Full wwPDB X-ray Structure Validation Report ⓘ

Aug 23, 2023 – 02:11 PM JST

PDB ID	:	8JJ6
Title	:	Structure of the NELF-BCE complex
Authors	:	Wang, Z.; Cao, Y.; Qin, Y.
Deposited on	:	2023-05-29
Resolution	:	2.72 Å(reported)

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

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

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

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

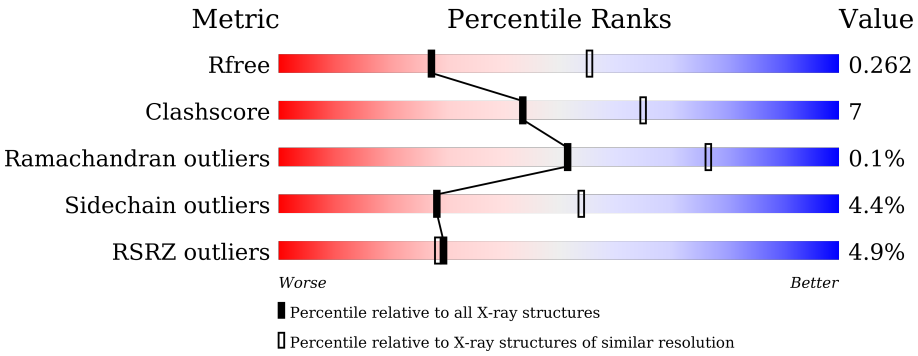
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.35
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35

1 Overall quality at a glance

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.72 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	3359 (2.74-2.70)
Clashscore	141614	3686 (2.74-2.70)
Ramachandran outliers	138981	3622 (2.74-2.70)
Sidechain outliers	138945	3623 (2.74-2.70)
RSRZ outliers	127900	3276 (2.74-2.70)

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	560	3% 82% 15% ••
1	B	560	4% 82% 16% ••
2	C	147	7% 80% 18% ••
2	D	147	8% 74% 24% ••
3	E	51	10% 51% 8% • 39%
3	F	51	8% 49% 10% • 39%

2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 11833 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 Negative elongation factor B.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	554	Total	C	N	O	S	0	0	0
			4438	2844	755	814	25			
1	B	554	Total	C	N	O	S	0	0	0
			4438	2844	755	814	25			

- Molecule 2 is a protein called Negative elongation factor complex member C/D.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	D	146	Total	C	N	O	S	0	0	0
			1179	752	193	229	5			
2	C	146	Total	C	N	O	S	0	0	0
			1179	752	193	229	5			

- Molecule 3 is a protein called NELF-E.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	E	31	Total	C	N	O	S	0	0	0
			246	162	40	41	3			
3	F	31	Total	C	N	O	S	0	0	0
			246	162	40	41	3			

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	48	Total	O	0	0
			48	48		
4	D	7	Total	O	0	0
			7	7		
4	B	41	Total	O	0	0
			41	41		
4	C	9	Total	O	0	0
			9	9		

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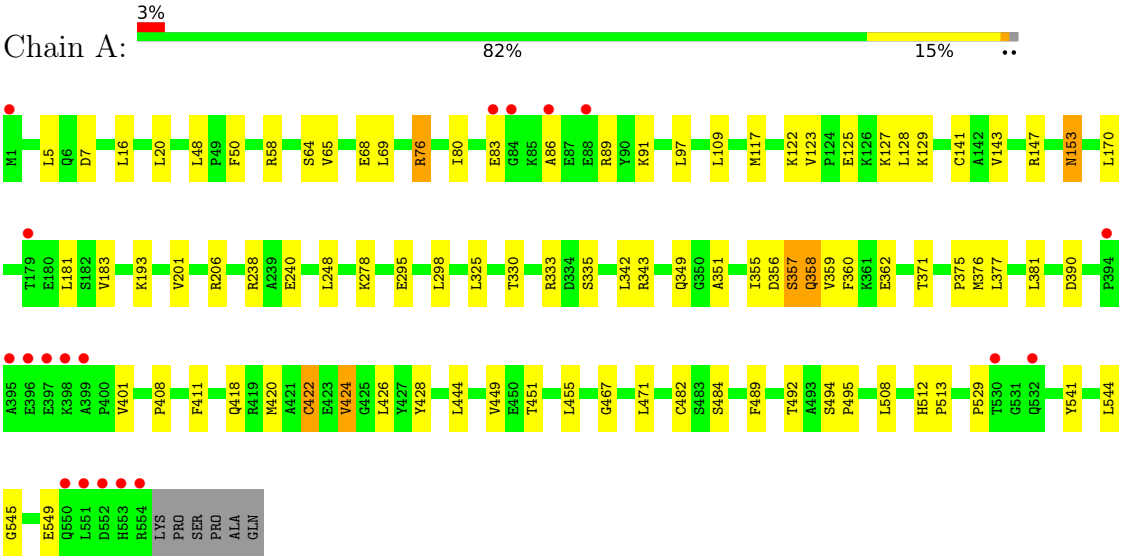
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	E	1	Total O 1 1	0	0
4	F	1	Total O 1 1	0	0

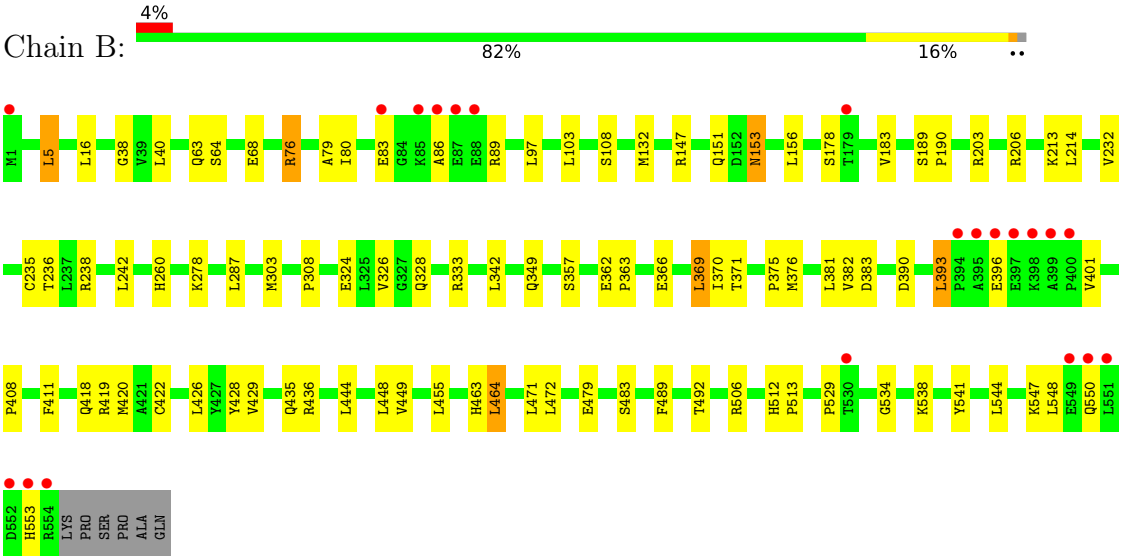
3 Residue-property plots (i)

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: Negative elongation factor B

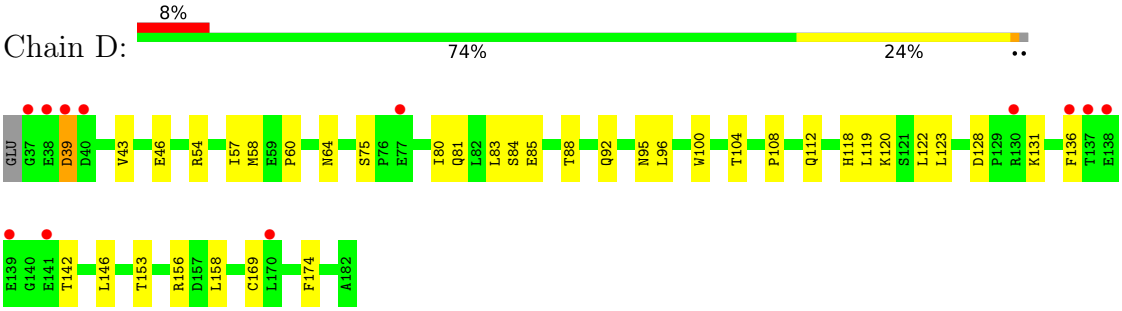


• Molecule 1: Negative elongation factor B



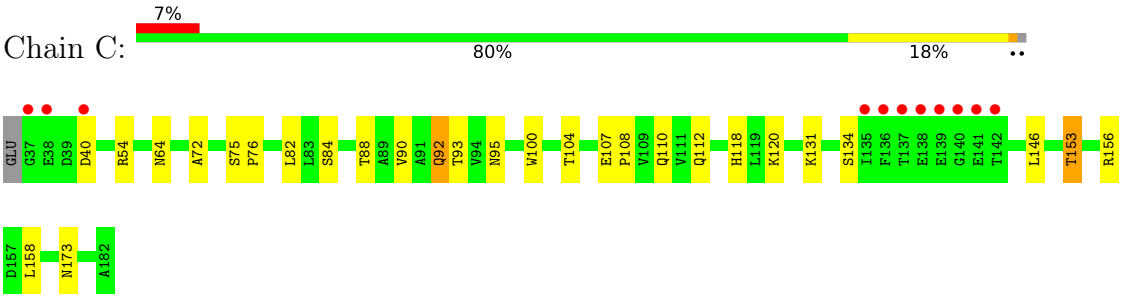
• Molecule 2: Negative elongation factor complex member C/D

Chain D:



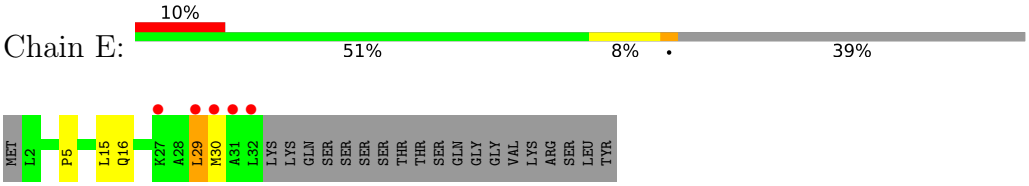
• Molecule 2: Negative elongation factor complex member C/D

Chain C:



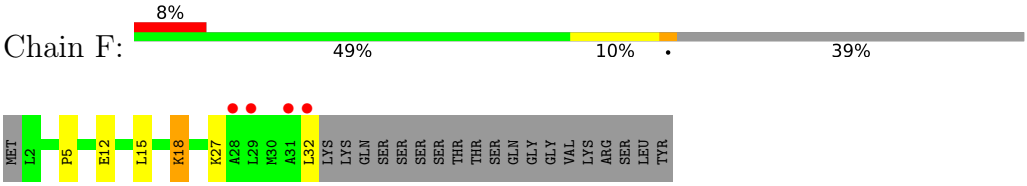
• Molecule 3: NELF-E

Chain E:



• Molecule 3: NELF-E

Chain F:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, α, β, γ	156.61Å 166.71Å 75.03Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	37.51 – 2.72 37.51 – 2.72	Depositor EDS
% Data completeness (in resolution range)	98.1 (37.51-2.72) 98.1 (37.51-2.72)	Depositor EDS
R_{merge}	0.29	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.71 (at 2.72Å)	Xtriage
Refinement program	PHENIX 1.13_2998, PHENIX 1.13_2998	Depositor
R, R_{free}	0.206 , 0.262 0.206 , 0.262	Depositor DCC
R_{free} test set	2565 reflections (4.87%)	wwPDB-VP
Wilson B-factor (Å^2)	41.5	Xtriage
Anisotropy	0.472	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.32 , 44.5	EDS
L-test for twinning[2]	$< \|L\| > = 0.52$, $< L^2 > = 0.35$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	11833	wwPDB-VP
Average B, all atoms (Å^2)	43.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 49.46 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 7.4402e-05. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

[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	0.47	1/4524 (0.0%)	0.60	0/6112
1	B	0.46	0/4524	0.60	1/6112 (0.0%)
2	C	0.45	0/1206	0.54	0/1640
2	D	0.46	0/1206	0.57	1/1640 (0.1%)
3	E	0.53	0/248	0.60	0/325
3	F	0.53	0/248	0.57	0/325
All	All	0.47	1/11956 (0.0%)	0.59	2/16154 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
2	D	0	1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	422	CYS	CB-SG	-5.19	1.73	1.81

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	D	58	MET	C-N-CA	-7.04	104.09	121.70
1	B	393	LEU	CA-CB-CG	5.03	126.86	115.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	D	39	ASP	Peptide

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	4438	0	4530	65	0
1	B	4438	0	4530	65	0
2	C	1179	0	1142	22	0
2	D	1179	0	1142	28	0
3	E	246	0	283	2	0
3	F	246	0	283	4	0
4	A	48	0	0	0	0
4	B	41	0	0	0	0
4	C	9	0	0	0	0
4	D	7	0	0	0	0
4	E	1	0	0	0	0
4	F	1	0	0	0	0
All	All	11833	0	11910	159	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 7.

All (159) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:76:ARG:NH1	2:C:104:THR:O	1.80	1.12
1:A:20:LEU:HB3	2:D:80:ILE:CD1	1.97	0.95
2:D:54:ARG:HH21	2:D:88:THR:HG21	1.42	0.85
1:B:449:VAL:HG13	1:B:492:THR:HG21	1.65	0.78
1:A:449:VAL:HG13	1:A:492:THR:HG21	1.68	0.76
1:A:20:LEU:CB	2:D:80:ILE:CD1	2.65	0.73
1:B:178:SER:O	1:B:506:ARG:NH2	2.18	0.71
1:B:390:ASP:HB3	1:B:401:VAL:HG11	1.72	0.70
1:A:512:HIS:CD2	1:A:513:PRO:HD3	2.27	0.68
1:A:50:PHE:CD2	2:D:123:LEU:HD21	2.30	0.67
1:A:381:LEU:HD11	1:A:428:TYR:HE1	1.60	0.67
1:B:383:ASP:OD2	3:F:18:LYS:HE3	1.94	0.67
2:C:54:ARG:NH2	2:C:88:THR:HG21	2.09	0.66
2:C:92:GLN:HA	2:C:95:ASN:HD22	1.61	0.65
1:B:76:ARG:NH1	2:C:104:THR:C	2.50	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:333:ARG:NH2	3:E:5:PRO:O	2.30	0.64
3:E:29:LEU:HD22	3:E:29:LEU:O	1.98	0.64
2:C:131:LYS:O	2:C:134:SER:OG	2.16	0.63
1:A:50:PHE:HD2	2:D:123:LEU:HD21	1.63	0.63
2:D:120:LYS:HG2	2:D:158:LEU:HD13	1.79	0.63
1:A:20:LEU:HB3	2:D:80:ILE:HD11	1.80	0.63
1:A:183:VAL:HG21	1:A:471:LEU:HD13	1.81	0.62
1:B:153:ASN:HD22	1:B:156:LEU:H	1.46	0.62
2:D:54:ARG:NH2	2:D:88:THR:HG21	2.15	0.61
2:C:40:ASP:HB3	2:C:72:ALA:HB1	1.83	0.61
1:A:20:LEU:HB3	2:D:80:ILE:HD13	1.80	0.60
2:C:100:TRP:O	2:C:104:THR:HG23	2.02	0.60
1:A:376:MET:HE3	1:A:408:PRO:HB2	1.84	0.59
1:B:382:VAL:HG21	3:F:18:LYS:HB3	1.86	0.58
1:B:151:GLN:HG2	1:B:213:LYS:HD3	1.84	0.58
1:B:76:ARG:HH11	2:C:104:THR:CB	2.16	0.58
2:D:108:PRO:O	2:D:112:GLN:HG3	2.03	0.57
1:A:343:ARG:NH1	1:A:362:GLU:OE2	2.38	0.56
1:B:544:LEU:O	1:B:548:LEU:HG	2.06	0.56
1:B:376:MET:HE1	1:B:411:PHE:N	2.22	0.55
1:B:435:GLN:O	1:B:436:ARG:HG2	2.06	0.55
1:B:512:HIS:NE2	1:B:548:LEU:HD23	2.22	0.55
1:B:436:ARG:HB2	1:B:472:LEU:HD21	1.89	0.55
1:A:20:LEU:CB	2:D:80:ILE:HD13	2.36	0.55
2:D:142:THR:HG21	2:D:174:PHE:CE2	2.42	0.55
1:A:147:ARG:NH1	1:A:206:ARG:O	2.40	0.54
1:B:333:ARG:NH2	3:F:5:PRO:O	2.39	0.54
1:B:76:ARG:NH1	1:B:80:ILE:HD11	2.23	0.54
1:B:76:ARG:NH1	2:C:104:THR:OG1	2.40	0.53
1:A:381:LEU:HD11	1:A:428:TYR:CE1	2.41	0.53
1:B:38:GLY:O	1:B:40:LEU:HD13	2.09	0.53
1:A:68:GLU:CD	2:D:118:HIS:HE1	2.13	0.53
1:A:122:LYS:HE2	1:A:125:GLU:OE2	2.09	0.52
2:D:153:THR:HG22	2:D:156:ARG:HH22	1.74	0.52
1:B:16:LEU:HD23	2:C:84:SER:HA	1.92	0.52
1:A:381:LEU:CD1	1:A:428:TYR:HE1	2.22	0.51
1:A:117:MET:HE3	1:A:123:VAL:HG11	1.91	0.51
1:A:428:TYR:HE2	1:A:444:LEU:CD1	2.23	0.51
1:B:63:GLN:OE1	2:C:54:ARG:NH1	2.44	0.51
1:B:376:MET:HE3	1:B:408:PRO:HB2	1.93	0.50
1:B:76:ARG:HD3	2:C:104:THR:OG1	2.12	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:79:ALA:O	1:B:83:GLU:HB2	2.11	0.49
1:B:5:LEU:HD13	1:B:103:LEU:HD11	1.94	0.49
2:C:120:LYS:HG2	2:C:158:LEU:HD13	1.95	0.49
2:D:153:THR:HG22	2:D:156:ARG:NH2	2.27	0.49
1:B:547:LYS:O	1:B:550:GLN:HG3	2.13	0.49
1:A:125:GLU:N	1:A:125:GLU:OE1	2.43	0.49
1:B:463:HIS:HD2	1:B:464:LEU:HD13	1.76	0.49
1:A:76:ARG:HG2	1:A:76:ARG:HH11	1.77	0.49
1:A:357:SER:HB2	1:B:278:LYS:HD2	1.94	0.48
1:B:376:MET:HE2	1:B:411:PHE:HB2	1.94	0.48
1:B:489:PHE:O	1:B:492:THR:HB	2.13	0.48
1:B:534:GLY:O	1:B:538:LYS:HG3	2.12	0.48
1:B:236:THR:OG1	1:B:308:PRO:HD2	2.14	0.48
1:A:125:GLU:O	1:A:129:LYS:HG3	2.13	0.48
1:A:420:MET:O	1:A:424:VAL:HG13	2.14	0.48
1:A:201:VAL:HG21	1:A:240:GLU:HB3	1.96	0.48
2:D:92:GLN:HA	2:D:95:ASN:HD22	1.79	0.47
1:A:86:ALA:O	1:A:89:ARG:HB3	2.15	0.47
1:B:76:ARG:NH1	2:C:104:THR:CB	2.77	0.47
1:B:86:ALA:HA	1:B:89:ARG:HE	1.80	0.47
1:B:479:GLU:O	1:B:483:SER:OG	2.29	0.46
1:A:181:LEU:HD22	1:A:467:GLY:HA2	1.96	0.46
1:A:428:TYR:HE2	1:A:444:LEU:HD13	1.81	0.46
1:A:58:ARG:HG3	2:D:60:PRO:HD3	1.98	0.46
1:B:147:ARG:HG3	1:B:214:LEU:CD1	2.46	0.46
1:B:429:VAL:HG21	1:B:448:LEU:HD11	1.97	0.46
1:A:76:ARG:HH12	2:D:104:THR:C	2.19	0.46
1:A:183:VAL:HG11	1:A:471:LEU:HD22	1.97	0.46
1:A:325:LEU:HD22	1:A:330:THR:HB	1.97	0.46
1:A:16:LEU:HD23	2:D:84:SER:HA	1.98	0.46
1:B:362:GLU:HG3	1:B:363:PRO:HD2	1.98	0.46
1:A:422:CYS:SG	1:A:451:THR:HB	2.56	0.45
1:A:489:PHE:O	1:A:492:THR:HB	2.16	0.45
1:B:512:HIS:CE1	1:B:547:LYS:HB3	2.52	0.45
1:B:147:ARG:NH1	1:B:206:ARG:O	2.50	0.45
1:A:508:LEU:HD23	1:A:508:LEU:HA	1.73	0.45
1:B:349:GLN:HE22	1:B:420:MET:HA	1.81	0.45
1:B:369:LEU:HD23	1:B:370:ILE:HD13	1.99	0.45
2:C:90:VAL:O	2:C:93:THR:HB	2.17	0.45
1:A:48:LEU:HD13	1:A:58:ARG:NH1	2.31	0.45
1:A:153:ASN:C	1:A:153:ASN:HD22	2.20	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:108:PRO:O	2:C:112:GLN:HG3	2.17	0.45
1:A:20:LEU:CB	2:D:80:ILE:HD12	2.47	0.44
1:A:80:ILE:O	1:A:89:ARG:HG3	2.16	0.44
1:B:366:GLU:HG2	1:B:418:GLN:HE22	1.82	0.44
1:A:295:GLU:O	1:A:298:LEU:HB2	2.17	0.44
1:A:545:GLY:O	1:A:549:GLU:HG3	2.17	0.44
1:B:324:GLU:O	1:B:328:GLN:HG3	2.17	0.44
2:D:92:GLN:HA	2:D:95:ASN:ND2	2.32	0.44
2:C:92:GLN:HA	2:C:92:GLN:HE21	1.83	0.44
2:C:54:ARG:HH21	2:C:88:THR:HG21	1.81	0.44
1:B:512:HIS:HE1	1:B:547:LYS:C	2.21	0.44
1:A:349:GLN:HE22	1:A:420:MET:HA	1.82	0.44
1:A:381:LEU:CD1	1:A:428:TYR:CE1	2.99	0.44
1:B:512:HIS:HB3	1:B:513:PRO:HD3	1.99	0.44
1:A:371:THR:O	1:A:375:PRO:HG2	2.18	0.44
1:B:472:LEU:HA	1:B:472:LEU:HD23	1.72	0.44
1:B:381:LEU:CD2	1:B:428:TYR:HE1	2.31	0.43
1:A:529:PRO:HD3	1:A:541:TYR:CD1	2.53	0.43
2:D:122:LEU:HD23	2:D:122:LEU:HA	1.80	0.43
2:D:57:ILE:HD13	2:D:83:LEU:HD13	1.99	0.43
1:B:371:THR:O	1:B:375:PRO:HG2	2.18	0.43
1:B:512:HIS:HE1	1:B:547:LYS:O	2.00	0.43
1:B:326:VAL:HG13	1:B:382:VAL:HG12	1.99	0.43
2:D:119:LEU:O	2:D:119:LEU:HD23	2.18	0.43
1:A:193:LYS:HE3	1:A:193:LYS:HB2	1.93	0.43
2:D:128:ASP:HB3	2:D:131:LYS:HG3	2.01	0.43
2:D:100:TRP:O	2:D:104:THR:HG23	2.19	0.42
1:B:183:VAL:HG11	1:B:471:LEU:HD11	2.01	0.42
1:B:235:CYS:SG	1:B:303:MET:HG3	2.60	0.42
1:A:351:ALA:O	1:A:355:ILE:HG12	2.20	0.42
1:A:83:GLU:O	1:A:89:ARG:HD3	2.20	0.42
1:B:455:LEU:HA	1:B:455:LEU:HD23	1.67	0.42
1:B:242:LEU:HD21	1:B:260:HIS:HA	2.02	0.42
2:D:81:GLN:NE2	2:D:85:GLU:HG2	2.34	0.42
1:B:287:LEU:HD23	1:B:287:LEU:HA	1.80	0.41
1:B:232:VAL:CG2	1:B:308:PRO:HG3	2.50	0.41
1:A:377:LEU:HD23	1:A:377:LEU:HA	1.69	0.41
1:B:147:ARG:HG3	1:B:214:LEU:HD11	2.02	0.41
2:C:75:SER:HA	2:C:76:PRO:HD3	1.86	0.41
1:A:358:GLN:HB3	1:A:360:PHE:CE2	2.55	0.41
1:A:376:MET:HE1	1:A:411:PHE:HB2	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:494:SER:OG	1:A:495:PRO:HD3	2.21	0.41
1:A:544:LEU:HD23	1:A:544:LEU:HA	1.90	0.41
1:B:422:CYS:O	1:B:426:LEU:HG	2.20	0.41
1:A:390:ASP:HB3	1:A:401:VAL:HG11	2.02	0.41
1:A:422:CYS:O	1:A:426:LEU:HG	2.21	0.41
2:D:39:ASP:HB2	2:D:43:VAL:HG23	2.03	0.41
1:A:123:VAL:HB	1:A:128:LEU:HD21	2.03	0.41
1:A:248:LEU:HD23	1:A:248:LEU:HA	1.79	0.41
1:A:357:SER:O	1:A:359:VAL:N	2.51	0.41
1:B:512:HIS:ND1	1:B:547:LYS:HB3	2.36	0.41
1:A:143:VAL:O	1:A:147:ARG:HG3	2.21	0.41
1:B:529:PRO:HD3	1:B:541:TYR:CD1	2.56	0.41
1:B:68:GLU:OE1	2:C:118:HIS:CE1	2.73	0.40
1:B:333:ARG:HD2	3:F:12:GLU:OE2	2.21	0.40
1:B:444:LEU:HD13	1:B:444:LEU:HA	1.93	0.40
2:C:153:THR:HB	2:C:156:ARG:NH1	2.36	0.40
1:A:325:LEU:HD21	1:A:335:SER:HB2	2.02	0.40
1:A:418:GLN:HE21	1:A:418:GLN:HB3	1.65	0.40
1:A:65:VAL:HG12	1:A:69:LEU:HD22	2.03	0.40
1:B:189:SER:N	1:B:190:PRO:HD2	2.36	0.40
2:C:107:GLU:HB3	2:C:110:GLN:HG2	2.04	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	552/560 (99%)	529 (96%)	21 (4%)	2 (0%)	34 58
1	B	552/560 (99%)	535 (97%)	17 (3%)	0	100 100
2	C	144/147 (98%)	142 (99%)	2 (1%)	0	100 100
2	D	144/147 (98%)	142 (99%)	2 (1%)	0	100 100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
3	E	29/51 (57%)	28 (97%)	1 (3%)	0	100 100
3	F	29/51 (57%)	29 (100%)	0	0	100 100
All	All	1450/1516 (96%)	1405 (97%)	43 (3%)	2 (0%)	51 77

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	358	GLN
1	A	356	ASP

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	495/500 (99%)	476 (96%)	19 (4%)	33 60
1	B	495/500 (99%)	478 (97%)	17 (3%)	37 65
2	C	130/131 (99%)	124 (95%)	6 (5%)	27 52
2	D	130/131 (99%)	123 (95%)	7 (5%)	22 45
3	E	27/45 (60%)	23 (85%)	4 (15%)	3 7
3	F	27/45 (60%)	23 (85%)	4 (15%)	3 7
All	All	1304/1352 (96%)	1247 (96%)	57 (4%)	28 54

All (57) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	5	LEU
1	A	7	ASP
1	A	64	SER
1	A	76	ARG
1	A	91	LYS
1	A	97	LEU
1	A	109	LEU
1	A	127	LYS

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Mol	Chain	Res	Type
1	A	141	CYS
1	A	153	ASN
1	A	170	LEU
1	A	238	ARG
1	A	278	LYS
1	A	342	LEU
1	A	357	SER
1	A	424	VAL
1	A	455	LEU
1	A	482	CYS
1	A	484	SER
2	D	46	GLU
2	D	64	ASN
2	D	75	SER
2	D	96	LEU
2	D	136	PHE
2	D	146	LEU
2	D	169	CYS
1	B	5	LEU
1	B	64	SER
1	B	76	ARG
1	B	97	LEU
1	B	108	SER
1	B	132	MET
1	B	153	ASN
1	B	203	ARG
1	B	238	ARG
1	B	342	LEU
1	B	357	SER
1	B	369	LEU
1	B	393	LEU
1	B	396	GLU
1	B	419	ARG
1	B	464	LEU
1	B	553	HIS
2	C	64	ASN
2	C	82	LEU
2	C	92	GLN
2	C	146	LEU
2	C	153	THR
2	C	173	ASN
3	E	15	LEU

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Mol	Chain	Res	Type
3	E	16	GLN
3	E	29	LEU
3	E	30	MET
3	F	15	LEU
3	F	18	LYS
3	F	27	LYS
3	F	32	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (33) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	6	GLN
1	A	22	ASN
1	A	119	HIS
1	A	153	ASN
1	A	349	GLN
1	A	510	HIS
1	A	512	HIS
1	A	524	GLN
1	A	550	GLN
2	D	44	GLN
2	D	81	GLN
2	D	86	ASN
2	D	118	HIS
2	D	126	HIS
1	B	6	GLN
1	B	54	HIS
1	B	119	HIS
1	B	151	GLN
1	B	153	ASN
1	B	154	GLN
1	B	220	GLN
1	B	321	HIS
1	B	323	GLN
1	B	349	GLN
1	B	388	ASN
1	B	439	ASN
1	B	512	HIS
1	B	532	GLN
2	C	64	ASN
2	C	92	GLN
2	C	112	GLN

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Mol	Chain	Res	Type
2	C	118	HIS
2	C	173	ASN

5.3.3 RNA

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates

There are no monosaccharides in this entry.

5.6 Ligand geometry

There are no ligands in this entry.

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
1	A	554/560 (98%)	-0.18	19 (3%)	45	45	19, 36, 73, 119	0
1	B	554/560 (98%)	-0.18	21 (3%)	40	40	19, 36, 76, 117	0
2	C	146/147 (99%)	0.14	11 (7%)	14	13	24, 47, 90, 116	0
2	D	146/147 (99%)	0.23	12 (8%)	11	10	24, 48, 87, 107	0
3	E	31/51 (60%)	0.30	5 (16%)	1	1	36, 49, 86, 89	0
3	F	31/51 (60%)	0.26	4 (12%)	3	3	35, 49, 89, 94	0
All	All	1462/1516 (96%)	-0.09	72 (4%)	29	28	19, 38, 82, 119	0

All (72) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	C	137	THR	9.2
1	A	554	ARG	9.0
1	B	551	LEU	8.5
2	D	37	GLY	7.9
2	D	137	THR	7.2
1	B	397	GLU	6.6
2	D	138	GLU	6.3
1	A	553	HIS	6.3
2	C	138	GLU	6.1
1	B	550	GLN	6.0
1	B	553	HIS	6.0
1	B	552	ASP	5.6
1	A	398	LYS	5.6
1	A	551	LEU	5.5
1	B	398	LYS	5.3
1	A	396	GLU	5.1
1	A	550	GLN	5.0
2	C	38	GLU	4.9
1	B	554	ARG	4.9

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Mol	Chain	Res	Type	RSRZ
1	A	395	ALA	4.7
2	C	37	GLY	4.6
1	A	399	ALA	4.1
1	A	552	ASP	4.1
2	D	39	ASP	4.0
3	E	32	LEU	3.8
2	C	139	GLU	3.8
1	A	394	PRO	3.7
1	A	397	GLU	3.7
2	D	77	GLU	3.4
1	B	179	THR	3.4
1	B	399	ALA	3.3
3	F	32	LEU	3.2
1	B	395	ALA	3.2
3	F	29	LEU	3.1
2	D	141	GLU	3.1
1	A	179	THR	3.0
2	D	139	GLU	3.0
1	B	1	MET	2.9
2	C	141	GLU	2.9
2	D	170	LEU	2.9
1	B	85	LYS	2.9
2	C	136	PHE	2.8
1	B	394	PRO	2.7
2	D	38	GLU	2.7
2	C	40	ASP	2.7
1	A	532	GLN	2.7
1	A	86	ALA	2.7
1	B	83	GLU	2.7
1	B	549	GLU	2.6
3	E	29	LEU	2.6
1	A	1	MET	2.5
3	F	31	ALA	2.5
2	D	136	PHE	2.5
1	B	530	THR	2.5
3	F	28	ALA	2.4
1	B	88	GLU	2.4
3	E	30	MET	2.4
2	D	40	ASP	2.4
2	C	140	GLY	2.4
1	A	530	THR	2.3
2	C	142	THR	2.3

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Mol	Chain	Res	Type	RSRZ
1	B	396	GLU	2.3
1	A	83	GLU	2.2
2	D	130	ARG	2.2
1	A	88	GLU	2.2
2	C	135	ILE	2.1
1	B	400	PRO	2.1
1	B	87	GLU	2.1
3	E	31	ALA	2.1
1	A	84	GLY	2.1
1	B	86	ALA	2.0
3	E	27	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)

There are no ligands in this entry.

6.5 Other polymers (i)

There are no such residues in this entry.