



Full wwPDB X-ray Structure Validation Report ⓘ

May 16, 2020 – 05:04 am BST

PDB ID : 1ONI
Title : Crystal structure of a human p14.5, a translational inhibitor reveals different mode of ligand binding near the invariant residues of the Yjgf/UK114 protein family
Authors : Manjasetty, B.A.; Delbrueck, H.; Mueller, U.; Erdmann, M.F.; Heinemann, U.
Deposited on : 2003-02-28
Resolution : 1.90 Å(reported)

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

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.11
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)	:	2.11

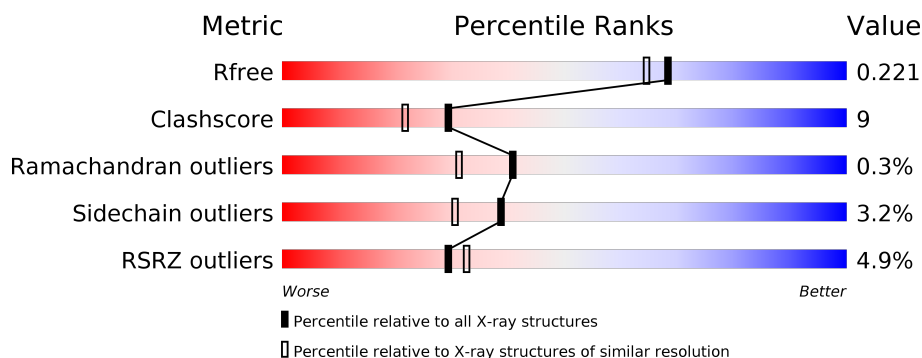
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.90 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	6207 (1.90-1.90)
Clashscore	141614	6847 (1.90-1.90)
Ramachandran outliers	138981	6760 (1.90-1.90)
Sidechain outliers	138945	6760 (1.90-1.90)
RSRZ outliers	127900	6082 (1.90-1.90)

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 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 $\leq 5\%$. 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	138	<div> <div>4%</div> <div> <div></div> <div>79%</div> <div>17%</div> <div>..</div> </div> </div>
1	B	138	<div> <div>4%</div> <div> <div></div> <div>81%</div> <div>14%</div> <div>..</div> </div> </div>
1	C	138	<div> <div>4%</div> <div> <div></div> <div>88%</div> <div>9%</div> <div>..</div> </div> </div>
1	D	138	<div> <div>6%</div> <div> <div></div> <div>84%</div> <div>12%</div> <div>..</div> </div> </div>
1	E	138	<div> <div>5%</div> <div> <div></div> <div>82%</div> <div>13%</div> <div>..</div> </div> </div>
1	F	138	<div> <div>5%</div> <div> <div></div> <div>83%</div> <div>12%</div> <div>..</div> </div> </div>

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Mol	Chain	Length	Quality of chain
1	G	138	
1	H	138	
1	I	138	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	BEZ	B	504	-	-	-	X
2	BEZ	H	515	-	-	X	-
2	BEZ	I	518	-	-	X	-

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 9553 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 14.5 kDa translational inhibitor protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	136	Total	C	N	O	S	6	2	0
			1015	641	174	197	3			
1	B	134	Total	C	N	O	S	5	0	0
			995	630	170	192	3			
1	C	134	Total	C	N	O	S	1	0	0
			995	630	170	192	3			
1	D	134	Total	C	N	O	S	0	0	0
			995	630	170	192	3			
1	E	134	Total	C	N	O	S	0	0	0
			995	630	170	192	3			
1	F	134	Total	C	N	O	S	0	0	0
			995	630	170	192	3			
1	G	134	Total	C	N	O	S	0	1	0
			998	631	171	193	3			
1	H	135	Total	C	N	O	S	0	0	0
			1001	633	171	194	3			
1	I	135	Total	C	N	O	S	0	1	0
			1004	634	172	195	3			

There are 18 discrepancies between the modelled and reference sequences:

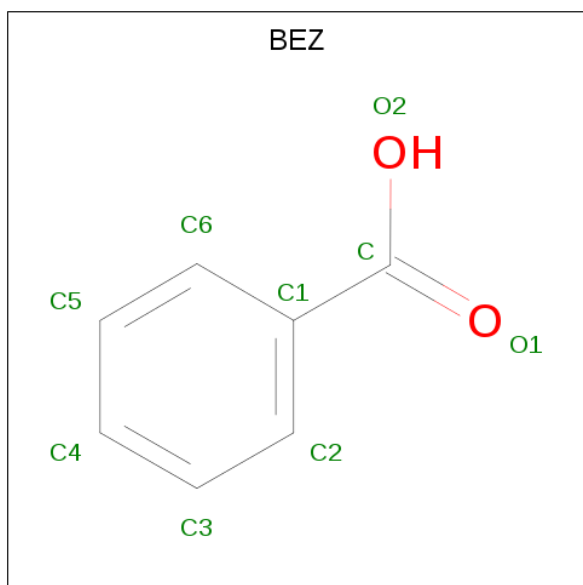
Chain	Residue	Modelled	Actual	Comment	Reference
A	0	GLY	-	CLONING ARTIFACT	UNP P52758
A	1	SER	-	CLONING ARTIFACT	UNP P52758
B	0	GLY	-	CLONING ARTIFACT	UNP P52758
B	1	SER	-	CLONING ARTIFACT	UNP P52758
C	0	GLY	-	CLONING ARTIFACT	UNP P52758
C	1	SER	-	CLONING ARTIFACT	UNP P52758
D	0	GLY	-	CLONING ARTIFACT	UNP P52758
D	1	SER	-	CLONING ARTIFACT	UNP P52758
E	0	GLY	-	CLONING ARTIFACT	UNP P52758
E	1	SER	-	CLONING ARTIFACT	UNP P52758
F	0	GLY	-	CLONING ARTIFACT	UNP P52758

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Chain	Residue	Modelled	Actual	Comment	Reference
F	1	SER	-	CLONING ARTIFACT	UNP P52758
G	0	GLY	-	CLONING ARTIFACT	UNP P52758
G	1	SER	-	CLONING ARTIFACT	UNP P52758
H	0	GLY	-	CLONING ARTIFACT	UNP P52758
H	1	SER	-	CLONING ARTIFACT	UNP P52758
I	0	GLY	-	CLONING ARTIFACT	UNP P52758
I	1	SER	-	CLONING ARTIFACT	UNP P52758

- Molecule 2 is BENZOIC ACID (three-letter code: BEZ) (formula: C₇H₆O₂).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	C	O	0	0
			9	7	2		
2	A	1	Total	C	O	0	0
			9	7	2		
2	B	1	Total	C	O	0	0
			9	7	2		
2	B	1	Total	C	O	0	0
			9	7	2		
2	C	1	Total	C	O	0	0
			9	7	2		
2	D	1	Total	C	O	0	0
			9	7	2		
2	D	1	Total	C	O	0	0
			9	7	2		
2	E	1	Total	C	O	0	0
			9	7	2		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	F	1	Total	C	O	0	0
			9	7	2		
2	G	1	Total	C	O	0	0
			9	7	2		
2	H	1	Total	C	O	0	0
			9	7	2		
2	I	1	Total	C	O	0	0
			9	7	2		
2	I	1	Total	C	O	0	0
			9	7	2		

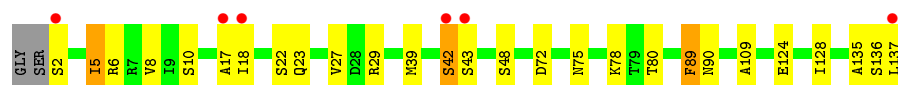
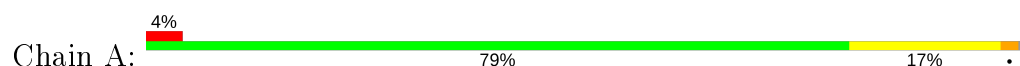
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	65	Total	O	0	0
			65	65		
3	B	58	Total	O	0	0
			58	58		
3	C	41	Total	O	0	0
			41	41		
3	D	64	Total	O	0	0
			64	64		
3	E	58	Total	O	0	0
			58	58		
3	F	55	Total	O	0	0
			55	55		
3	G	43	Total	O	0	0
			43	43		
3	H	24	Total	O	0	0
			24	24		
3	I	35	Total	O	0	0
			35	35		

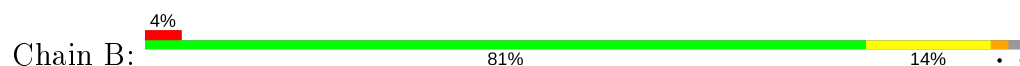
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of 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.

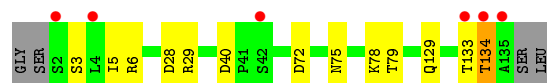
- Molecule 1: 14.5 kDa translational inhibitor protein



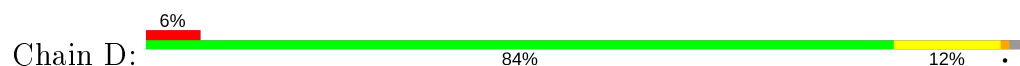
- Molecule 1: 14.5 kDa translational inhibitor protein



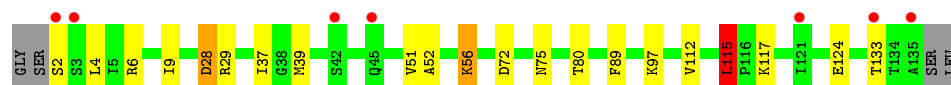
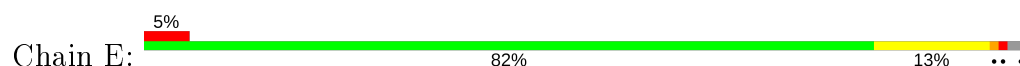
- Molecule 1: 14.5 kDa translational inhibitor protein



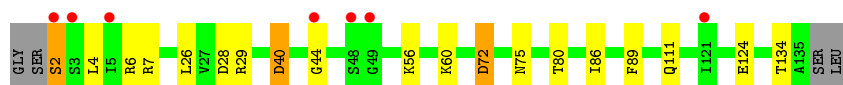
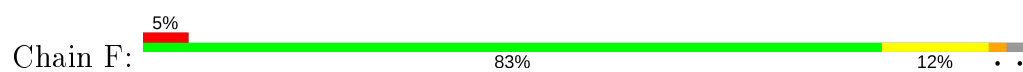
- Molecule 1: 14.5 kDa translational inhibitor protein



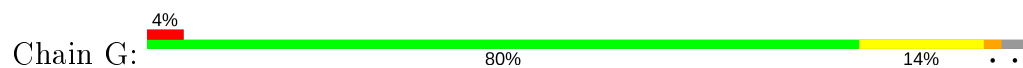
- Molecule 1: 14.5 kDa translational inhibitor protein



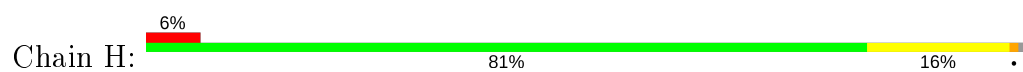
- Molecule 1: 14.5 kDa translational inhibitor protein



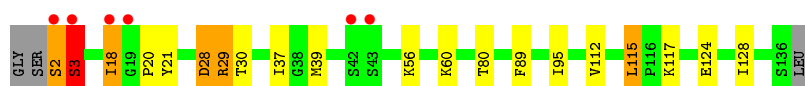
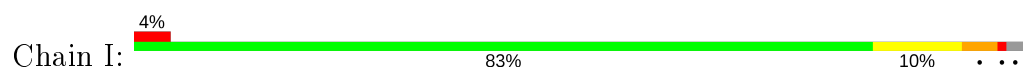
- Molecule 1: 14.5 kDa translational inhibitor protein



- Molecule 1: 14.5 kDa translational inhibitor protein



- Molecule 1: 14.5 kDa translational inhibitor protein



4 Data and refinement statistics

Property	Value	Source
Space group	P 31 2 1	Depositor
Cell constants a, b, c, α , β , γ	154.16Å 154.16Å 104.56Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	20.00 – 1.90 19.98 – 1.90	Depositor EDS
% Data completeness (in resolution range)	98.2 (20.00-1.90) 98.3 (19.98-1.90)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	0.08	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.95 (at 1.90Å)	Xtriage
Refinement program	REFMAC 5.0	Depositor
R, R_{free}	0.185 , 0.216 0.191 , 0.221	Depositor DCC
R_{free} test set	10758 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	30.8	Xtriage
Anisotropy	0.011	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 44.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.022 for -h,-k,l	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	9553	wwPDB-VP
Average B, all atoms (Å ²)	22.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.18% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ 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 ⓘ

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

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	0.65	0/1039	0.80	1/1409 (0.1%)
1	B	0.65	0/1009	0.86	5/1368 (0.4%)
1	C	0.62	0/1009	0.80	1/1368 (0.1%)
1	D	0.64	0/1009	0.82	2/1368 (0.1%)
1	E	0.67	0/1009	0.87	2/1368 (0.1%)
1	F	0.63	0/1009	0.84	2/1368 (0.1%)
1	G	0.65	1/1017 (0.1%)	0.83	2/1379 (0.1%)
1	H	0.53	0/1015	0.80	2/1376 (0.1%)
1	I	0.56	0/1023	0.80	2/1387 (0.1%)
All	All	0.62	1/9139 (0.0%)	0.82	19/12391 (0.2%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	G	130	GLY	CA-C	5.10	1.60	1.51

All (19) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	88	ASP	CB-CG-OD2	7.28	124.85	118.30
1	B	29	ARG	NE-CZ-NH2	-6.77	116.91	120.30
1	F	40	ASP	CB-CG-OD2	6.44	124.09	118.30
1	E	28	ASP	CB-CG-OD2	6.37	124.03	118.30
1	H	40	ASP	CB-CG-OD2	6.20	123.88	118.30
1	G	28	ASP	CB-CG-OD2	6.20	123.88	118.30
1	C	40	ASP	CB-CG-OD2	5.94	123.65	118.30
1	B	5	ILE	CB-CG1-CD1	-5.70	97.93	113.90
1	I	28	ASP	CB-CG-OD2	5.65	123.38	118.30
1	E	115	LEU	CB-CG-CD1	5.51	120.37	111.00
1	G	29	ARG	NE-CZ-NH2	-5.47	117.56	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	28	ASP	CB-CG-OD2	5.41	123.17	118.30
1	I	29	ARG	NE-CZ-NH1	-5.26	117.67	120.30
1	B	85	ASP	CB-CG-OD1	5.26	123.03	118.30
1	B	40	ASP	CB-CG-OD2	5.22	123.00	118.30
1	F	72	ASP	CB-CG-OD2	5.06	122.86	118.30
1	H	88	ASP	CB-CG-OD2	5.05	122.85	118.30
1	D	40	ASP	CB-CG-OD2	5.03	122.83	118.30
1	A	29	ARG	N-CA-CB	5.03	119.65	110.60

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1015	0	1041	22	0
1	B	995	0	1021	17	0
1	C	995	0	1021	14	0
1	D	995	0	1021	16	0
1	E	995	0	1021	21	0
1	F	995	0	1021	25	0
1	G	998	0	1023	24	0
1	H	1001	0	1026	19	0
1	I	1004	0	1028	24	0
2	A	18	0	10	1	0
2	B	18	0	10	3	0
2	C	9	0	5	3	0
2	D	18	0	10	1	0
2	E	9	0	5	3	0
2	F	9	0	5	1	0
2	G	9	0	5	0	0
2	H	9	0	5	9	0
2	I	18	0	10	4	0
3	A	65	0	0	0	0
3	B	58	0	0	3	0
3	C	41	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	D	64	0	0	0	0
3	E	58	0	0	4	0
3	F	55	0	0	2	0
3	G	43	0	0	2	0
3	H	24	0	0	0	0
3	I	35	0	0	3	0
All	All	9553	0	9288	174	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 9.

All (174) 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:H:515:BEZ:C	2:H:515:BEZ:C1	1.75	1.62
2:C:505:BEZ:C	2:C:505:BEZ:C1	1.76	1.56
2:E:509:BEZ:C	2:E:509:BEZ:C1	1.76	1.56
2:I:518:BEZ:C	2:I:518:BEZ:C1	1.77	1.54
2:B:504:BEZ:C1	2:B:504:BEZ:C	1.83	1.52
1:B:133:THR:HG23	1:C:5:ILE:HG12	1.53	0.91
1:D:56:LYS:HG2	1:D:60:LYS:HE3	1.53	0.89
1:C:28:ASP:O	1:C:29:ARG:HB2	1.76	0.86
1:G:93[A]:ASN:HD21	1:H:20:PRO:HG3	1.40	0.85
1:F:7:ARG:HD3	1:F:26:LEU:HD23	1.58	0.85
1:F:4:LEU:HD22	1:F:28:ASP:HB2	1.60	0.84
1:G:28:ASP:O	1:G:29:ARG:HB2	1.75	0.83
1:I:18:ILE:HG22	1:I:18:ILE:O	1.80	0.81
1:I:2:SER:O	1:I:3:SER:HB2	1.81	0.81
1:B:134:THR:HG22	1:C:6:ARG:HE	1.46	0.78
1:G:93[A]:ASN:HD21	1:H:20:PRO:CG	1.97	0.77
2:H:515:BEZ:C6	3:I:545:HOH:O	2.32	0.76
1:E:89:PHE:HZ	3:E:542:HOH:O	1.67	0.75
2:H:515:BEZ:H4	1:I:37:ILE:HG12	1.70	0.73
1:F:86:ILE:H	1:F:111:GLN:HE21	1.34	0.73
1:A:5:ILE:HA	1:C:133:THR:O	1.89	0.73
1:I:2:SER:O	1:I:3:SER:CB	2.38	0.72
1:I:18:ILE:H	1:I:21:TYR:HE1	1.38	0.71
1:H:18:ILE:O	1:H:18:ILE:HG13	1.88	0.71
1:I:18:ILE:O	1:I:18:ILE:CG2	2.39	0.71
1:D:29:ARG:NH2	1:F:2:SER:O	2.23	0.71
1:F:86:ILE:H	1:F:111:GLN:NE2	1.87	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:8:VAL:HG13	1:A:22:SER:HB3	1.73	0.69
1:E:80:THR:HB	1:E:124:GLU:HG2	1.75	0.69
1:B:72:ASP:H	1:B:75:ASN:HD22	1.42	0.67
1:I:112:VAL:HG21	1:I:115:LEU:HD13	1.76	0.67
1:D:29:ARG:NH2	1:F:4:LEU:HG	2.12	0.65
2:H:515:BEZ:C	2:H:515:BEZ:C2	2.69	0.65
1:C:72:ASP:H	1:C:75:ASN:HD22	1.43	0.65
1:G:52:ALA:O	1:G:56:LYS:HG3	1.96	0.65
1:C:28:ASP:O	1:C:29:ARG:CB	2.47	0.63
1:F:80:THR:HB	1:F:124:GLU:HG2	1.81	0.63
1:G:80:THR:HB	1:G:124:GLU:HG2	1.80	0.63
1:A:80:THR:HB	1:A:124:GLU:HG2	1.79	0.63
1:G:89:PHE:HE1	1:G:109:ALA:HB1	1.62	0.63
2:C:505:BEZ:C2	2:C:505:BEZ:C	2.71	0.63
1:E:72:ASP:H	1:E:75:ASN:HD22	1.47	0.61
1:H:86:ILE:H	1:H:111:GLN:NE2	1.98	0.61
1:H:97:LYS:HG3	1:I:20:PRO:HG3	1.82	0.61
1:A:128:ILE:HG13	1:B:27:VAL:HG21	1.80	0.61
1:E:39:MET:HE3	3:E:533:HOH:O	1.99	0.61
1:B:133:THR:HG23	1:C:5:ILE:CG1	2.29	0.60
1:E:6:ARG:HE	1:F:134:THR:HG22	1.67	0.60
1:F:89:PHE:HE2	3:F:565:HOH:O	1.83	0.60
1:E:112:VAL:HG21	1:E:115:LEU:HD13	1.83	0.60
1:E:2:SER:O	1:F:29:ARG:NH1	2.34	0.60
1:E:6:ARG:HE	1:F:134:THR:CG2	2.14	0.59
1:G:83:LEU:HD11	1:G:89:PHE:HD1	1.66	0.59
2:I:518:BEZ:C	2:I:518:BEZ:C2	2.73	0.59
1:B:120:ARG:HD3	3:B:517:HOH:O	2.02	0.59
1:G:78:LYS:NZ	3:G:531:HOH:O	2.35	0.59
1:F:28:ASP:O	1:F:29:ARG:HB2	2.04	0.58
1:D:2:SER:O	1:E:29:ARG:NH1	2.33	0.58
1:A:8:VAL:HG13	1:A:22:SER:CB	2.33	0.57
2:C:505:BEZ:C6	2:C:505:BEZ:C	2.72	0.57
1:I:80:THR:HB	1:I:124:GLU:HG2	1.86	0.57
1:A:72:ASP:H	1:A:75:ASN:HD22	1.53	0.56
2:B:504:BEZ:C6	2:B:504:BEZ:C	2.75	0.56
1:E:2:SER:N	3:E:529:HOH:O	2.38	0.56
1:G:72:ASP:H	1:G:75:ASN:HD22	1.54	0.56
1:F:72:ASP:H	1:F:75:ASN:HD22	1.54	0.56
1:I:56:LYS:HE2	1:I:60:LYS:HE3	1.87	0.55
2:E:509:BEZ:C2	2:E:509:BEZ:C	2.72	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:89:PHE:CD2	1:G:93[B]:ASN:ND2	2.74	0.55
1:I:56:LYS:HE2	1:I:60:LYS:CE	2.37	0.55
1:F:56:LYS:HG2	1:F:60:LYS:HE3	1.88	0.55
1:F:7:ARG:CD	1:F:26:LEU:HD23	2.34	0.55
1:G:83:LEU:HD11	1:G:89:PHE:CD1	2.42	0.55
1:G:29:ARG:NH2	1:H:2:SER:O	2.33	0.55
3:B:551:HOH:O	1:G:13:LYS:HD2	2.06	0.54
1:D:28:ASP:O	1:D:29:ARG:HB2	2.07	0.54
1:A:2:SER:O	1:C:29:ARG:NH2	2.35	0.53
1:E:37:ILE:HD11	1:E:39:MET:CE	2.38	0.53
1:G:89:PHE:CE1	1:G:109:ALA:HB1	2.43	0.53
1:G:27:VAL:HG21	1:I:128:ILE:HG13	1.90	0.53
1:H:18:ILE:O	1:H:18:ILE:CG1	2.56	0.53
1:A:89:PHE:HZ	1:A:109:ALA:CB	2.22	0.53
1:E:72:ASP:H	1:E:75:ASN:ND2	2.05	0.52
1:A:89:PHE:CZ	1:A:109:ALA:HB1	2.45	0.52
1:G:49:GLY:HA3	1:G:53:GLU:HG3	1.92	0.51
1:A:5:ILE:HG12	1:A:6:ARG:N	2.24	0.51
1:H:86:ILE:HB	1:H:111:GLN:HE21	1.75	0.51
1:A:42:SER:OG	1:A:43:SER:N	2.43	0.50
1:E:97:LYS:HD3	3:E:540:HOH:O	2.11	0.50
1:A:72:ASP:H	1:A:75:ASN:ND2	2.09	0.50
2:I:518:BEZ:C6	2:I:518:BEZ:C	2.75	0.50
1:H:107:ARG:NH2	2:H:515:BEZ:O1	2.40	0.50
2:H:515:BEZ:H4	1:I:37:ILE:CG1	2.39	0.50
1:B:72:ASP:H	1:B:75:ASN:ND2	2.09	0.50
1:G:93[A]:ASN:ND2	1:H:20:PRO:HG3	2.19	0.50
1:I:30:THR:OG1	3:I:547:HOH:O	2.20	0.50
2:E:509:BEZ:C6	2:E:509:BEZ:C	2.74	0.49
1:E:37:ILE:HD11	1:E:39:MET:HE3	1.93	0.49
1:D:56:LYS:HG2	1:D:60:LYS:CE	2.36	0.49
1:G:5:ILE:O	1:G:27:VAL:HA	2.13	0.49
1:A:80:THR:HB	1:A:124:GLU:CG	2.42	0.49
1:E:28:ASP:O	1:E:29:ARG:HB2	2.13	0.48
1:E:39:MET:HE1	1:E:117:LYS:HE3	1.95	0.48
1:B:80:THR:HB	1:B:124:GLU:HG2	1.96	0.48
1:A:27:VAL:O	1:A:27:VAL:HG13	2.13	0.48
1:F:89:PHE:HZ	2:F:511:BEZ:O2	1.97	0.48
1:F:89:PHE:CE2	3:F:565:HOH:O	2.54	0.48
1:H:53:GLU:OE1	1:H:56:LYS:NZ	2.43	0.47
1:I:39:MET:SD	1:I:117:LYS:HE3	2.55	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:97:LYS:CG	1:I:20:PRO:HG3	2.44	0.47
1:G:2:SER:O	1:I:29:ARG:NH1	2.41	0.47
1:A:89:PHE:HZ	1:A:109:ALA:HB1	1.78	0.47
1:E:133:THR:HG23	1:E:133:THR:O	2.15	0.47
1:B:18:ILE:HD12	1:B:117:LYS:HE2	1.95	0.47
1:B:40:ASP:OD2	1:B:42:SER:HB2	2.14	0.47
1:E:4:LEU:HG	1:F:29:ARG:NH1	2.30	0.47
1:H:28:ASP:O	1:H:29:ARG:HB2	2.14	0.47
2:H:515:BEZ:H6	3:I:545:HOH:O	2.09	0.47
1:A:48:SER:HB3	1:D:43:SER:O	2.14	0.46
1:D:56:LYS:O	1:D:60:LYS:HG3	2.16	0.46
2:H:515:BEZ:C	2:H:515:BEZ:C6	2.73	0.46
1:H:9:ILE:HB	1:H:24:ALA:HB3	1.97	0.46
1:F:40:ASP:O	1:F:44:GLY:N	2.40	0.46
1:F:72:ASP:H	1:F:75:ASN:ND2	2.14	0.46
1:I:80:THR:HB	1:I:124:GLU:CG	2.46	0.46
1:B:134:THR:CG2	1:C:6:ARG:HE	2.21	0.45
1:C:72:ASP:H	1:C:75:ASN:ND2	2.11	0.45
1:A:135:ALA:C	1:A:137:LEU:H	2.20	0.45
1:G:78:LYS:HE2	1:G:79:THR:O	2.16	0.45
1:H:102:SER:O	1:H:103:ASN:C	2.55	0.45
1:B:133:THR:O	1:C:5:ILE:HA	2.17	0.45
1:D:26:LEU:HB2	1:D:31:ILE:HG12	1.99	0.45
1:B:102:SER:O	1:B:103:ASN:C	2.55	0.45
1:C:78:LYS:HE2	1:C:79:THR:O	2.16	0.45
1:D:56:LYS:CG	1:D:60:LYS:HE3	2.34	0.45
1:G:119:SER:HB3	3:G:532:HOH:O	2.15	0.45
1:I:95:ILE:N	1:I:95:ILE:HD12	2.32	0.45
1:C:133:THR:OG1	1:C:134:THR:N	2.50	0.44
2:H:515:BEZ:H4	1:I:37:ILE:CD1	2.48	0.44
1:I:18:ILE:N	1:I:21:TYR:HE1	2.11	0.44
1:I:56:LYS:HE2	1:I:60:LYS:NZ	2.33	0.44
1:E:51:VAL:HG13	1:E:52:ALA:N	2.33	0.43
1:H:86:ILE:H	1:H:111:GLN:HE21	1.65	0.43
1:I:28:ASP:O	1:I:29:ARG:HB2	2.18	0.43
1:H:56:LYS:HB2	1:H:56:LYS:HE3	1.76	0.43
2:B:503:BEZ:O1	2:B:504:BEZ:H5	2.18	0.43
1:B:133:THR:CG2	1:C:5:ILE:HG12	2.38	0.43
2:I:517:BEZ:O2	2:I:518:BEZ:O1	2.37	0.43
1:H:43:SER:O	1:H:45:GLN:HG3	2.19	0.43
1:D:29:ARG:CZ	1:F:4:LEU:HD12	2.49	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:80:THR:HB	1:B:124:GLU:CG	2.50	0.42
1:F:86:ILE:N	1:F:111:GLN:HE21	2.10	0.42
1:E:56:LYS:HE3	1:E:56:LYS:HB2	1.53	0.42
1:F:7:ARG:HG3	1:F:26:LEU:HB3	2.01	0.42
1:F:56:LYS:HE2	1:F:60:LYS:CE	2.50	0.42
1:H:83:LEU:O	1:H:111:GLN:HA	2.20	0.42
1:A:10:SER:HA	1:A:23:GLN:OE1	2.19	0.41
1:B:37:ILE:HD11	1:B:39:MET:HE3	2.01	0.41
1:B:5:ILE:O	1:B:27:VAL:HA	2.20	0.41
1:G:72:ASP:H	1:G:75:ASN:ND2	2.16	0.41
1:D:102:SER:O	1:D:103:ASN:C	2.58	0.41
1:G:89:PHE:HD2	1:G:93[B]:ASN:ND2	2.18	0.41
1:D:29:ARG:CZ	1:F:4:LEU:CD1	2.98	0.41
1:I:18:ILE:HA	1:I:18:ILE:HD13	1.55	0.41
1:E:9:ILE:HD12	1:E:9:ILE:N	2.36	0.41
1:D:90:ASN:HD21	2:D:508:BEZ:H3	1.87	0.40
1:D:56:LYS:HE2	1:D:60:LYS:HE2	2.02	0.40
1:A:78:LYS:HE3	3:B:548:HOH:O	2.20	0.40
2:A:501:BEZ:O1	2:A:502:BEZ:O2	2.40	0.40
1:D:71:CYS:HB3	1:D:75:ASN:CG	2.42	0.40
1:G:89:PHE:CE1	1:G:109:ALA:CB	3.04	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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	136/138 (99%)	128 (94%)	6 (4%)	2 (2%)	10	3
1	B	132/138 (96%)	129 (98%)	3 (2%)	0	100	100
1	C	132/138 (96%)	129 (98%)	3 (2%)	0	100	100
1	D	132/138 (96%)	129 (98%)	3 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	E	132/138 (96%)	129 (98%)	3 (2%)	0	100	100
1	F	132/138 (96%)	131 (99%)	1 (1%)	0	100	100
1	G	133/138 (96%)	131 (98%)	2 (2%)	0	100	100
1	H	133/138 (96%)	128 (96%)	5 (4%)	0	100	100
1	I	134/138 (97%)	129 (96%)	4 (3%)	1 (1%)	22	12
All	All	1196/1242 (96%)	1163 (97%)	30 (2%)	3 (0%)	41	31

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	I	3	SER
1	A	17	ALA
1	A	18	ILE

5.3.2 Protein sidechains ⓘ

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	109/108 (101%)	104 (95%)	5 (5%)	27	17
1	B	105/108 (97%)	102 (97%)	3 (3%)	42	35
1	C	105/108 (97%)	102 (97%)	3 (3%)	42	35
1	D	105/108 (97%)	101 (96%)	4 (4%)	33	24
1	E	105/108 (97%)	103 (98%)	2 (2%)	57	53
1	F	105/108 (97%)	103 (98%)	2 (2%)	57	53
1	G	106/108 (98%)	104 (98%)	2 (2%)	57	53
1	H	106/108 (98%)	102 (96%)	4 (4%)	33	24
1	I	107/108 (99%)	102 (95%)	5 (5%)	26	16
All	All	953/972 (98%)	923 (97%)	30 (3%)	39	32

All (30) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	5	ILE
1	A	39	MET
1	A	42	SER
1	A	89	PHE
1	A	136	SER
1	B	94	GLU
1	B	101	LYS
1	B	133	THR
1	C	3	SER
1	C	129	GLN
1	C	134	THR
1	D	3	SER
1	D	89	PHE
1	D	101	LYS
1	D	133	THR
1	E	56	LYS
1	E	115	LEU
1	F	2	SER
1	F	6	ARG
1	G	13	LYS
1	G	117	LYS
1	H	7	ARG
1	H	56	LYS
1	H	119	SER
1	H	120	ARG
1	I	2	SER
1	I	3	SER
1	I	18	ILE
1	I	89	PHE
1	I	115	LEU

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

Mol	Chain	Res	Type
1	A	45	GLN
1	A	75	ASN
1	A	87	ASN
1	B	75	ASN
1	B	90	ASN
1	C	45	GLN
1	C	75	ASN
1	C	103	ASN
1	C	129	GLN

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Mol	Chain	Res	Type
1	D	90	ASN
1	E	75	ASN
1	E	103	ASN
1	F	75	ASN
1	F	111	GLN
1	G	75	ASN
1	G	103	ASN
1	H	45	GLN
1	H	90	ASN
1	H	111	GLN
1	H	129	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 ⓘ

13 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
2	BEZ	A	501	-	7,9,9	2.43	1 (14%)	8,11,11	1.31	1 (12%)
2	BEZ	D	507	-	7,9,9	3.44	1 (14%)	8,11,11	1.02	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	BEZ	D	508	-	7,9,9	10.10	1 (14%)	8,11,11	0.84	0
2	BEZ	I	518	-	7,9,9	11.92	1 (14%)	8,11,11	0.95	0
2	BEZ	C	505	-	7,9,9	11.20	1 (14%)	8,11,11	0.99	0
2	BEZ	G	513	-	7,9,9	5.39	1 (14%)	8,11,11	1.18	1 (12%)
2	BEZ	E	509	-	7,9,9	11.43	1 (14%)	8,11,11	0.68	0
2	BEZ	B	504	-	7,9,9	14.20	1 (14%)	8,11,11	1.52	1 (12%)
2	BEZ	H	515	-	7,9,9	10.92	1 (14%)	8,11,11	1.01	0
2	BEZ	F	511	-	7,9,9	4.95	1 (14%)	8,11,11	1.17	0
2	BEZ	A	502	-	7,9,9	6.54	1 (14%)	8,11,11	0.85	0
2	BEZ	I	517	-	7,9,9	0.78	0	8,11,11	0.93	0
2	BEZ	B	503	-	7,9,9	2.00	1 (14%)	8,11,11	1.14	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	BEZ	A	501	-	-	0/0/4/4	0/1/1/1
2	BEZ	D	507	-	-	0/0/4/4	0/1/1/1
2	BEZ	D	508	-	-	0/0/4/4	0/1/1/1
2	BEZ	I	518	-	-	0/0/4/4	0/1/1/1
2	BEZ	C	505	-	-	0/0/4/4	0/1/1/1
2	BEZ	G	513	-	-	0/0/4/4	0/1/1/1
2	BEZ	E	509	-	-	0/0/4/4	0/1/1/1
2	BEZ	B	504	-	-	0/0/4/4	0/1/1/1
2	BEZ	H	515	-	-	0/0/4/4	0/1/1/1
2	BEZ	F	511	-	-	0/0/4/4	0/1/1/1
2	BEZ	A	502	-	-	0/0/4/4	0/1/1/1
2	BEZ	I	517	-	-	0/0/4/4	0/1/1/1
2	BEZ	B	503	-	-	0/0/4/4	0/1/1/1

All (12) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	504	BEZ	C1-C	37.56	1.83	1.47
2	I	518	BEZ	C1-C	31.53	1.77	1.47
2	E	509	BEZ	C1-C	30.24	1.76	1.47
2	C	505	BEZ	C1-C	29.62	1.76	1.47
2	H	515	BEZ	C1-C	28.88	1.75	1.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	508	BEZ	C1-C	26.72	1.73	1.47
2	A	502	BEZ	C1-C	17.26	1.64	1.47
2	G	513	BEZ	C1-C	14.23	1.61	1.47
2	F	511	BEZ	C1-C	13.09	1.60	1.47
2	D	507	BEZ	C1-C	9.00	1.56	1.47
2	A	501	BEZ	C1-C	6.32	1.53	1.47
2	B	503	BEZ	C1-C	5.21	1.52	1.47

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	504	BEZ	C6-C1-C	-3.07	116.25	120.37
2	A	501	BEZ	C6-C1-C2	2.28	122.12	117.59
2	G	513	BEZ	C6-C1-C2	2.01	121.60	117.59

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

11 monomers are involved in 25 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	501	BEZ	1	0
2	D	508	BEZ	1	0
2	I	518	BEZ	4	0
2	C	505	BEZ	3	0
2	E	509	BEZ	3	0
2	B	504	BEZ	3	0
2	H	515	BEZ	9	0
2	F	511	BEZ	1	0
2	A	502	BEZ	1	0
2	I	517	BEZ	1	0
2	B	503	BEZ	1	0

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	136/138 (98%)	0.11	6 (4%)	34	37	10, 16, 45, 65	7 (5%)
1	B	134/138 (97%)	-0.11	6 (4%)	33	36	10, 15, 43, 67	6 (4%)
1	C	134/138 (97%)	-0.00	6 (4%)	33	36	9, 16, 47, 58	9 (6%)
1	D	134/138 (97%)	0.09	8 (5%)	21	24	10, 16, 52, 66	7 (5%)
1	E	134/138 (97%)	0.11	7 (5%)	27	30	9, 16, 48, 65	10 (7%)
1	F	134/138 (97%)	0.19	7 (5%)	27	30	10, 16, 50, 66	6 (4%)
1	G	134/138 (97%)	0.01	5 (3%)	41	44	10, 16, 49, 64	6 (4%)
1	H	135/138 (97%)	0.30	8 (5%)	22	25	10, 16, 58, 65	10 (7%)
1	I	135/138 (97%)	0.25	6 (4%)	34	37	10, 15, 52, 68	12 (8%)
All	All	1210/1242 (97%)	0.11	59 (4%)	29	33	9, 16, 52, 68	73 (6%)

All (59) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	135	ALA	9.4
1	A	137	LEU	8.0
1	I	18	ILE	7.8
1	D	2	SER	7.4
1	I	2	SER	6.6
1	A	18	ILE	5.8
1	G	2	SER	5.3
1	I	42	SER	5.2
1	C	134	THR	4.7
1	D	3	SER	4.4
1	D	135	ALA	4.4
1	G	135	ALA	4.0
1	B	134	THR	3.8
1	A	42	SER	3.7
1	C	2	SER	3.7

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Mol	Chain	Res	Type	RSRZ
1	H	42	SER	3.7
1	I	43	SER	3.5
1	B	133	THR	3.5
1	F	48	SER	3.3
1	F	2	SER	3.3
1	H	133	THR	3.2
1	H	136	SER	3.2
1	E	2	SER	3.2
1	I	3	SER	3.2
1	F	3	SER	3.1
1	B	135	ALA	3.0
1	F	5	ILE	3.0
1	A	17	ALA	3.0
1	G	3	SER	3.0
1	A	2	SER	2.9
1	D	133	THR	2.9
1	I	19	GLY	2.9
1	C	4	LEU	2.8
1	F	44	GLY	2.8
1	B	3	SER	2.8
1	H	19	GLY	2.6
1	A	43	SER	2.6
1	C	42	SER	2.6
1	F	121	ILE	2.5
1	D	76	VAL	2.5
1	D	131	PRO	2.5
1	H	13	LYS	2.5
1	G	102	SER	2.5
1	E	133	THR	2.4
1	F	49	GLY	2.4
1	E	135	ALA	2.3
1	E	42	SER	2.3
1	E	3	SER	2.3
1	H	87	ASN	2.3
1	E	121	ILE	2.2
1	D	134	THR	2.2
1	C	133	THR	2.2
1	B	2	SER	2.1
1	H	3	SER	2.1
1	B	49	GLY	2.1
1	E	45	GLN	2.1
1	H	2	SER	2.1

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Mol	Chain	Res	Type	RSRZ
1	D	5	ILE	2.1
1	G	133	THR	2.0

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

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

6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. 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
2	BEZ	I	518	9/9	0.63	0.32	30,35,38,38	9
2	BEZ	B	504	9/9	0.77	0.41	35,35,36,36	9
2	BEZ	D	508	9/9	0.80	0.25	29,31,34,34	9
2	BEZ	H	515	9/9	0.82	0.56	47,48,49,50	9
2	BEZ	C	505	9/9	0.84	0.49	39,40,40,40	9
2	BEZ	A	502	9/9	0.87	0.16	35,42,45,46	0
2	BEZ	G	513	9/9	0.91	0.13	48,49,50,51	0
2	BEZ	F	511	9/9	0.92	0.10	38,39,40,41	0
2	BEZ	A	501	9/9	0.94	0.09	29,31,32,32	0
2	BEZ	E	509	9/9	0.94	0.11	42,43,45,45	0
2	BEZ	D	507	9/9	0.95	0.11	31,33,35,35	0
2	BEZ	B	503	9/9	0.95	0.09	35,37,39,40	0
2	BEZ	I	517	9/9	0.96	0.09	34,35,37,37	0

6.5 Other polymers [i](#)

There are no such residues in this entry.