expression tag	UNP P03420
K	519	PHE	-	expression tag	UNP P03420
K	520	GLN	-	expression tag	UNP P03420
K	521	GLY	-	expression tag	UNP P03420
K	522	PRO	-	expression tag	UNP P03420
K	523	HIS	-	expression tag	UNP P03420
K	524	HIS	-	expression tag	UNP P03420
K	525	HIS	-	expression tag	UNP P03420
K	526	HIS	-	expression tag	UNP P03420
K	527	HIS	-	expression tag	UNP P03420
K	528	HIS	-	expression tag	UNP P03420
K	529	HIS	-	expression tag	UNP P03420

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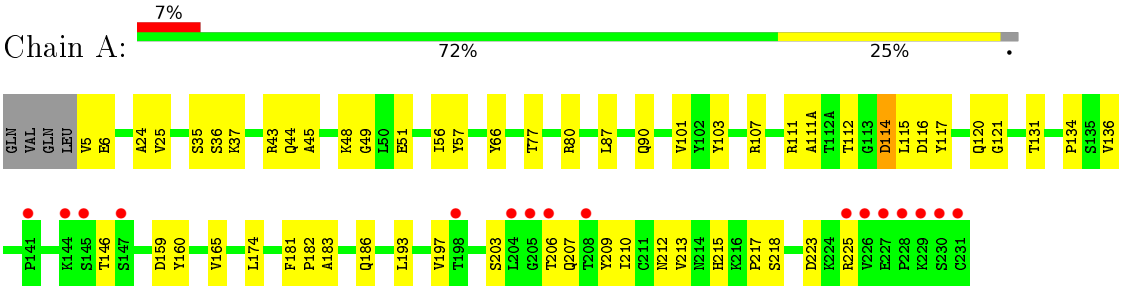
Chain	Residue	Modelled	Actual	Comment	Reference
K	530	HIS	-	expression tag	UNP P03420
K	531	SER	-	expression tag	UNP P03420
K	532	ALA	-	expression tag	UNP P03420
K	533	TRP	-	expression tag	UNP P03420
K	534	SER	-	expression tag	UNP P03420
K	535	HIS	-	expression tag	UNP P03420
K	536	PRO	-	expression tag	UNP P03420
K	537	GLN	-	expression tag	UNP P03420
K	538	PHE	-	expression tag	UNP P03420
K	539	GLU	-	expression tag	UNP P03420
K	540	LYS	-	expression tag	UNP P03420

3 Residue-property plots (i)

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

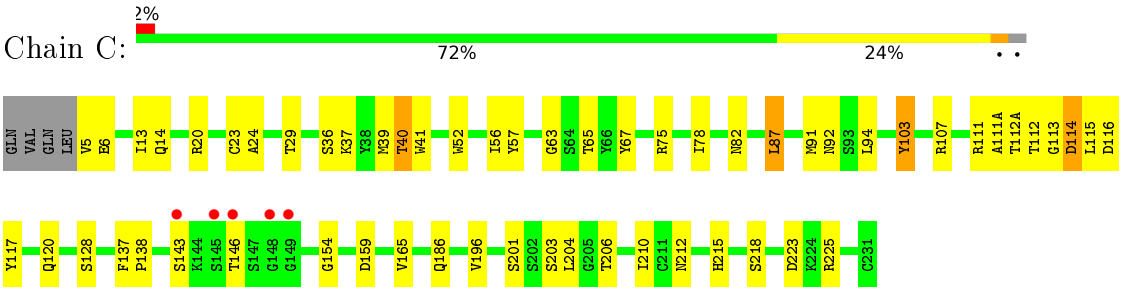
- Molecule 1: 14N4 heavy chain

Chain A:



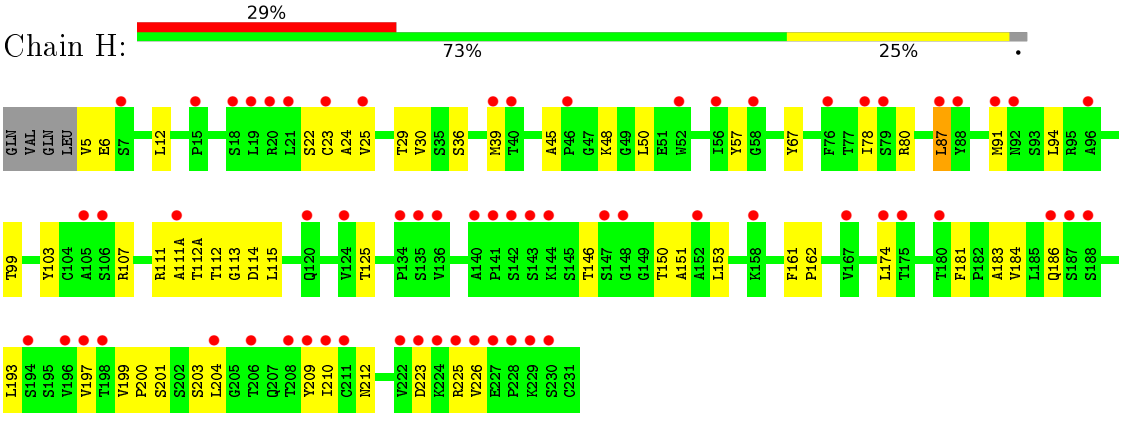
- Molecule 1: 14N4 heavy chain

Chain C:



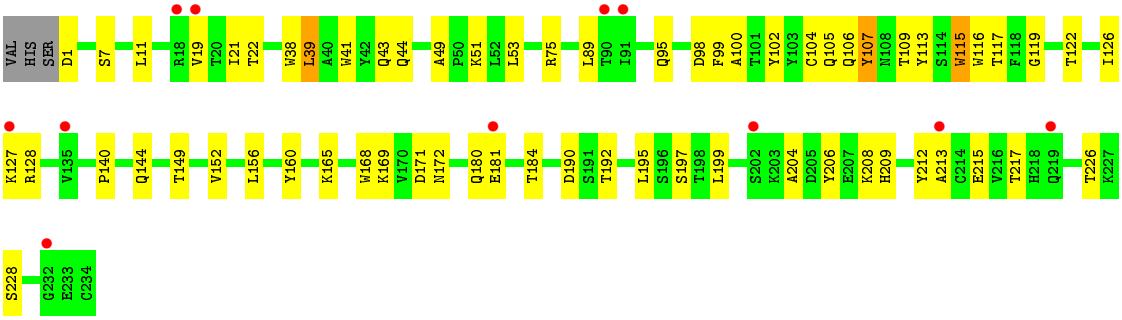
- Molecule 1: 14N4 heavy chain

Chain H:



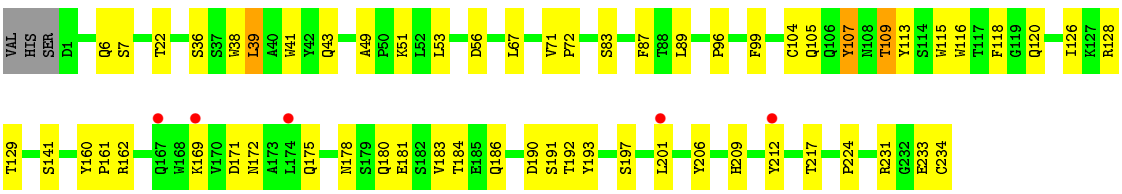
- Molecule 2: 14N4 light chain

Chain B:



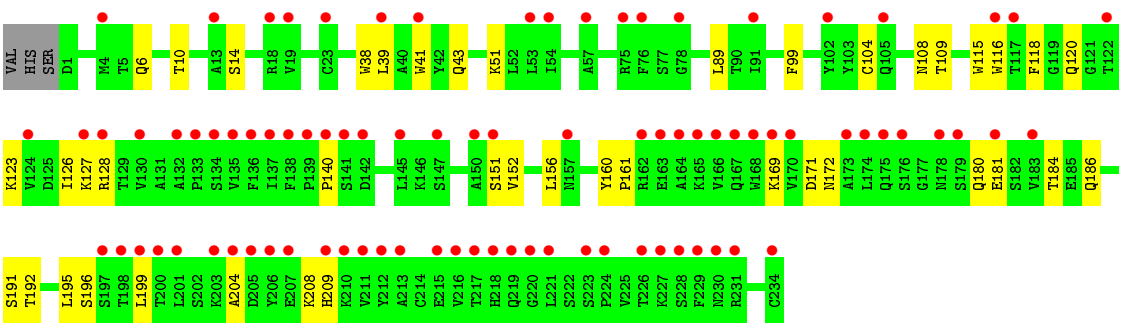
- Molecule 2: 14N4 light chain

Chain D:



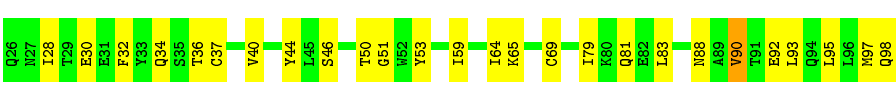
- Molecule 2: 14N4 light chain

Chain L:



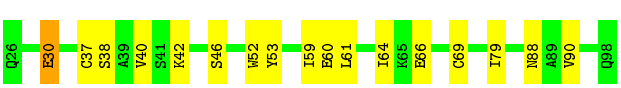
- Molecule 3: Fusion glycoprotein F0

Chain E:



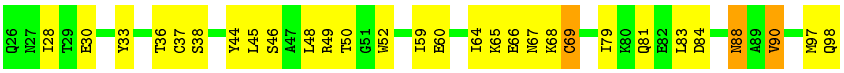
- Molecule 3: Fusion glycoprotein F0

Chain G:



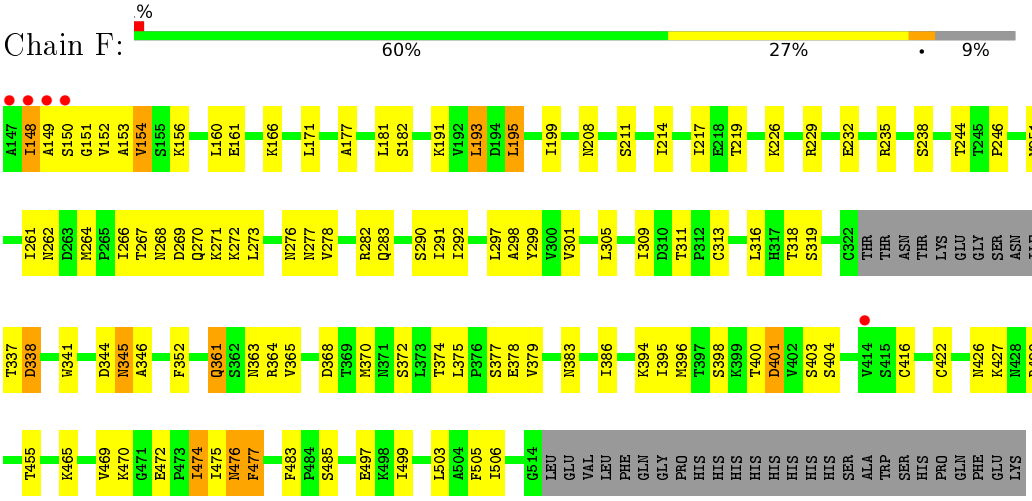
- Molecule 3: Fusion glycoprotein F0

Chain J:



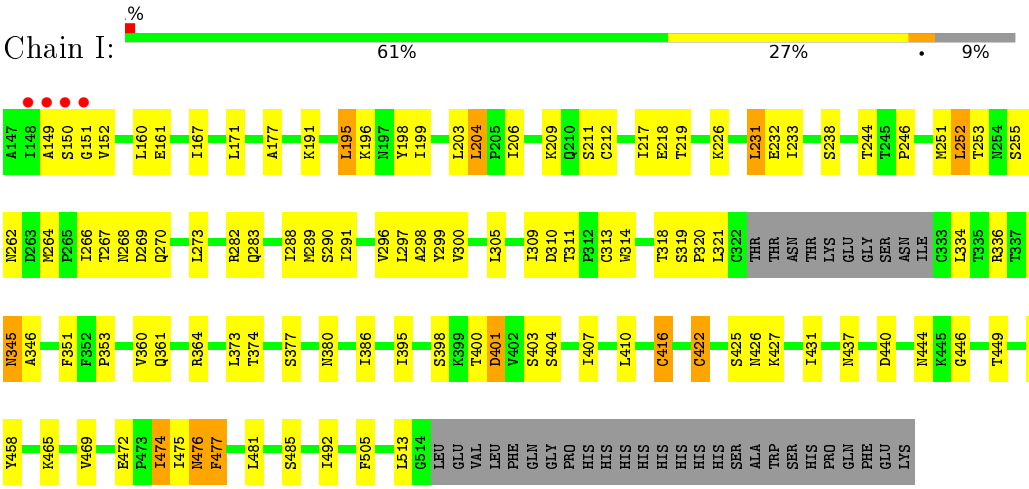
• Molecule 4: Fusion glycoprotein F0

Chain F:



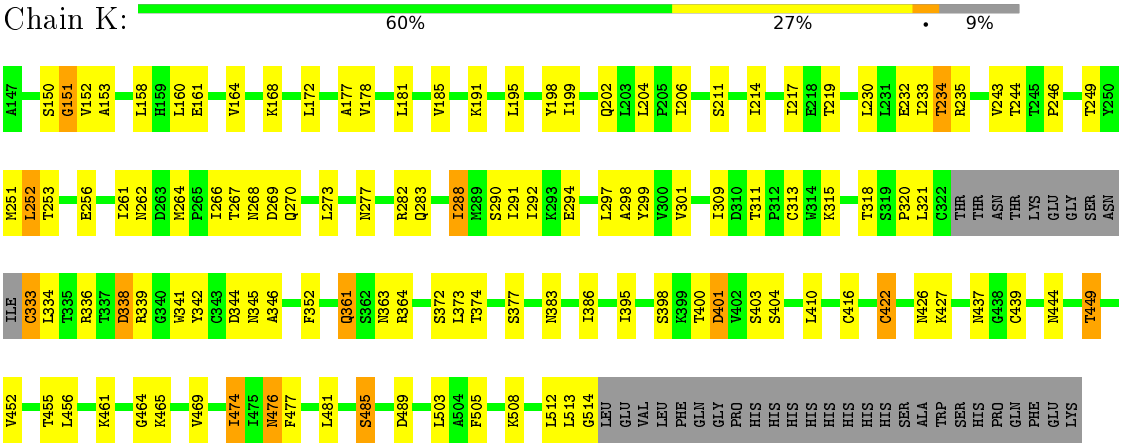
• Molecule 4: Fusion glycoprotein F0

Chain I:



• Molecule 4: Fusion glycoprotein F0

Chain K:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 42 21 2	Depositor
Cell constants a, b, c, α, β, γ	235.13Å 235.13Å 220.14Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.50 – 4.08 49.50 – 4.08	Depositor EDS
% Data completeness (in resolution range)	97.3 (49.50-4.08) 84.8 (49.50-4.08)	Depositor EDS
R_{merge}	0.30	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.82 (at 4.14Å)	Xtriage
Refinement program	PHENIX (1.10.1_2155: ???)	Depositor
R, R_{free}	0.257 , 0.282 0.262 , 0.289	Depositor DCC
R_{free} test set	1808 reflections (4.13%)	DCC
Wilson B-factor (Å^2)	101.3	Xtriage
Anisotropy	0.063	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.32 , 105.9	EDS
L-test for twinning[2]	$< \|L\| > = 0.39$, $< L^2 > = 0.22$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.85	EDS
Total number of atoms	19902	wwPDB-VP
Average B, all atoms (Å^2)	153.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.43% 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	0.34	0/1660	0.56	0/2262
1	C	0.45	0/1660	0.63	0/2262
1	H	0.27	0/1660	0.51	0/2262
2	B	0.34	0/1704	0.55	0/2317
2	D	0.42	0/1704	0.59	0/2317
2	L	0.29	0/1704	0.50	0/2317
3	E	0.50	0/586	0.75	0/789
3	G	0.64	0/586	0.85	1/789 (0.1%)
3	J	0.50	0/586	0.73	0/789
4	F	0.50	0/2805	0.74	2/3803 (0.1%)
4	I	0.54	0/2805	0.81	4/3803 (0.1%)
4	K	0.56	1/2805 (0.0%)	0.80	5/3803 (0.1%)
All	All	0.46	1/20265 (0.0%)	0.68	12/27513 (0.0%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	K	439	CYS	CB-SG	-6.17	1.71	1.82

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	I	212	CYS	CA-CB-SG	12.46	136.43	114.00
4	K	172	LEU	CA-CB-CG	-6.41	100.56	115.30
4	I	231	LEU	CA-CB-CG	-6.26	100.91	115.30
4	I	373	LEU	CA-CB-CG	-6.26	100.90	115.30
4	I	305	LEU	CB-CG-CD1	-5.41	101.80	111.00
4	K	172	LEU	CB-CG-CD2	-5.39	101.83	111.00
4	F	333	CYS	CA-CB-SG	5.34	123.61	114.00
4	K	373	LEU	CA-CB-CG	-5.31	103.09	115.30
4	K	333	CYS	CA-CB-SG	5.22	123.39	114.00
4	F	193	LEU	CB-CG-CD1	-5.19	102.17	111.00
3	G	61	LEU	CB-CG-CD2	-5.14	102.27	111.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	K	151	GLY	N-CA-C	5.07	125.78	113.10

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	1624	0	1599	43	0
1	C	1624	0	1599	45	1
1	H	1624	0	1599	36	0
2	B	1665	0	1600	48	0
2	D	1665	0	1600	65	0
2	L	1665	0	1600	33	0
3	E	580	0	589	25	0
3	G	580	0	589	13	0
3	J	580	0	589	26	0
4	F	2765	0	2798	112	0
4	I	2765	0	2798	122	0
4	K	2765	0	2798	109	0
All	All	19902	0	19758	514	1

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 13.

All (514) 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:D:38:TRP:CE2	4:I:268:ASN:HB3	1.81	1.15
2:D:38:TRP:HH2	4:I:269:ASP:HA	1.35	0.89
1:A:35:SER:O	4:I:465:LYS:NZ	2.09	0.86
2:D:109:THR:HG23	4:I:267:THR:HA	1.55	0.85
4:F:345:ASN:HD22	4:I:455:THR:HG21	1.42	0.84
4:F:272:LYS:O	4:F:276:ASN:ND2	2.12	0.82
2:B:109:THR:O	2:B:116:TRP:NE1	2.13	0.81

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:212:ASN:ND2	1:C:223:ASP:OD1	2.13	0.80
3:E:59:ILE:HG23	4:I:469:VAL:HB	1.64	0.79
4:K:318:THR:HG21	4:K:336:ARG:HB2	1.65	0.78
4:F:261:ILE:HG12	4:F:264:MET:HE1	1.65	0.77
4:I:152:VAL:HG11	4:K:152:VAL:HB	1.67	0.77
4:K:270:GLN:HG2	4:K:309:ILE:HD12	1.67	0.76
2:D:107:TYR:O	4:I:268:ASN:ND2	2.18	0.76
4:F:290:SER:OG	4:F:291:ILE:N	2.19	0.75
4:F:171:LEU:HD23	4:I:513:LEU:HD11	1.68	0.75
2:D:38:TRP:CZ2	4:I:268:ASN:C	2.61	0.74
2:D:38:TRP:CH2	4:I:269:ASP:HA	2.22	0.74
1:C:36:SER:HA	4:K:465:LYS:NZ	2.03	0.73
4:F:270:GLN:HG2	4:F:309:ILE:HD12	1.69	0.73
2:D:38:TRP:CZ2	4:I:268:ASN:HB3	2.23	0.73
2:B:107:TYR:O	4:F:268:ASN:ND2	2.22	0.72
4:K:252:LEU:O	4:K:282:ARG:NH1	2.23	0.71
4:F:318:THR:HG21	4:F:336:ARG:HB2	1.73	0.71
2:D:38:TRP:CH2	4:I:268:ASN:C	2.64	0.71
1:A:212:ASN:ND2	1:A:223:ASP:OD1	2.23	0.70
2:L:6:GLN:HB2	2:L:120:GLN:HE22	1.56	0.70
1:H:5:VAL:N	1:H:24:ALA:O	2.24	0.70
4:F:166:LYS:NZ	4:K:514:GLY:HA3	2.06	0.70
4:I:270:GLN:HG2	4:I:309:ILE:HD12	1.73	0.70
2:D:43:GLN:HB2	2:D:53:LEU:HD11	1.73	0.69
2:D:96:PRO:HA	2:D:99:PHE:CD2	2.28	0.69
4:I:266:ILE:HD12	4:I:270:GLN:HB2	1.75	0.69
2:D:38:TRP:CD2	4:I:268:ASN:HB3	2.28	0.68
1:C:186:GLN:HA	2:D:180:GLN:HE22	1.58	0.68
1:A:174:LEU:HD21	1:A:197:VAL:HG21	1.74	0.68
2:D:38:TRP:CZ2	4:I:268:ASN:O	2.47	0.68
4:K:449:THR:HG23	4:K:456:LEU:HD11	1.76	0.68
1:C:39:MET:HE3	1:C:87:LEU:HD22	1.75	0.68
2:D:38:TRP:HH2	4:I:269:ASP:CA	2.05	0.68
4:F:148:ILE:HB	4:F:154:VAL:HG12	1.74	0.68
4:K:261:ILE:HG12	4:K:264:MET:HE1	1.75	0.68
4:K:334:LEU:HD22	4:K:395:ILE:HD13	1.75	0.67
4:K:230:LEU:O	4:K:234:THR:HG23	1.95	0.66
1:C:23:CYS:HB3	1:C:87:LEU:HD23	1.78	0.66
2:B:43:GLN:O	2:B:51:LYS:N	2.27	0.66
4:F:266:ILE:HD12	4:F:270:GLN:HB2	1.78	0.66
2:D:171:ASP:OD2	2:D:209:HIS:ND1	2.27	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:F:277:ASN:OD1	4:F:361:GLN:HG2	1.94	0.66
1:A:77:THR:HB	1:A:90:GLN:HB3	1.77	0.66
1:A:43:ARG:NE	1:A:51:GLU:OE1	2.24	0.66
1:A:183:ALA:HA	1:A:193:LEU:HB3	1.79	0.65
4:F:149:ALA:HB3	4:K:152:VAL:HG22	1.78	0.65
1:H:151:ALA:HB3	1:H:204:LEU:HD21	1.78	0.65
4:K:290:SER:OG	4:K:291:ILE:N	2.29	0.65
4:I:318:THR:HG21	4:I:336:ARG:HB2	1.77	0.65
2:B:171:ASP:OD2	2:B:209:HIS:ND1	2.21	0.65
1:A:5:VAL:N	1:A:24:ALA:O	2.30	0.65
3:J:66:GLU:HA	3:J:79:ILE:HG21	1.78	0.65
3:G:52:TRP:HB2	4:K:461:LYS:HG2	1.80	0.64
1:C:5:VAL:N	1:C:117:TYR:HH	1.95	0.64
2:D:41:TRP:CZ3	2:D:104:CYS:HB3	2.32	0.64
2:L:171:ASP:OD2	2:L:209:HIS:ND1	2.29	0.64
1:A:114:ASP:N	1:A:114:ASP:OD1	2.31	0.64
2:D:169:LYS:HE2	2:D:172:ASN:HA	1.79	0.64
4:F:345:ASN:ND2	4:I:455:THR:HG21	2.12	0.64
2:B:41:TRP:CE2	2:B:89:LEU:HB2	2.32	0.64
4:I:351:PHE:CE2	4:I:353:PRO:HB3	2.32	0.63
3:E:46:SER:HB3	4:F:313:CYS:SG	2.38	0.63
3:E:64:ILE:HG22	4:I:474:ILE:HG13	1.80	0.63
1:C:107:ARG:HD3	1:C:114:ASP:OD1	1.99	0.63
3:E:64:ILE:HD12	3:E:79:ILE:HG23	1.81	0.63
1:A:210:ILE:HG12	1:A:225:ARG:HG2	1.80	0.63
1:A:36:SER:HA	4:I:465:LYS:NZ	2.13	0.62
4:F:251:MET:HG3	4:F:299:TYR:CE1	2.35	0.62
1:C:210:ILE:HG12	1:C:225:ARG:HG2	1.82	0.62
3:E:28:ILE:HD11	4:F:363:ASN:HA	1.80	0.62
4:F:199:ILE:HD11	4:I:199:ILE:HD11	1.81	0.62
4:F:199:ILE:HD11	4:K:199:ILE:HD11	1.82	0.62
1:A:57:TYR:HE1	1:A:112:THR:HG21	1.64	0.61
4:I:264:MET:HE3	4:I:266:ILE:HD11	1.82	0.61
2:D:105:GLN:HB2	2:D:118:PHE:CE1	2.34	0.61
4:F:152:VAL:HG11	4:I:152:VAL:HG21	1.81	0.61
1:A:182:PRO:HD3	2:B:184:THR:HG22	1.82	0.61
2:D:6:GLN:H	2:D:120:GLN:HE22	1.49	0.61
4:F:166:LYS:HZ1	4:K:514:GLY:HA3	1.65	0.61
1:C:114:ASP:N	1:C:114:ASP:OD1	2.27	0.61
1:C:40:THR:OG1	1:C:41:TRP:N	2.33	0.61
4:F:253:THR:OG1	4:F:256:GLU:HG3	1.99	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:K:246:PRO:HB3	4:K:283:GLN:HA	1.81	0.61
4:K:336:ARG:NH1	4:K:383:ASN:OD1	2.34	0.61
1:H:30:VAL:O	1:H:80:ARG:NH1	2.34	0.61
2:B:169:LYS:HE2	2:B:172:ASN:HA	1.83	0.61
4:F:229:ARG:NH2	4:F:256:GLU:OE1	2.29	0.61
2:D:56:ASP:OD1	2:D:107:TYR:OH	2.17	0.60
2:L:126:ILE:O	2:L:160:TYR:OH	2.17	0.60
4:K:277:ASN:OD1	4:K:361:GLN:HG2	2.02	0.60
2:D:38:TRP:CH2	4:I:269:ASP:CA	2.83	0.60
4:I:345:ASN:OD1	4:K:455:THR:HG21	2.01	0.60
4:I:251:MET:HG3	4:I:299:TYR:CE1	2.37	0.60
4:K:252:LEU:HD22	4:K:301:VAL:HG21	1.82	0.60
1:C:5:VAL:N	1:C:117:TYR:OH	2.35	0.60
4:F:469:VAL:HB	3:J:59:ILE:HG23	1.83	0.59
4:I:426:ASN:ND2	4:I:446:GLY:O	2.36	0.59
4:F:474:ILE:HG13	3:J:64:ILE:HG22	1.84	0.59
4:I:199:ILE:HD11	4:K:199:ILE:HD11	1.83	0.59
2:L:156:LEU:HB2	2:L:195:LEU:HB3	1.84	0.59
1:A:57:TYR:CE1	1:A:112:THR:HG21	2.36	0.59
4:I:252:LEU:HD23	4:I:256:GLU:HB2	1.83	0.59
2:B:11:LEU:HD23	2:B:19:VAL:HG13	1.82	0.59
4:F:465:LYS:NZ	1:H:36:SER:HA	2.18	0.59
4:I:246:PRO:HB3	4:I:283:GLN:HA	1.83	0.59
4:K:164:VAL:O	4:K:168:LYS:HB2	2.03	0.58
4:I:253:THR:OG1	4:I:256:GLU:HG3	2.03	0.58
2:L:43:GLN:HB3	2:L:51:LYS:HB3	1.84	0.58
1:C:112(A):THR:CG2	2:D:38:TRP:HE1	2.17	0.58
4:K:253:THR:OG1	4:K:256:GLU:HG3	2.04	0.58
1:A:35:SER:HA	1:A:80:ARG:NH1	2.19	0.58
1:C:107:ARG:NH1	1:C:111:ARG:HG3	2.18	0.58
2:D:175:GLN:OE1	2:D:178:ASN:ND2	2.35	0.57
4:F:278:VAL:HG22	3:J:98:GLN:NE2	2.20	0.57
2:B:1:ASP:HB3	2:B:115:TRP:CE2	2.39	0.57
3:J:46:SER:HB3	4:K:313:CYS:SG	2.45	0.57
1:C:36:SER:HA	4:K:465:LYS:HZ2	1.69	0.57
3:G:40:VAL:HG11	3:G:42:LYS:HE2	1.86	0.57
4:F:152:VAL:HB	4:K:152:VAL:HG21	1.86	0.57
4:K:426:ASN:OD1	4:K:427:LYS:N	2.38	0.57
1:C:114:ASP:O	1:C:115:LEU:HD13	2.05	0.57
2:D:38:TRP:CH2	4:I:269:ASP:N	2.73	0.57
2:B:99:PHE:CE1	2:B:126:ILE:HG12	2.40	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:57:TYR:CE1	1:C:112:THR:HG21	2.39	0.57
3:G:46:SER:HB3	4:I:313:CYS:SG	2.46	0.56
1:A:5:VAL:N	1:A:117:TYR:HH	2.03	0.56
1:A:165:VAL:HG23	1:A:215:HIS:HB2	1.87	0.56
4:I:374:THR:HG21	4:K:404:SER:HB3	1.86	0.56
4:I:171:LEU:HD23	4:K:513:LEU:HD11	1.87	0.56
4:I:297:LEU:HD12	4:I:298:ALA:H	1.70	0.56
4:F:226:LYS:HE2	3:J:81:GLN:NE2	2.21	0.56
4:K:251:MET:HG3	4:K:299:TYR:CE1	2.40	0.56
3:J:36:THR:HB	4:K:336:ARG:HD2	1.87	0.56
4:I:261:ILE:HG12	4:I:264:MET:HE1	1.87	0.56
2:D:38:TRP:CH2	4:I:269:ASP:OD1	2.59	0.56
3:J:90:VAL:HG11	4:K:294:GLU:HG2	1.88	0.56
1:C:103:TYR:HE1	2:D:49:ALA:HA	1.71	0.55
2:L:10:THR:HG22	2:L:123:LYS:HB3	1.87	0.55
4:I:334:LEU:HB3	4:I:395:ILE:HD11	1.88	0.55
1:H:186:GLN:HA	2:L:180:GLN:HE22	1.71	0.55
2:B:156:LEU:HD22	2:B:195:LEU:HD13	1.87	0.55
4:F:161:GLU:HA	4:K:160:LEU:HD21	1.88	0.55
4:K:269:ASP:OD1	2:L:38:TRP:CH2	2.60	0.55
1:A:186:GLN:HA	2:B:180:GLN:HE22	1.72	0.55
1:C:111(A):ALA:HB2	4:I:258:LEU:HD22	1.89	0.55
1:A:134:PRO:HB3	1:A:160:TYR:HB3	1.89	0.55
2:B:156:LEU:HB2	2:B:195:LEU:HB3	1.89	0.55
1:C:91:MET:HB3	1:C:94:LEU:HD21	1.88	0.54
4:I:311:THR:HG23	4:I:344:ASP:HB2	1.90	0.54
4:I:422:CYS:HB3	4:I:452:VAL:HG22	1.89	0.54
2:D:160:TYR:CD2	2:D:161:PRO:HA	2.42	0.54
2:B:38:TRP:HH2	4:F:269:ASP:OD1	1.90	0.54
2:D:99:PHE:CE1	2:D:126:ILE:HG12	2.42	0.54
2:D:38:TRP:CZ3	4:I:269:ASP:OD1	2.59	0.54
4:F:475:ILE:CD1	3:J:65:LYS:HE2	2.37	0.54
1:H:107:ARG:NH1	1:H:111:ARG:HG3	2.22	0.54
3:J:28:ILE:HD11	4:K:363:ASN:HA	1.88	0.54
1:C:36:SER:O	1:C:37:LYS:HG3	2.07	0.54
3:G:64:ILE:HD12	3:G:79:ILE:HG23	1.90	0.54
1:A:215:HIS:CE1	1:A:218:SER:HG	2.23	0.54
1:A:103:TYR:HE1	2:B:49:ALA:HA	1.73	0.53
1:A:203:SER:HB2	1:A:206:THR:HB	1.90	0.53
4:K:338:ASP:HB2	4:K:342:TYR:OH	2.08	0.53
3:E:40:VAL:HG22	4:F:316:LEU:HD12	1.90	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:128:ARG:NH1	2:B:190:ASP:O	2.41	0.53
4:I:204:LEU:HD22	4:K:481:LEU:O	2.08	0.53
3:E:46:SER:OG	4:F:311:THR:HB	2.08	0.53
1:H:114:ASP:N	1:H:114:ASP:OD1	2.41	0.53
2:L:41:TRP:CZ3	2:L:104:CYS:HB3	2.43	0.53
2:D:178:ASN:HD22	2:D:201:LEU:HD21	1.74	0.53
1:A:136:VAL:HG21	1:A:213:VAL:HG21	1.89	0.53
1:A:6:GLU:OE1	1:A:120:GLN:N	2.42	0.53
4:F:374:THR:HG21	4:I:404:SER:HB3	1.91	0.53
1:H:91:MET:HB3	1:H:94:LEU:HD21	1.91	0.53
4:I:505:PHE:HB2	4:K:177:ALA:HB2	1.91	0.53
4:K:266:ILE:HD12	4:K:270:GLN:HB2	1.91	0.53
2:B:75:ARG:CZ	2:B:95:GLN:HG3	2.38	0.52
1:C:113:GLY:HA2	2:D:116:TRP:CZ2	2.44	0.52
4:F:182:SER:OG	4:K:181:LEU:HD13	2.09	0.52
2:B:7:SER:OG	2:B:22:THR:OG1	2.27	0.52
1:C:159:ASP:OD1	1:C:186:GLN:NE2	2.42	0.52
4:K:269:ASP:OD1	2:L:38:TRP:HH2	1.92	0.52
4:F:318:THR:CG2	4:F:336:ARG:HB2	2.38	0.52
2:D:99:PHE:CD1	2:D:126:ILE:HG12	2.45	0.52
3:E:51:GLY:HA3	4:I:458:TYR:HB2	1.91	0.52
2:L:128:ARG:NH1	2:L:192:THR:HG23	2.25	0.52
2:L:169:LYS:HE2	2:L:172:ASN:HA	1.92	0.52
1:A:159:ASP:OD1	1:A:186:GLN:NE2	2.43	0.52
4:F:336:ARG:NH1	4:F:383:ASN:OD1	2.39	0.52
2:D:109:THR:HG22	2:D:113:TYR:CD2	2.45	0.51
4:F:152:VAL:HG13	4:I:149:ALA:HB3	1.92	0.51
4:F:219:THR:OG1	4:I:476:ASN:HB3	2.10	0.51
4:I:290:SER:OG	4:I:291:ILE:N	2.43	0.51
1:C:112(A):THR:HG22	2:D:38:TRP:HE1	1.75	0.51
1:A:112:THR:CB	4:F:271:LYS:HZ3	2.24	0.51
4:F:416:CYS:O	4:F:437:ASN:HA	2.10	0.51
2:D:160:TYR:CG	2:D:161:PRO:HA	2.45	0.51
4:K:321:LEU:O	4:K:333:CYS:HA	2.11	0.51
3:G:59:ILE:HG23	4:K:469:VAL:HB	1.92	0.51
4:F:426:ASN:OD1	4:F:427:LYS:N	2.44	0.51
1:H:99:THR:HG23	1:H:125:THR:HA	1.92	0.51
3:E:65:LYS:HE2	4:I:475:ILE:CD1	2.41	0.51
1:C:113:GLY:HA3	2:D:107:TYR:CD1	2.45	0.51
1:C:154:GLY:HA3	1:C:196:VAL:HG12	1.93	0.51
4:F:470:LYS:HE2	3:J:60:GLU:OE2	2.10	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:I:410:LEU:HA	4:I:444:ASN:ND2	2.26	0.51
2:B:113:TYR:H	2:B:113:TYR:HD2	1.59	0.51
1:C:203:SER:HB2	1:C:206:THR:HB	1.93	0.51
4:F:232:GLU:OE1	4:K:235:ARG:NH1	2.44	0.51
3:E:53:TYR:HB2	4:F:305:LEU:HD11	1.91	0.51
1:H:113:GLY:HA2	2:L:116:TRP:CZ2	2.46	0.51
4:F:193:LEU:HD13	4:I:492:ILE:HG21	1.92	0.51
4:F:273:LEU:HD11	4:F:364:ARG:HG2	1.92	0.50
3:G:46:SER:OG	4:I:311:THR:HB	2.11	0.50
4:I:426:ASN:OD1	4:I:427:LYS:N	2.44	0.50
2:B:126:ILE:O	2:B:160:TYR:OH	2.29	0.50
4:F:246:PRO:HB3	4:F:283:GLN:HA	1.93	0.50
4:F:311:THR:HG23	4:F:344:ASP:HB2	1.93	0.50
4:I:152:VAL:CG1	4:K:152:VAL:HB	2.40	0.50
3:J:84:ASP:O	3:J:88:ASN:HB3	2.11	0.50
4:F:214:ILE:HD11	4:K:214:ILE:HD11	1.93	0.50
3:J:38:SER:HB3	4:K:318:THR:HG22	1.93	0.50
2:B:38:TRP:CH2	4:F:269:ASP:OD1	2.64	0.50
4:K:311:THR:HG23	4:K:344:ASP:HB2	1.94	0.50
4:K:264:MET:HE3	4:K:266:ILE:HD11	1.94	0.50
4:I:233:ILE:HD13	4:I:299:TYR:CE2	2.47	0.50
4:K:266:ILE:HD12	4:K:270:GLN:CB	2.41	0.50
2:B:144:GLN:HG2	2:B:149:THR:O	2.12	0.50
4:F:352:PHE:CD1	4:F:372:SER:HB3	2.46	0.50
3:J:49:ARG:NH1	3:J:52:TRP:CE2	2.80	0.50
2:B:140:PRO:HD3	2:B:152:VAL:HG22	1.94	0.49
2:D:181:GLU:HG2	2:D:197:SER:HB2	1.95	0.49
4:F:177:ALA:HB2	4:K:505:PHE:HB2	1.94	0.49
2:D:36:SER:HB2	2:D:38:TRP:CE3	2.47	0.49
2:D:96:PRO:HA	2:D:99:PHE:HD2	1.75	0.49
4:K:320:PRO:HA	4:K:334:LEU:O	2.11	0.49
2:B:204:ALA:O	2:B:208:LYS:HG3	2.12	0.49
1:C:201:SER:HA	1:C:204:LEU:HG	1.94	0.49
4:I:297:LEU:HD12	4:I:298:ALA:N	2.27	0.49
4:I:321:LEU:HB3	4:I:334:LEU:HB2	1.95	0.49
4:I:449:THR:HG23	4:I:456:LEU:HD11	1.94	0.49
4:K:318:THR:H	4:K:339:ARG:HD3	1.78	0.49
4:K:334:LEU:HD22	4:K:395:ILE:CD1	2.42	0.49
1:A:101:VAL:HG12	1:A:103:TYR:HE2	1.77	0.49
2:D:126:ILE:HD12	2:D:191:SER:HB3	1.95	0.49
4:K:318:THR:CG2	4:K:336:ARG:HB2	2.40	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:143:SER:OG	2:D:234:CYS:SG	2.71	0.49
4:F:465:LYS:HZ1	1:H:36:SER:HA	1.78	0.49
1:C:63:GLY:O	1:C:65:THR:HG23	2.12	0.49
4:I:346:ALA:HB2	4:K:455:THR:HG23	1.95	0.49
2:L:160:TYR:CG	2:L:161:PRO:HA	2.48	0.49
2:B:41:TRP:CZ3	2:B:104:CYS:HB3	2.47	0.48
2:D:162:ARG:HB2	2:D:193:TYR:CZ	2.48	0.48
3:E:32:PHE:CE2	3:E:34:GLN:HG2	2.48	0.48
1:C:112(A):THR:O	4:I:262:ASN:ND2	2.46	0.48
1:H:174:LEU:HD21	1:H:197:VAL:HG21	1.95	0.48
4:I:206:ILE:HD13	4:I:209:LYS:HD2	1.93	0.48
1:C:111(A):ALA:HA	4:I:262:ASN:OD1	2.14	0.48
4:F:252:LEU:O	4:F:282:ARG:NH1	2.43	0.48
3:J:97:MET:SD	4:K:292:ILE:HG22	2.52	0.48
4:F:426:ASN:ND2	4:F:429:ARG:HD2	2.28	0.48
1:H:39:MET:HE2	1:H:87:LEU:HB3	1.95	0.48
4:K:416:CYS:O	4:K:437:ASN:HA	2.14	0.48
3:E:92:GLU:HA	3:E:95:LEU:HD12	1.94	0.48
4:K:243:VAL:HG22	4:K:288:ILE:HG23	1.95	0.48
4:K:400:THR:HG22	4:K:401:ASP:N	2.29	0.48
2:D:105:GLN:HB2	2:D:118:PHE:CD1	2.49	0.48
3:E:64:ILE:HG12	3:E:83:LEU:HD21	1.95	0.48
1:H:201:SER:HA	1:H:204:LEU:HG	1.96	0.48
4:I:314:TRP:HZ2	4:I:380:ASN:HD21	1.58	0.48
1:A:5:VAL:N	1:A:117:TYR:OH	2.47	0.48
4:F:297:LEU:HD12	4:F:298:ALA:H	1.79	0.48
4:F:368:ASP:OD2	4:F:370:MET:HE2	2.13	0.48
2:L:99:PHE:CD1	2:L:126:ILE:HG12	2.49	0.48
3:E:36:THR:HB	4:F:336:ARG:HD2	1.96	0.47
4:F:338:ASP:HB3	4:F:394:LYS:HE3	1.95	0.47
4:I:425:SER:HA	4:I:431:ILE:HA	1.95	0.47
1:A:107:ARG:NH1	1:A:111:ARG:HG3	2.30	0.47
2:B:104:CYS:O	2:B:119:GLY:N	2.36	0.47
2:L:156:LEU:HD22	2:L:195:LEU:HD13	1.97	0.47
2:D:67:LEU:HD21	2:D:71:VAL:HB	1.95	0.47
3:G:60:GLU:HA	4:I:296:VAL:HG23	1.97	0.47
3:G:66:GLU:HA	3:G:79:ILE:HG21	1.95	0.47
1:H:111(A):ALA:HA	4:K:262:ASN:OD1	2.13	0.47
2:D:39:LEU:HA	2:D:105:GLN:O	2.15	0.47
4:I:238:SER:HB3	4:K:249:THR:OG1	2.14	0.47
1:C:5:VAL:N	1:C:24:ALA:O	2.47	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:F:150:SER:HB2	4:F:151:GLY:HA2	1.97	0.47
3:E:90:VAL:HG22	4:F:292:ILE:HD11	1.96	0.47
3:E:36:THR:HG22	4:F:386:ILE:CG1	2.45	0.47
4:K:422:CYS:HB3	4:K:452:VAL:HG22	1.97	0.47
1:H:210:ILE:HG12	1:H:225:ARG:HG2	1.97	0.47
4:I:321:LEU:O	4:I:334:LEU:N	2.39	0.47
4:I:341:TRP:CZ2	4:I:360:VAL:HG21	2.50	0.47
4:F:506:ILE:HD11	4:K:178:VAL:HG11	1.97	0.47
4:K:267:THR:HB	2:L:109:THR:HG22	1.97	0.47
2:B:206:TYR:O	2:B:212:TYR:OH	2.30	0.47
4:F:337:THR:HG21	4:F:396:MET:HB2	1.97	0.47
4:I:231:LEU:HD23	4:I:231:LEU:HA	1.67	0.47
4:I:481:LEU:HD22	4:K:206:ILE:HG13	1.96	0.47
2:B:165:LYS:HB3	2:B:217:THR:OG1	2.15	0.47
4:F:153:ALA:HB1	4:F:156:LYS:HB3	1.97	0.46
1:C:107:ARG:HA	1:C:116:ASP:OD1	2.15	0.46
3:E:50:THR:HB	4:I:457:TYR:HA	1.98	0.46
4:K:485:SER:O	4:K:489:ASP:N	2.42	0.46
2:D:206:TYR:O	2:D:212:TYR:OH	2.31	0.46
4:I:160:LEU:HD21	4:K:161:GLU:HB2	1.96	0.46
2:L:14:SER:OG	2:L:127:LYS:HB2	2.16	0.46
2:D:99:PHE:CZ	2:D:126:ILE:HG23	2.50	0.46
3:E:44:TYR:HB2	4:F:313:CYS:HB2	1.98	0.46
4:F:226:LYS:HE2	3:J:81:GLN:HE22	1.79	0.46
4:I:171:LEU:HG	4:I:171:LEU:O	2.15	0.46
4:I:318:THR:CG2	4:I:336:ARG:HB2	2.45	0.46
4:I:334:LEU:HD22	4:I:395:ILE:HD13	1.97	0.46
4:F:404:SER:HB3	4:K:374:THR:HG21	1.97	0.46
4:K:268:ASN:HB2	2:L:108:ASN:O	2.16	0.46
2:B:127:LYS:HA	2:B:160:TYR:OH	2.16	0.46
2:B:215:GLU:HG2	2:B:226:THR:OG1	2.16	0.46
4:F:266:ILE:HD12	4:F:270:GLN:CB	2.46	0.46
4:K:474:ILE:HG12	4:K:474:ILE:H	1.52	0.46
3:E:37:CYS:SG	4:F:319:SER:HB3	2.55	0.46
4:F:152:VAL:HG11	4:I:152:VAL:CG2	2.45	0.46
1:H:181:PHE:CZ	2:L:196:SER:HB3	2.51	0.45
4:I:195:LEU:HD23	4:I:195:LEU:HA	1.68	0.45
4:I:252:LEU:O	4:I:282:ARG:NH1	2.45	0.45
3:J:36:THR:HG22	4:K:386:ILE:HG12	1.97	0.45
2:L:41:TRP:CE2	2:L:89:LEU:HB2	2.50	0.45
2:B:213:ALA:HB2	2:B:228:SER:HB3	1.97	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:109:THR:HG22	2:D:113:TYR:HD2	1.82	0.45
2:L:43:GLN:O	2:L:51:LYS:N	2.41	0.45
4:F:346:ALA:HB2	4:I:455:THR:HG23	1.97	0.45
4:K:297:LEU:HD12	4:K:298:ALA:H	1.82	0.45
4:K:352:PHE:CE1	4:K:372:SER:HB3	2.52	0.45
2:D:128:ARG:NH1	2:D:192:THR:HG23	2.31	0.45
4:F:334:LEU:HD22	4:F:395:ILE:HD13	1.99	0.45
1:H:183:ALA:HA	1:H:193:LEU:HB3	1.98	0.45
2:B:39:LEU:HA	2:B:105:GLN:O	2.16	0.45
4:F:161:GLU:HG3	4:K:160:LEU:HD11	1.99	0.45
3:G:64:ILE:HG22	4:K:474:ILE:HG13	1.98	0.45
4:F:476:ASN:ND2	3:J:67:ASN:HB2	2.32	0.45
4:K:191:LYS:HA	4:K:191:LYS:HD3	1.59	0.45
2:B:128:ARG:NH1	2:B:192:THR:HG23	2.32	0.45
2:D:96:PRO:HA	2:D:99:PHE:CE2	2.51	0.45
1:C:6:GLU:OE2	1:C:103:TYR:HA	2.17	0.45
4:I:219:THR:OG1	4:K:476:ASN:HB3	2.17	0.45
3:E:97:MET:O	3:E:98:GLN:HG3	2.17	0.45
4:K:508:LYS:O	4:K:512:LEU:HD13	2.15	0.45
4:I:351:PHE:O	4:I:353:PRO:HD3	2.17	0.44
3:J:44:TYR:HB2	4:K:313:CYS:HB2	1.99	0.44
4:K:352:PHE:CD1	4:K:372:SER:HB3	2.52	0.44
1:H:184:VAL:HG11	2:L:180:GLN:HB3	1.99	0.44
2:L:151:SER:HA	2:L:199:LEU:O	2.16	0.44
4:F:252:LEU:CD2	4:F:301:VAL:HG11	2.48	0.44
4:F:476:ASN:HB3	4:K:219:THR:OG1	2.16	0.44
1:H:45:ALA:HB3	1:H:48:LYS:HB2	1.99	0.44
1:A:66:TYR:CE1	2:B:113:TYR:HD1	2.36	0.44
1:H:181:PHE:HA	2:L:184:THR:HG22	1.99	0.44
1:A:44:GLN:HG3	1:A:49:GLY:O	2.17	0.44
1:A:103:TYR:CE1	2:B:49:ALA:HA	2.53	0.44
1:C:67:TYR:OH	1:C:78:ILE:HG22	2.17	0.44
1:H:12:LEU:HA	1:H:125:THR:O	2.16	0.44
1:C:75:ARG:HB3	1:C:92:ASN:O	2.17	0.44
4:I:266:ILE:HD12	4:I:270:GLN:CB	2.45	0.44
4:I:386:ILE:HD13	4:I:395:ILE:CD1	2.48	0.44
1:H:186:GLN:HG2	2:L:180:GLN:OE1	2.18	0.44
1:H:150:THR:HB	1:H:199:VAL:O	2.18	0.44
4:F:150:SER:HB3	4:F:154:VAL:HG11	2.00	0.44
4:I:196:LYS:C	4:I:196:LYS:HD3	2.38	0.44
4:K:150:SER:HB2	4:K:151:GLY:HA2	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:F:455:THR:HG21	4:K:345:ASN:OD1	2.18	0.44
4:I:407:ILE:HD11	4:I:457:TYR:HB3	1.99	0.44
4:F:252:LEU:HD22	4:F:301:VAL:HG21	1.99	0.43
4:F:497:GLU:O	4:F:497:GLU:HG2	2.17	0.43
4:I:290:SER:HB3	4:I:300:VAL:HG23	2.00	0.43
1:A:36:SER:HA	4:I:465:LYS:HZ2	1.81	0.43
1:C:57:TYR:HE1	1:C:112:THR:HG21	1.83	0.43
2:D:67:LEU:CD2	2:D:71:VAL:HB	2.48	0.43
4:F:499:ILE:HD11	4:K:185:VAL:HG12	2.00	0.43
4:I:309:ILE:CG2	4:I:310:ASP:N	2.80	0.43
3:J:68:LYS:O	3:J:69:CYS:HB3	2.17	0.43
2:B:43:GLN:HB2	2:B:53:LEU:HD21	2.00	0.43
4:F:235:ARG:NH1	4:I:232:GLU:OE2	2.51	0.43
4:I:416:CYS:O	4:I:437:ASN:HA	2.18	0.43
1:C:116:ASP:OD1	1:C:116:ASP:N	2.51	0.43
1:C:165:VAL:HG23	1:C:215:HIS:HB2	2.00	0.43
3:J:48:LEU:O	3:J:50:THR:HG23	2.18	0.43
3:J:49:ARG:NH1	3:J:52:TRP:NE1	2.67	0.43
1:A:183:ALA:HB2	1:A:193:LEU:HD23	1.99	0.43
2:D:38:TRP:HZ2	4:I:268:ASN:O	1.97	0.43
1:H:212:ASN:ND2	1:H:223:ASP:OD1	2.51	0.43
4:F:161:GLU:CA	4:K:160:LEU:HD21	2.49	0.43
1:A:6:GLU:CD	1:A:121:GLY:H	2.22	0.43
4:F:195:LEU:HA	4:F:195:LEU:HD23	1.57	0.43
3:G:38:SER:HB3	4:I:318:THR:HG22	2.00	0.43
1:H:57:TYR:HE1	1:H:112:THR:HG21	1.83	0.43
4:K:252:LEU:HA	4:K:252:LEU:HD12	1.81	0.43
2:B:109:THR:HG22	4:F:267:THR:HA	2.01	0.43
2:B:1:ASP:HB3	2:B:115:TRP:CD2	2.54	0.43
2:B:44:GLN:O	2:B:100:ALA:HB1	2.18	0.43
1:C:13:ILE:HD12	1:C:14:GLN:H	1.84	0.43
4:I:477:PHE:CD2	4:I:477:PHE:C	2.91	0.43
1:A:111(A):ALA:HA	4:F:262:ASN:OD1	2.18	0.43
1:A:207:GLN:HB3	1:A:209:TYR:CZ	2.54	0.43
4:F:217:ILE:HD13	4:I:217:ILE:CG2	2.49	0.43
4:F:217:ILE:HD11	4:I:218:GLU:HG3	2.00	0.43
3:J:46:SER:OG	4:K:311:THR:HB	2.19	0.43
2:B:128:ARG:HH12	2:B:192:THR:HG23	1.84	0.43
2:D:43:GLN:O	2:D:51:LYS:N	2.45	0.43
3:E:81:GLN:HE22	4:I:226:LYS:HE2	1.84	0.42
4:F:364:ARG:HD3	4:F:364:ARG:HA	1.78	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:K:481:LEU:HD12	4:K:481:LEU:HA	1.70	0.42
1:C:6:GLU:OE1	1:C:120:GLN:N	2.53	0.42
2:D:175:GLN:HB3	2:D:178:ASN:OD1	2.19	0.42
3:E:83:LEU:HA	3:E:83:LEU:HD23	1.84	0.42
1:A:114:ASP:O	1:A:115:LEU:HD13	2.19	0.42
4:F:483:PHE:HD1	4:I:198:TYR:CE2	2.38	0.42
3:E:93:LEU:HD11	4:F:238:SER:OG	2.20	0.42
4:K:181:LEU:O	4:K:181:LEU:HG	2.20	0.42
4:K:410:LEU:HA	4:K:444:ASN:ND2	2.34	0.42
3:G:30:GLU:HG3	3:G:40:VAL:O	2.20	0.42
1:H:67:TYR:CE1	1:H:78:ILE:HG22	2.54	0.42
1:H:161:PHE:HA	1:H:162:PRO:HA	1.81	0.42
1:H:50:LEU:O	2:L:118:PHE:HB2	2.20	0.42
2:L:160:TYR:CD2	2:L:161:PRO:HA	2.55	0.42
2:L:204:ALA:O	2:L:208:LYS:HG3	2.19	0.42
4:F:375:LEU:HD13	4:F:379:VAL:HG11	2.02	0.42
1:A:116:ASP:OD1	1:A:116:ASP:N	2.50	0.42
1:H:23:CYS:HB3	1:H:87:LEU:HD23	2.00	0.42
4:I:217:ILE:HD13	4:K:217:ILE:HG21	2.02	0.42
4:I:273:LEU:HD11	4:I:364:ARG:HG2	2.02	0.42
2:L:99:PHE:CZ	2:L:126:ILE:HG23	2.55	0.42
2:D:71:VAL:HG12	2:D:72:PRO:HD2	2.01	0.42
1:H:114:ASP:O	1:H:115:LEU:HD13	2.20	0.42
4:I:203:LEU:HG	4:I:203:LEU:O	2.19	0.42
4:I:264:MET:O	4:I:266:ILE:N	2.53	0.42
1:H:39:MET:HB2	1:H:87:LEU:HD13	2.02	0.41
4:I:264:MET:HE3	4:I:266:ILE:CD1	2.49	0.41
4:I:334:LEU:HA	4:I:334:LEU:HD23	1.65	0.41
3:J:83:LEU:HA	3:J:83:LEU:HD23	1.85	0.41
1:A:37:LYS:HD3	1:A:107:ARG:O	2.19	0.41
2:B:181:GLU:HG2	2:B:197:SER:HB2	2.02	0.41
4:F:455:THR:HG23	4:K:346:ALA:HB2	2.02	0.41
1:H:200:PRO:HG2	1:H:203:SER:OG	2.21	0.41
4:I:150:SER:HB2	4:I:151:GLY:HA2	2.02	0.41
4:I:400:THR:HG22	4:I:401:ASP:N	2.35	0.41
4:F:191:LYS:HA	4:F:191:LYS:HD3	1.68	0.41
4:F:503:LEU:HA	4:F:503:LEU:HD23	1.85	0.41
3:E:65:LYS:HE2	4:I:475:ILE:HD11	2.02	0.41
3:J:33:TYR:O	3:J:37:CYS:N	2.53	0.41
4:K:400:THR:HG22	4:K:401:ASP:H	1.85	0.41
2:D:41:TRP:CD2	2:D:89:LEU:HB2	2.56	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:G:37:CYS:SG	4:I:319:SER:HB3	2.61	0.41
4:I:505:PHE:CB	4:K:177:ALA:HB2	2.50	0.41
2:B:41:TRP:CD2	2:B:89:LEU:HB2	2.55	0.41
2:D:6:GLN:HB2	2:D:120:GLN:NE2	2.35	0.41
2:D:217:THR:HG22	2:D:224:PRO:HG3	2.02	0.41
4:F:208:ASN:HD21	4:I:481:LEU:H	1.69	0.41
4:K:198:TYR:O	4:K:202:GLN:HB2	2.20	0.41
2:B:21:ILE:HD13	2:B:122:THR:HB	2.03	0.41
4:K:232:GLU:O	4:K:233:ILE:C	2.59	0.41
4:K:315:LYS:HD2	4:K:341:TRP:CZ2	2.55	0.41
4:I:204:LEU:CD2	4:K:481:LEU:HB3	2.51	0.41
4:K:158:LEU:HD23	4:K:161:GLU:OE2	2.21	0.41
3:J:45:LEU:HA	4:K:311:THR:O	2.20	0.41
4:F:166:LYS:HZ2	4:K:514:GLY:HA3	1.83	0.41
3:E:53:TYR:CD2	4:F:264:MET:HG2	2.56	0.41
4:F:400:THR:HG22	4:F:401:ASP:N	2.36	0.41
1:A:45:ALA:HB3	1:A:48:LYS:HB2	2.03	0.41
1:C:137:PHE:HB3	2:D:141:SER:OG	2.21	0.41
2:D:190:ASP:OD1	2:D:191:SER:N	2.54	0.41
4:F:252:LEU:HD22	4:F:301:VAL:HG11	2.02	0.41
2:L:140:PRO:HD3	2:L:152:VAL:HG22	2.02	0.41
2:L:126:ILE:HD12	2:L:191:SER:HB3	2.03	0.41
1:A:131:THR:HG21	1:A:217:PRO:O	2.21	0.41
4:F:261:ILE:HA	4:F:264:MET:HE2	2.03	0.41
1:H:153:LEU:HB2	1:H:226:VAL:HG11	2.03	0.41
4:K:321:LEU:HB3	4:K:334:LEU:HB2	2.03	0.41
4:K:334:LEU:HD13	4:K:386:ILE:HD12	2.03	0.41
2:B:98:ASP:HB3	2:B:102:TYR:OH	2.20	0.41
1:C:138:PRO:O	2:D:141:SER:HB3	2.21	0.41
1:H:153:LEU:HD21	1:H:209:TYR:CD2	2.56	0.41
4:K:273:LEU:HD11	4:K:364:ARG:HG2	2.03	0.41
2:B:168:TRP:CE2	2:B:199:LEU:HB2	2.57	0.40
4:F:334:LEU:HD23	4:F:334:LEU:HA	1.82	0.40
4:F:505:PHE:CB	4:I:177:ALA:HB2	2.51	0.40
4:I:191:LYS:HD3	4:I:191:LYS:HA	1.78	0.40
4:F:181:LEU:HD23	4:K:181:LEU:CD2	2.51	0.40
1:A:181:PHE:CD2	2:B:184:THR:HG23	2.57	0.40
2:D:128:ARG:NH2	2:D:129:THR:O	2.51	0.40
2:D:83:SER:HA	2:D:87:PHE:CE1	2.56	0.40
4:F:378:GLU:OE1	4:I:400:THR:HG21	2.22	0.40
4:K:503:LEU:HD23	4:K:503:LEU:HA	1.84	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:107:ARG:HA	1:A:116:ASP:OD1	2.21	0.40
2:B:38:TRP:CE2	4:F:268:ASN:HB3	2.56	0.40
1:C:215:HIS:ND1	1:C:218:SER:OG	2.49	0.40
2:D:7:SER:OG	2:D:22:THR:OG1	2.39	0.40
4:F:341:TRP:CZ3	4:F:365:VAL:HG21	2.56	0.40
4:I:167:ILE:CD1	4:K:164:VAL:HG13	2.52	0.40
4:I:386:ILE:HD13	4:I:395:ILE:HD12	2.04	0.40
2:L:181:GLU:CD	2:L:195:LEU:HD21	2.41	0.40
1:H:6:GLU:HA	1:H:22:SER:O	2.21	0.40
4:I:320:PRO:HA	4:I:334:LEU:O	2.21	0.40
2:B:106:GLN:HE21	2:B:117:THR:N	2.19	0.40
1:C:52:TRP:HB3	2:D:116:TRP:O	2.22	0.40
4:F:477:PHE:CD2	4:F:477:PHE:C	2.94	0.40
4:F:160:LEU:HD21	4:I:161:GLU:HB2	2.03	0.40
3:G:53:TYR:CE1	4:K:464:GLY:HA3	2.56	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:14:GLN:OE1	1:C:20:ARG:NH1[8_554]	2.13	0.07

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	218/224 (97%)	198 (91%)	20 (9%)	0	100	100
1	C	218/224 (97%)	199 (91%)	19 (9%)	0	100	100
1	H	218/224 (97%)	199 (91%)	19 (9%)	0	100	100
2	B	213/218 (98%)	198 (93%)	15 (7%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
2	D	213/218 (98%)	198 (93%)	13 (6%)	2 (1%)	21 67
2	L	213/218 (98%)	198 (93%)	15 (7%)	0	100 100
3	E	71/73 (97%)	65 (92%)	5 (7%)	1 (1%)	14 59
3	G	71/73 (97%)	65 (92%)	5 (7%)	1 (1%)	14 59
3	J	71/73 (97%)	65 (92%)	5 (7%)	1 (1%)	14 59
4	F	354/394 (90%)	333 (94%)	21 (6%)	0	100 100
4	I	354/394 (90%)	334 (94%)	20 (6%)	0	100 100
4	K	354/394 (90%)	332 (94%)	21 (6%)	1 (0%)	46 82
All	All	2568/2727 (94%)	2384 (93%)	178 (7%)	6 (0%)	52 86

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	G	69	CYS
3	J	69	CYS
3	E	69	CYS
4	K	153	ALA
2	D	233	GLU
2	D	231	ARG

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	183/187 (98%)	178 (97%)	5 (3%)	52 80
1	C	183/187 (98%)	174 (95%)	9 (5%)	31 69
1	H	183/187 (98%)	177 (97%)	6 (3%)	45 78
2	B	190/193 (98%)	187 (98%)	3 (2%)	70 88
2	D	190/193 (98%)	183 (96%)	7 (4%)	41 75
2	L	190/193 (98%)	187 (98%)	3 (2%)	70 88
3	E	66/66 (100%)	63 (96%)	3 (4%)	34 71

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
3	G	66/66 (100%)	63 (96%)	3 (4%)	34 71
3	J	66/66 (100%)	63 (96%)	3 (4%)	34 71
4	F	329/362 (91%)	309 (94%)	20 (6%)	23 63
4	I	329/362 (91%)	306 (93%)	23 (7%)	19 59
4	K	329/362 (91%)	310 (94%)	19 (6%)	25 65
All	All	2304/2424 (95%)	2200 (96%)	104 (4%)	34 71

All (104) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	25	VAL
1	A	56	ILE
1	A	87	LEU
1	A	114	ASP
1	A	146	THR
2	B	39	LEU
2	B	107	TYR
2	B	115	TRP
1	C	29	THR
1	C	40	THR
1	C	56	ILE
1	C	82	ASN
1	C	87	LEU
1	C	103	TYR
1	C	114	ASP
1	C	128	SER
1	C	146	THR
2	D	39	LEU
2	D	107	TYR
2	D	109	THR
2	D	115	TRP
2	D	183	VAL
2	D	184	THR
2	D	186	GLN
3	E	30	GLU
3	E	88	ASN
3	E	90	VAL
4	F	148	ILE
4	F	154	VAL
4	F	195	LEU

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Mol	Chain	Res	Type
4	F	211	SER
4	F	244	THR
4	F	252	LEU
4	F	338	ASP
4	F	345	ASN
4	F	361	GLN
4	F	377	SER
4	F	398	SER
4	F	401	ASP
4	F	403	SER
4	F	422	CYS
4	F	449	THR
4	F	472	GLU
4	F	474	ILE
4	F	476	ASN
4	F	477	PHE
4	F	485	SER
3	G	30	GLU
3	G	88	ASN
3	G	90	VAL
1	H	25	VAL
1	H	29	THR
1	H	87	LEU
1	H	103	TYR
1	H	112(A)	THR
1	H	146	THR
4	I	195	LEU
4	I	204	LEU
4	I	211	SER
4	I	244	THR
4	I	252	LEU
4	I	255	SER
4	I	288	ILE
4	I	289	MET
4	I	338	ASP
4	I	345	ASN
4	I	361	GLN
4	I	377	SER
4	I	398	SER
4	I	401	ASP
4	I	403	SER
4	I	416	CYS

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Mol	Chain	Res	Type
4	I	422	CYS
4	I	440	ASP
4	I	472	GLU
4	I	474	ILE
4	I	476	ASN
4	I	477	PHE
4	I	485	SER
3	J	30	GLU
3	J	88	ASN
3	J	90	VAL
4	K	195	LEU
4	K	204	LEU
4	K	211	SER
4	K	234	THR
4	K	244	THR
4	K	252	LEU
4	K	288	ILE
4	K	338	ASP
4	K	361	GLN
4	K	377	SER
4	K	398	SER
4	K	401	ASP
4	K	403	SER
4	K	422	CYS
4	K	449	THR
4	K	474	ILE
4	K	476	ASN
4	K	477	PHE
4	K	485	SER
2	L	39	LEU
2	L	115	TRP
2	L	186	GLN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (12) such sidechains are listed below:

Mol	Chain	Res	Type
2	B	6	GLN
2	D	180	GLN
3	E	26	GLN
3	E	81	GLN
4	F	345	ASN
4	F	380	ASN

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Mol	Chain	Res	Type
3	G	26	GLN
3	G	81	GLN
4	I	225	GLN
3	J	26	GLN
3	J	81	GLN
2	L	6	GLN

5.3.3 RNA

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates

There are no carbohydrates in this entry.

5.6 Ligand geometry

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, 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	220/224 (98%)	0.32	16 (7%) 18 13	125, 169, 259, 296	0
1	C	220/224 (98%)	-0.04	5 (2%) 64 53	71, 108, 207, 239	0
1	H	220/224 (98%)	1.54	65 (29%) 1 1	162, 259, 353, 380	0
2	B	215/218 (98%)	0.51	11 (5%) 32 24	130, 208, 264, 282	0
2	D	215/218 (98%)	0.04	5 (2%) 64 53	86, 143, 209, 223	0
2	L	215/218 (98%)	1.79	87 (40%) 0 1	167, 277, 375, 387	0
3	E	73/73 (100%)	-0.18	0 100 100	82, 108, 139, 163	0
3	G	73/73 (100%)	-0.23	0 100 100	79, 102, 128, 162	0
3	J	73/73 (100%)	-0.29	0 100 100	86, 110, 143, 169	0
4	F	358/394 (90%)	-0.07	5 (1%) 78 68	74, 109, 145, 185	0
4	I	358/394 (90%)	-0.13	4 (1%) 82 75	72, 97, 137, 195	0
4	K	358/394 (90%)	-0.17	0 100 100	76, 99, 133, 170	0
All	All	2598/2727 (95%)	0.28	198 (7%) 17 12	71, 125, 323, 387	0

All (198) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
4	F	147	ALA	7.1
1	H	228	PRO	7.0
4	I	149	ALA	6.5
1	H	229	LYS	6.2
2	L	142	ASP	5.7
2	L	216	VAL	5.6
1	A	205	GLY	5.5
2	L	165	LYS	5.4
1	H	148	GLY	5.4
2	L	134	SER	5.3
1	H	227	GLU	5.3

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Mol	Chain	Res	Type	RSRZ
1	C	145	SER	5.2
2	L	132	ALA	5.1
2	L	166	VAL	5.0
2	L	210	LYS	5.0
2	L	176	SER	4.9
1	A	204	LEU	4.9
1	H	141	PRO	4.9
2	L	133	PRO	4.8
2	L	164	ALA	4.8
4	F	148	ILE	4.7
1	H	39	MET	4.5
2	L	220	GLY	4.5
1	H	136	VAL	4.5
1	A	229	LYS	4.4
2	L	175	GLN	4.3
2	L	78	GLY	4.2
2	L	219	GLN	4.1
1	H	230	SER	4.1
2	L	169	LYS	4.1
2	L	147	SER	4.1
2	L	76	PHE	4.1
1	H	223	ASP	4.0
2	L	23	CYS	4.0
2	L	217	THR	4.0
1	H	106	SER	3.9
1	A	147	SER	3.9
1	H	144	LYS	3.8
1	H	188	SER	3.7
2	L	230	ASN	3.7
1	H	91	MET	3.7
2	L	204	ALA	3.7
1	H	167	VAL	3.6
2	B	127	LYS	3.6
2	B	18	ARG	3.6
2	L	13	ALA	3.6
4	I	148	ILE	3.6
2	L	229	PHE	3.6
1	H	20	ARG	3.6
1	H	143	SER	3.5
1	A	226	VAL	3.5
2	B	19	VAL	3.5
1	C	148	GLY	3.5

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Mol	Chain	Res	Type	RSRZ
2	L	137	ILE	3.5
2	L	198	THR	3.4
2	L	178	ASN	3.4
1	H	25	VAL	3.3
1	C	149	GLY	3.3
1	H	225	ARG	3.3
1	H	135	SER	3.3
1	H	209	TYR	3.3
4	I	151	GLY	3.3
2	L	170	VAL	3.3
2	L	221	LEU	3.3
1	H	40	THR	3.3
2	L	157	ASN	3.3
2	L	212	TYR	3.2
1	H	140	ALA	3.2
1	A	198	THR	3.2
2	L	140	PRO	3.2
2	L	141	SER	3.2
2	L	227	LYS	3.2
2	L	197	SER	3.1
1	H	187	SER	3.1
4	I	150	SER	3.1
2	L	138	PHE	3.1
1	H	194	SER	3.1
4	F	150	SER	3.1
1	H	92	ASN	3.1
1	H	152	ALA	3.0
2	L	201	LEU	3.0
2	L	145	LEU	3.0
2	L	228	SER	3.0
2	B	202	SER	3.0
1	H	196	VAL	3.0
1	H	180	THR	3.0
1	H	222	VAL	2.9
2	L	167	GLN	2.9
1	H	158	LYS	2.9
1	H	134	PRO	2.9
1	H	206	THR	2.9
2	B	91	ILE	2.9
1	H	197	VAL	2.9
2	L	102	TYR	2.9
2	L	215	GLU	2.9

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Mol	Chain	Res	Type	RSRZ
1	H	76	PHE	2.9
2	L	218	HIS	2.8
1	H	147	SER	2.8
1	H	174	LEU	2.8
2	L	162	ARG	2.8
2	L	203	LYS	2.8
1	H	210	ILE	2.8
2	B	232	GLY	2.7
2	L	183	VAL	2.7
2	L	234	CYS	2.7
1	H	226	VAL	2.7
2	L	122	THR	2.7
1	A	206	THR	2.7
1	H	19	LEU	2.7
1	A	230	SER	2.7
1	H	18	SER	2.7
1	C	146	THR	2.6
2	L	209	HIS	2.6
4	F	149	ALA	2.6
2	L	223	SER	2.6
2	D	169	LYS	2.6
2	L	206	TYR	2.6
1	A	231	CYS	2.6
1	H	7	SER	2.6
1	H	56	ILE	2.6
2	D	174	LEU	2.6
2	L	128	ARG	2.6
2	L	205	ASP	2.6
2	L	174	LEU	2.5
1	H	198	THR	2.5
2	L	211	VAL	2.5
2	L	39	LEU	2.5
2	L	150	ALA	2.4
2	L	130	VAL	2.4
1	A	208	THR	2.4
1	H	15	PRO	2.4
2	L	75	ARG	2.4
2	L	53	LEU	2.4
2	L	135	VAL	2.4
2	L	116	TRP	2.4
2	B	213	ALA	2.4
2	L	200	THR	2.4

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Mol	Chain	Res	Type	RSRZ
2	L	41	TRP	2.4
1	H	21	LEU	2.3
1	H	142	SER	2.3
2	L	124	VAL	2.3
1	H	105	ALA	2.3
2	B	135	VAL	2.3
2	L	226	THR	2.3
2	L	179	SER	2.3
2	D	201	LEU	2.3
2	L	168	TRP	2.3
1	A	228	PRO	2.3
2	L	54	ILE	2.3
2	L	163	GLU	2.3
1	H	124	VAL	2.3
1	H	78	ILE	2.3
2	L	151	SER	2.3
2	L	213	ALA	2.3
1	H	52	TRP	2.3
1	A	145	SER	2.3
1	H	204	LEU	2.2
1	H	88	TYR	2.2
2	L	181	GLU	2.2
1	A	141	PRO	2.2
1	H	120	GLN	2.2
1	H	208	THR	2.2
2	L	199	LEU	2.2
1	H	23	CYS	2.2
1	H	58	GLY	2.2
1	H	224	LYS	2.2
2	L	127	LYS	2.2
2	B	90	THR	2.2
2	L	105	GLN	2.2
1	H	87	LEU	2.1
2	L	19	VAL	2.1
1	H	186	GLN	2.1
2	L	224	PRO	2.1
2	D	167	GLN	2.1
2	L	18	ARG	2.1
2	L	57	ALA	2.1
1	C	143	SER	2.1
2	L	139	PRO	2.1
1	A	227	GLU	2.1

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Mol	Chain	Res	Type	RSRZ
2	B	181	GLU	2.1
1	A	225	ARG	2.1
1	H	175	THR	2.1
2	L	207	GLU	2.1
1	H	111(A)	ALA	2.1
2	L	173	ALA	2.1
1	H	46	PRO	2.1
1	A	144	LYS	2.1
1	H	211	CYS	2.1
2	D	212	TYR	2.1
2	L	231	ARG	2.0
2	B	219	GLN	2.0
2	L	91	ILE	2.0
2	L	4	MET	2.0
4	F	414	VAL	2.0
1	H	96	ALA	2.0
2	L	117	THR	2.0
1	H	79	SER	2.0
2	L	136	PHE	2.0

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

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

6.3 Carbohydrates (i)

There are no carbohydrates in this entry.

6.4 Ligands (i)

There are no ligands in this entry.

6.5 Other polymers (i)

There are no such residues in this entry.