Full wwPDB X-ray Structure Validation Report (i)

Jan 31, 2016 – 11:48 PM GMT

PDB ID	:	1YLO
Title	:	Crystal Structure of Protein of Unknown Function (Possible Aminopeptidase) S2589 from Shigella flexneri 2a str. 2457T
Authors	:	Nocek, B.P.; Midwest Center for Structural Genomics (MCSG)
Deposited on	:	2005-01-19
Resolution	:	2.15 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:

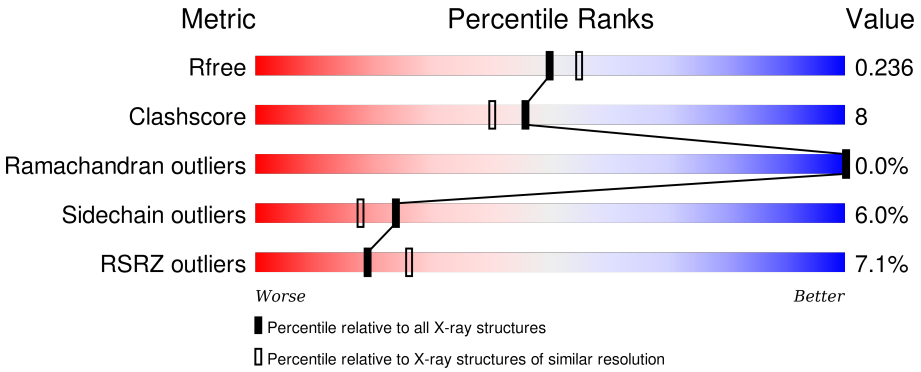
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	trunk26865

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 2.15 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	1045 (2.16-2.16)
Clashscore	102246	1152 (2.16-2.16)
Ramachandran outliers	100387	1131 (2.16-2.16)
Sidechain outliers	100360	1131 (2.16-2.16)
RSRZ outliers	91569	1050 (2.16-2.16)

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	348	7% 80% 18%
1	B	348	7% 82% 16%
1	C	348	7% 84% 14%
1	D	348	9% 84% 13%
1	E	348	6% 84% 13%

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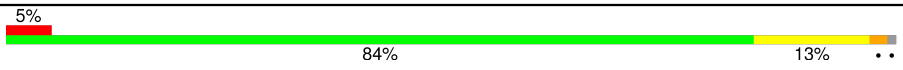
Mol	Chain	Length	Quality of chain
1	F	348	

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 16577 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 hypothetical protein SF2450.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	346	Total	C	N	O	S	Se	0	4	0
			2648	1647	475	508	6	12			
1	B	346	Total	C	N	O	S	Se	0	4	0
			2648	1647	475	508	6	12			
1	C	346	Total	C	N	O	S	Se	0	4	0
			2648	1647	475	508	6	12			
1	D	346	Total	C	N	O	S	Se	0	4	0
			2648	1647	475	508	6	12			
1	E	346	Total	C	N	O	S	Se	0	4	0
			2648	1647	475	508	6	12			
1	F	346	Total	C	N	O	S	Se	0	4	0
			2648	1647	475	508	6	12			

There are 90 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-2	SER	-	CLONING ARTIFACT	UNP Q83K87
A	-1	ASN	-	CLONING ARTIFACT	UNP Q83K87
A	0	ALA	-	CLONING ARTIFACT	UNP Q83K87
A	1	MSE	MET	MODIFIED RESIDUE	UNP Q83K87
A	58	MSE	MET	MODIFIED RESIDUE	UNP Q83K87
A	63	MSE	MET	MODIFIED RESIDUE	UNP Q83K87
A	69	MSE	MET	MODIFIED RESIDUE	UNP Q83K87
A	89	MSE	MET	MODIFIED RESIDUE	UNP Q83K87
A	123	MSE	MET	MODIFIED RESIDUE	UNP Q83K87
A	136	MSE	MET	MODIFIED RESIDUE	UNP Q83K87
A	161	MSE	MET	MODIFIED RESIDUE	UNP Q83K87
A	244	MSE	MET	MODIFIED RESIDUE	UNP Q83K87
A	277	MSE	MET	MODIFIED RESIDUE	UNP Q83K87
A	300	MSE	MET	MODIFIED RESIDUE	UNP Q83K87
A	322	MSE	MET	MODIFIED RESIDUE	UNP Q83K87
B	-2	SER	-	CLONING ARTIFACT	UNP Q83K87
B	-1	ASN	-	CLONING ARTIFACT	UNP Q83K87

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Chain	Residue	Modelled	Actual	Comment	Reference
B	0	ALA	-	CLONING ARTIFACT	UNP Q83K87
B	1	MSE	MET	MODIFIED RESIDUE	UNP Q83K87
B	58	MSE	MET	MODIFIED RESIDUE	UNP Q83K87
B	63	MSE	MET	MODIFIED RESIDUE	UNP Q83K87
B	69	MSE	MET	MODIFIED RESIDUE	UNP Q83K87
B	89	MSE	MET	MODIFIED RESIDUE	UNP Q83K87
B	123	MSE	MET	MODIFIED RESIDUE	UNP Q83K87
B	136	MSE	MET	MODIFIED RESIDUE	UNP Q83K87
B	161	MSE	MET	MODIFIED RESIDUE	UNP Q83K87
B	244	MSE	MET	MODIFIED RESIDUE	UNP Q83K87
B	277	MSE	MET	MODIFIED RESIDUE	UNP Q83K87
B	300	MSE	MET	MODIFIED RESIDUE	UNP Q83K87
B	322	MSE	MET	MODIFIED RESIDUE	UNP Q83K87
C	-2	SER	-	CLONING ARTIFACT	UNP Q83K87
C	-1	ASN	-	CLONING ARTIFACT	UNP Q83K87
C	0	ALA	-	CLONING ARTIFACT	UNP Q83K87
C	1	MSE	MET	MODIFIED RESIDUE	UNP Q83K87
C	58	MSE	MET	MODIFIED RESIDUE	UNP Q83K87
C	63	MSE	MET	MODIFIED RESIDUE	UNP Q83K87
C	69	MSE	MET	MODIFIED RESIDUE	UNP Q83K87
C	89	MSE	MET	MODIFIED RESIDUE	UNP Q83K87
C	123	MSE	MET	MODIFIED RESIDUE	UNP Q83K87
C	136	MSE	MET	MODIFIED RESIDUE	UNP Q83K87
C	161	MSE	MET	MODIFIED RESIDUE	UNP Q83K87
C	244	MSE	MET	MODIFIED RESIDUE	UNP Q83K87
C	277	MSE	MET	MODIFIED RESIDUE	UNP Q83K87
C	300	MSE	MET	MODIFIED RESIDUE	UNP Q83K87
C	322	MSE	MET	MODIFIED RESIDUE	UNP Q83K87
D	-2	SER	-	CLONING ARTIFACT	UNP Q83K87
D	-1	ASN	-	CLONING ARTIFACT	UNP Q83K87
D	0	ALA	-	CLONING ARTIFACT	UNP Q83K87
D	1	MSE	MET	MODIFIED RESIDUE	UNP Q83K87
D	58	MSE	MET	MODIFIED RESIDUE	UNP Q83K87
D	63	MSE	MET	MODIFIED RESIDUE	UNP Q83K87
D	69	MSE	MET	MODIFIED RESIDUE	UNP Q83K87
D	89	MSE	MET	MODIFIED RESIDUE	UNP Q83K87
D	123	MSE	MET	MODIFIED RESIDUE	UNP Q83K87
D	136	MSE	MET	MODIFIED RESIDUE	UNP Q83K87
D	161	MSE	MET	MODIFIED RESIDUE	UNP Q83K87
D	244	MSE	MET	MODIFIED RESIDUE	UNP Q83K87
D	277	MSE	MET	MODIFIED RESIDUE	UNP Q83K87
D	300	MSE	MET	MODIFIED RESIDUE	UNP Q83K87

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Chain	Residue	Modelled	Actual	Comment	Reference
D	322	MSE	MET	MODIFIED RESIDUE	UNP Q83K87
E	-2	SER	-	CLONING ARTIFACT	UNP Q83K87
E	-1	ASN	-	CLONING ARTIFACT	UNP Q83K87
E	0	ALA	-	CLONING ARTIFACT	UNP Q83K87
E	1	MSE	MET	MODIFIED RESIDUE	UNP Q83K87
E	58	MSE	MET	MODIFIED RESIDUE	UNP Q83K87
E	63	MSE	MET	MODIFIED RESIDUE	UNP Q83K87
E	69	MSE	MET	MODIFIED RESIDUE	UNP Q83K87
E	89	MSE	MET	MODIFIED RESIDUE	UNP Q83K87
E	123	MSE	MET	MODIFIED RESIDUE	UNP Q83K87
E	136	MSE	MET	MODIFIED RESIDUE	UNP Q83K87
E	161	MSE	MET	MODIFIED RESIDUE	UNP Q83K87
E	244	MSE	MET	MODIFIED RESIDUE	UNP Q83K87
E	277	MSE	MET	MODIFIED RESIDUE	UNP Q83K87
E	300	MSE	MET	MODIFIED RESIDUE	UNP Q83K87
E	322	MSE	MET	MODIFIED RESIDUE	UNP Q83K87
F	-2	SER	-	CLONING ARTIFACT	UNP Q83K87
F	-1	ASN	-	CLONING ARTIFACT	UNP Q83K87
F	0	ALA	-	CLONING ARTIFACT	UNP Q83K87
F	1	MSE	MET	MODIFIED RESIDUE	UNP Q83K87
F	58	MSE	MET	MODIFIED RESIDUE	UNP Q83K87
F	63	MSE	MET	MODIFIED RESIDUE	UNP Q83K87
F	69	MSE	MET	MODIFIED RESIDUE	UNP Q83K87
F	89	MSE	MET	MODIFIED RESIDUE	UNP Q83K87
F	123	MSE	MET	MODIFIED RESIDUE	UNP Q83K87
F	136	MSE	MET	MODIFIED RESIDUE	UNP Q83K87
F	161	MSE	MET	MODIFIED RESIDUE	UNP Q83K87
F	244	MSE	MET	MODIFIED RESIDUE	UNP Q83K87
F	277	MSE	MET	MODIFIED RESIDUE	UNP Q83K87
F	300	MSE	MET	MODIFIED RESIDUE	UNP Q83K87
F	322	MSE	MET	MODIFIED RESIDUE	UNP Q83K87

- Molecule 2 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	D	2	Total Zn 2 2	0	0
2	E	2	Total Zn 2 2	0	0
2	B	2	Total Zn 2 2	0	0
2	C	2	Total Zn 2 2	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	2	Total Zn 2 2	0	0
2	F	2	Total Zn 2 2	0	0

- Molecule 3 is water.

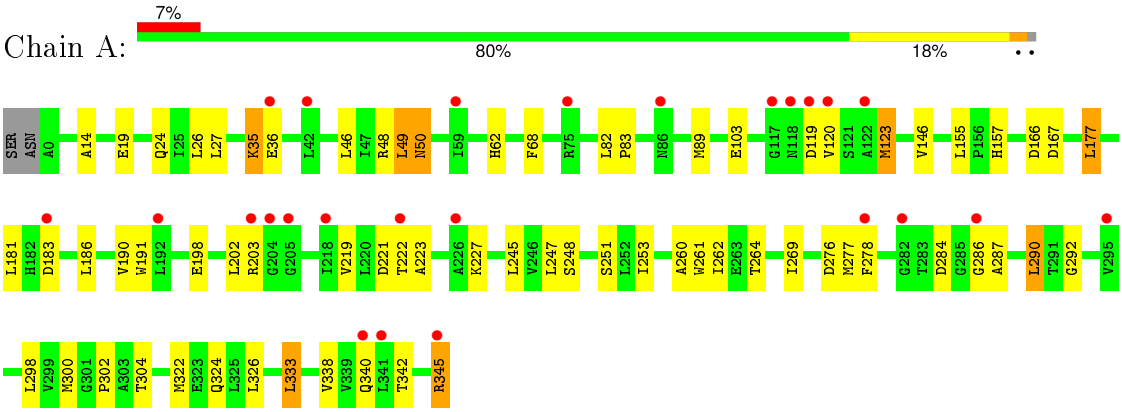
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	111	Total O 111 111	0	0
3	B	114	Total O 114 114	0	0
3	C	115	Total O 115 115	0	0
3	D	120	Total O 120 120	0	0
3	E	111	Total O 111 111	0	0
3	F	106	Total O 106 106	0	0

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.

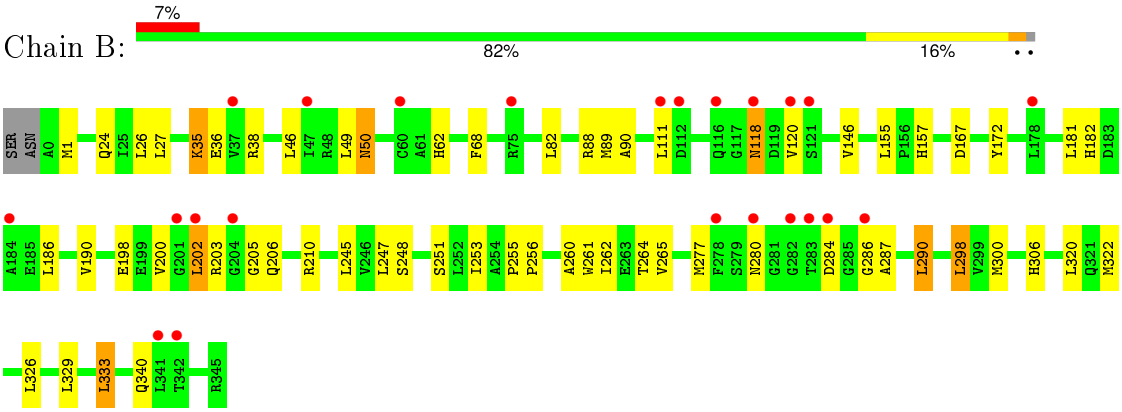
- Molecule 1: hypothetical protein SF2450

Chain A:



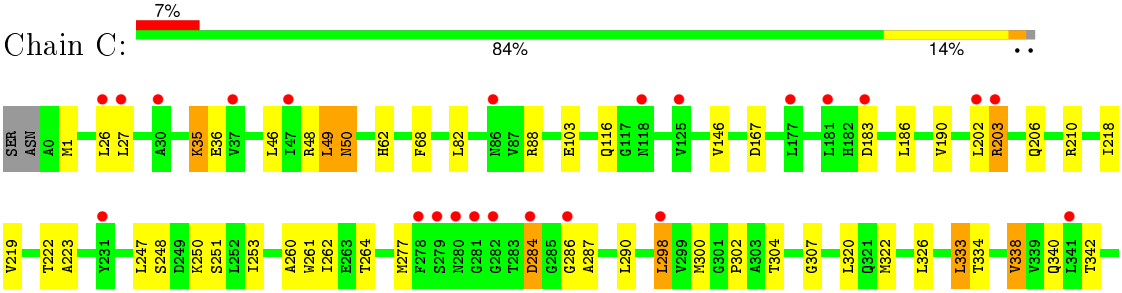
- Molecule 1: hypothetical protein SF2450

Chain B:

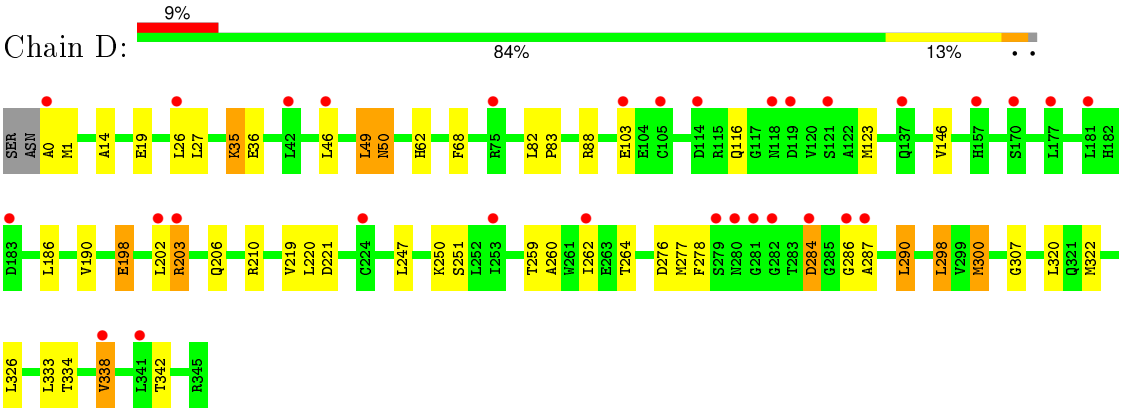


- Molecule 1: hypothetical protein SF2450

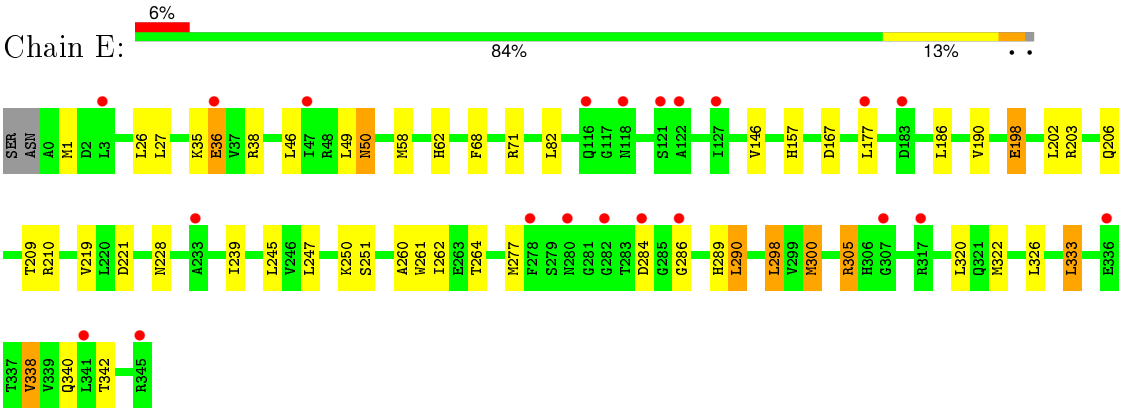
Chain C:



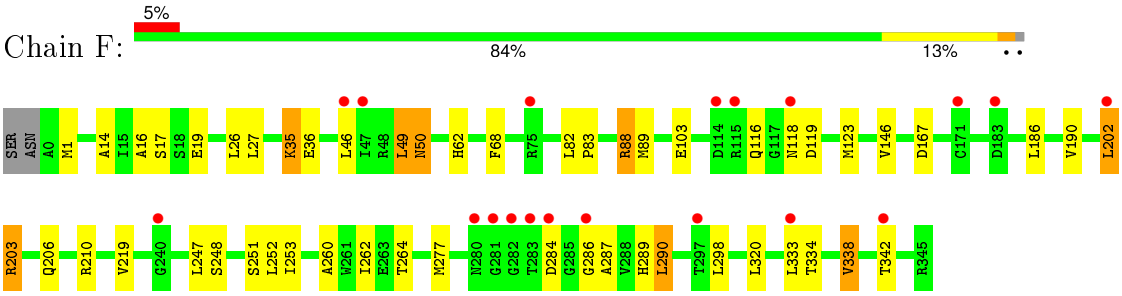
• Molecule 1: hypothetical protein SF2450



• Molecule 1: hypothetical protein SF2450



• Molecule 1: hypothetical protein SF2450



4 Data and refinement statistics (i)

Property	Value	Source
Space group	I 41	Depositor
Cell constants a, b, c, α, β, γ	161.83Å 161.83Å 228.57Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	50.00 – 2.15 36.19 – 2.15	Depositor EDS
% Data completeness (in resolution range)	99.7 (50.00-2.15) 99.4 (36.19-2.15)	Depositor EDS
R_{merge}	0.11	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.95 (at 2.16Å)	Xtriage
Refinement program	REFMAC 5.2.0005	Depositor
R, R_{free}	0.190 , 0.229 0.200 , 0.236	Depositor DCC
R_{free} test set	7909 reflections (5.28%)	DCC
Wilson B-factor (Å^2)	33.7	Xtriage
Anisotropy	0.035	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	(Not available) , (Not available)	EDS
Estimated twinning fraction	0.467 for -1/2*h+1/2*k-1/2*l,1/2*h-1/2*k-1/2*l,-h-k 0.467 for -1/2*h+1/2*k+1/2*l,1/2*h-1/2*k+1/2*l,h+k 0.469 for -1/2*h-1/2*k+1/2*l,-1/2*h-1/2*k-1/2*l,h-k 0.469 for -1/2*h-1/2*k-1/2*l,-1/2*h-1/2*k+1/2*l,-h+k 0.477 for -h,k,-l	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.33$	Xtriage
Outliers	1 of 157779 reflections (0.001%)	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	16577	wwPDB-VP
Average B, all atoms (Å^2)	35.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.10% 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, 0.375 respectively for untwinned datasets, and 0.333, 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: ZN

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\#\|Z\| > 5$	RMSZ	$\#\|Z\| > 5$
1	A	0.59	0/2685	0.68	1/3619 (0.0%)
1	B	0.60	0/2685	0.67	0/3619
1	C	0.60	0/2685	0.67	0/3619
1	D	0.59	0/2685	0.67	1/3619 (0.0%)
1	E	0.58	0/2685	0.69	2/3619 (0.1%)
1	F	0.60	0/2685	0.67	0/3619
All	All	0.59	0/16110	0.67	4/21714 (0.0%)

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	221	ASP	CB-CG-OD1	6.55	124.20	118.30
1	E	221	ASP	CB-CG-OD1	6.28	123.95	118.30
1	D	221	ASP	CB-CG-OD1	5.40	123.16	118.30
1	E	305	ARG	NE-CZ-NH1	5.17	122.88	120.30

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	2648	0	2680	56	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	B	2648	0	2680	42	0
1	C	2648	0	2680	43	0
1	D	2648	0	2680	41	0
1	E	2648	0	2680	40	0
1	F	2648	0	2680	39	0
2	A	2	0	0	0	0
2	B	2	0	0	0	0
2	C	2	0	0	0	0
2	D	2	0	0	0	0
2	E	2	0	0	0	0
2	F	2	0	0	0	0
3	A	111	0	0	3	0
3	B	114	0	0	2	0
3	C	115	0	0	2	0
3	D	120	0	0	3	0
3	E	111	0	0	4	0
3	F	106	0	0	3	0
All	All	16577	0	16080	245	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 8.

All (245) 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:A:89:MSE:CE	1:A:120:VAL:H	1.52	1.22
1:E:206:GLN:HE21	1:E:210:ARG:HH12	1.08	1.02
1:B:206:GLN:HE21	1:B:210:ARG:HH12	1.04	0.96
1:A:222:THR:HG21	1:A:304:THR:HG23	1.48	0.96
1:D:1:MSE:HE3	1:D:320:LEU:CD2	1.97	0.93
1:C:206:GLN:HE21	1:C:210:ARG:HH12	1.13	0.92
1:F:206:GLN:HE21	1:F:210:ARG:HH12	1.16	0.92
1:A:89:MSE:HE2	1:A:119:ASP:HA	1.54	0.90
1:D:277:MSE:HE2	1:E:82:LEU:HD12	1.54	0.89
1:B:50:ASN:HD21	1:B:190:VAL:H	1.20	0.89
1:D:206:GLN:HE21	1:D:210:ARG:NH1	1.70	0.89
1:D:206:GLN:HE21	1:D:210:ARG:HH12	0.89	0.88
1:A:89:MSE:HE1	1:A:120:VAL:H	1.35	0.88
1:C:222:THR:HG23	1:C:302:PRO:O	1.73	0.87
1:F:1:MSE:HE3	1:F:320:LEU:CD2	2.04	0.87
1:A:89:MSE:CE	1:A:120:VAL:N	2.36	0.87

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:206:GLN:NE2	1:D:210:ARG:HH12	1.72	0.86
1:A:277:MSE:HE2	1:B:82:LEU:HD12	1.56	0.86
1:C:50:ASN:HD21	1:C:190:VAL:H	1.24	0.86
1:C:202:LEU:HB2	1:C:287:ALA:HB2	1.55	0.86
1:A:222:THR:HG23	1:A:302:PRO:O	1.75	0.85
1:A:50:ASN:HD21	1:A:190:VAL:H	1.24	0.84
1:B:277:MSE:HE2	1:C:82:LEU:HD12	1.60	0.83
1:A:103[B]:GLU:OE1	3:A:1546:HOH:O	1.97	0.83
1:D:202:LEU:HB2	1:D:287:ALA:HB2	1.61	0.83
1:D:1:MSE:HE3	1:D:320:LEU:HD21	1.61	0.81
1:E:50:ASN:HD21	1:E:190:VAL:H	1.27	0.81
1:C:103[B]:GLU:OE1	3:C:1681:HOH:O	1.98	0.81
1:F:50:ASN:HD21	1:F:190:VAL:H	1.28	0.81
1:C:1:MSE:HE3	1:C:320:LEU:CD2	2.12	0.80
1:E:1:MSE:HE3	1:E:320:LEU:CD2	2.11	0.80
1:F:103[B]:GLU:OE1	3:F:1969:HOH:O	1.99	0.80
1:A:262:ILE:HG21	1:A:300:MSE:HE1	1.64	0.80
1:D:83:PRO:HG3	1:D:123:MSE:HE1	1.63	0.80
1:D:62:HIS:CD2	1:D:198[A]:GLU:HG2	2.18	0.79
1:E:62:HIS:CD2	1:E:198[A]:GLU:HG2	2.18	0.79
1:F:202:LEU:HB2	1:F:287:ALA:HB2	1.64	0.79
1:D:50:ASN:HD21	1:D:190:VAL:H	1.31	0.79
1:E:284:ASP:HB2	3:E:1907:HOH:O	1.83	0.78
1:D:103[B]:GLU:OE1	3:D:1816:HOH:O	2.00	0.78
1:C:206:GLN:NE2	1:C:210:ARG:HH12	1.81	0.78
1:B:262:ILE:HD12	1:B:298:LEU:HD11	1.66	0.76
1:B:1:MSE:HE3	1:B:320:LEU:CD2	2.15	0.76
1:A:251:SER:HB2	1:A:286:GLY:HA3	1.65	0.76
1:A:177:LEU:HD13	1:A:181:LEU:HD12	1.67	0.75
1:B:206:GLN:NE2	1:B:210:ARG:HH12	1.83	0.75
1:A:62:HIS:CD2	1:A:198[B]:GLU:HG2	2.21	0.75
1:B:206:GLN:HE21	1:B:210:ARG:NH1	1.83	0.75
1:C:206:GLN:HE21	1:C:210:ARG:NH1	1.85	0.74
1:C:222:THR:HG21	1:C:304:THR:HG23	1.67	0.73
1:F:1:MSE:HE3	1:F:320:LEU:HD21	1.68	0.73
1:A:345:ARG:HG2	1:A:345:ARG:HH21	1.53	0.73
1:E:62:HIS:CG	1:E:198[A]:GLU:HG2	2.24	0.72
1:E:262:ILE:HD12	1:E:298:LEU:HD11	1.70	0.72
1:E:228:ASN:OD1	1:E:305:ARG:HG2	1.90	0.72
1:A:202:LEU:HB2	1:A:287:ALA:HB2	1.71	0.71
1:D:82:LEU:HD12	1:F:277:MSE:HE2	1.73	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:262:ILE:HD12	1:C:298:LEU:HD11	1.75	0.69
1:D:1:MSE:HE3	1:D:320:LEU:HD23	1.74	0.69
1:D:251:SER:HB2	1:D:286:GLY:HA3	1.74	0.68
1:E:1:MSE:HE3	1:E:320:LEU:HD21	1.75	0.68
1:F:251:SER:HB2	1:F:286:GLY:HA3	1.76	0.67
1:B:200:VAL:HG23	1:B:203:ARG:HD3	1.75	0.66
1:B:251:SER:HB2	1:B:286:GLY:HA3	1.76	0.66
1:D:290:LEU:HD11	1:E:203:ARG:HB3	1.78	0.65
1:C:1:MSE:HE3	1:C:320:LEU:HD21	1.76	0.65
1:B:1:MSE:HE3	1:B:320:LEU:HD21	1.78	0.64
1:A:262:ILE:HD12	1:A:298:LEU:HD21	1.78	0.64
1:D:203:ARG:HG3	1:F:290:LEU:HD11	1.80	0.64
1:E:260:ALA:O	1:E:264:THR:HG23	1.98	0.63
1:E:305:ARG:HD2	3:E:1850:HOH:O	1.97	0.63
1:A:219:VAL:HG11	1:A:284:ASP:HB3	1.81	0.62
1:E:290:LEU:HD11	1:F:203:ARG:HG3	1.80	0.62
1:B:50:ASN:ND2	1:B:190:VAL:H	1.94	0.62
1:A:89:MSE:HE3	1:A:120:VAL:H	1.57	0.62
1:A:222:THR:HG21	1:A:304:THR:CG2	2.25	0.62
1:E:277:MSE:HE2	1:F:82:LEU:HD12	1.82	0.61
1:F:260:ALA:O	1:F:264:THR:HG23	2.01	0.61
1:A:89:MSE:HE2	1:A:120:VAL:H	1.60	0.61
1:E:251:SER:HB2	1:E:286:GLY:HA3	1.81	0.61
1:F:50:ASN:HD22	1:F:50:ASN:N	2.00	0.60
1:C:284:ASP:HB2	3:C:1708:HOH:O	2.01	0.60
1:F:1:MSE:HE3	1:F:320:LEU:HD23	1.84	0.60
1:F:206:GLN:NE2	1:F:210:ARG:HH12	1.95	0.60
1:A:260:ALA:O	1:A:264:THR:HG23	2.02	0.60
1:F:1:MSE:HE2	1:F:1:MSE:HA	1.82	0.59
1:E:50:ASN:ND2	1:E:190:VAL:H	1.98	0.59
1:A:253:ILE:H	1:B:203:ARG:HH22	1.51	0.59
1:C:50:ASN:HD22	1:C:50:ASN:N	2.01	0.59
1:A:50:ASN:HD22	1:A:50:ASN:N	2.00	0.59
1:A:82:LEU:HD12	1:C:277:MSE:HE2	1.85	0.58
1:A:83:PRO:HD3	1:A:123:MSE:HE3	1.86	0.58
1:E:1:MSE:HE2	1:E:1:MSE:HA	1.84	0.58
1:B:36:GLU:H	1:B:36:GLU:CD	2.05	0.58
1:B:260:ALA:O	1:B:264:THR:HG23	2.04	0.58
1:A:290:LEU:HD21	1:B:203:ARG:HG2	1.84	0.58
1:C:251:SER:HB2	1:C:286:GLY:HA3	1.85	0.58
1:B:1:MSE:HA	1:B:1:MSE:HE2	1.85	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:62:HIS:CG	1:A:198[B]:GLU:HG2	2.38	0.57
1:B:50:ASN:HD22	1:B:50:ASN:N	2.02	0.57
1:A:245:LEU:HD13	1:A:300:MSE:CE	2.34	0.57
1:D:260:ALA:O	1:D:264:THR:HG23	2.04	0.57
1:E:219:VAL:HG11	1:E:284:ASP:HB3	1.87	0.57
1:F:248:SER:HB2	1:F:253:ILE:HD13	1.85	0.57
1:C:260:ALA:O	1:C:264:THR:HG23	2.04	0.57
1:C:50:ASN:ND2	1:C:190:VAL:H	1.98	0.57
1:F:50:ASN:ND2	1:F:190:VAL:H	1.99	0.57
1:D:35:LYS:HE2	1:D:49:LEU:O	2.05	0.57
1:D:50:ASN:ND2	1:D:190:VAL:H	2.02	0.55
1:B:322:MSE:HE2	1:B:326:LEU:HG	1.88	0.55
1:A:35:LYS:HE2	1:A:49:LEU:O	2.06	0.55
1:A:342:THR:HB	3:A:1500:HOH:O	2.07	0.55
1:E:338:VAL:O	1:E:342:THR:HG22	2.06	0.55
1:C:218:ILE:HG21	1:C:300:MSE:HE2	1.88	0.55
1:D:1:MSE:HA	1:D:1:MSE:HE2	1.89	0.54
1:E:50:ASN:N	1:E:50:ASN:HD22	2.05	0.54
1:D:50:ASN:N	1:D:50:ASN:HD22	2.05	0.54
1:F:35:LYS:HE2	1:F:49:LEU:O	2.07	0.54
1:B:290:LEU:HD21	1:C:203:ARG:HG3	1.90	0.54
1:D:338:VAL:O	1:D:342:THR:HG22	2.07	0.53
1:A:248:SER:HB2	1:A:253:ILE:HD13	1.91	0.53
1:C:248:SER:HB2	1:C:253:ILE:HD13	1.91	0.53
1:C:36:GLU:H	1:C:36:GLU:CD	2.12	0.53
1:A:222:THR:HG22	1:A:223:ALA:N	2.23	0.53
1:A:219:VAL:CG1	1:A:284:ASP:HB3	2.38	0.53
1:D:36:GLU:H	1:D:36:GLU:CD	2.13	0.53
1:F:284:ASP:HB2	3:F:2017:HOH:O	2.09	0.52
1:E:245:LEU:HD13	1:E:300:MSE:HE3	1.92	0.52
1:D:262:ILE:HD12	1:D:298:LEU:HD11	1.90	0.52
1:A:50:ASN:ND2	1:A:190:VAL:H	1.99	0.52
1:B:68:PHE:HB2	1:B:146:VAL:HB	1.92	0.52
1:B:245:LEU:HD13	1:B:300:MSE:HE3	1.91	0.52
1:C:219:VAL:HG11	1:C:284:ASP:HB3	1.90	0.52
1:B:198[B]:GLU:OE2	1:B:284:ASP:HB3	2.09	0.52
1:D:88:ARG:HD2	1:D:307:GLY:O	2.10	0.51
1:E:322:MSE:HE2	1:E:326:LEU:HG	1.91	0.51
1:B:90:ALA:O	3:B:1619:HOH:O	2.18	0.51
1:B:261:TRP:CH2	1:B:333:LEU:HD13	2.45	0.51
1:B:202:LEU:HB2	1:B:287:ALA:HB2	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:177:LEU:CD1	1:A:181:LEU:HD12	2.41	0.51
1:F:338:VAL:O	1:F:342:THR:HG22	2.12	0.50
1:B:1:MSE:HE3	1:B:320:LEU:HD23	1.94	0.49
1:D:259:THR:HG22	1:D:298:LEU:HD12	1.95	0.49
1:A:89:MSE:HE1	1:A:120:VAL:N	2.16	0.49
1:C:300:MSE:HE3	1:C:322:MSE:CE	2.42	0.49
1:C:222:THR:HG21	1:C:304:THR:CG2	2.38	0.49
1:F:14:ALA:HB1	1:F:19:GLU:HA	1.95	0.49
1:F:206:GLN:HE21	1:F:210:ARG:NH1	1.99	0.48
1:A:50:ASN:HD22	1:A:50:ASN:H	1.61	0.48
1:D:83:PRO:CG	1:D:123:MSE:HE1	2.40	0.48
1:F:16:ALA:O	1:F:17:SER:HB2	2.12	0.48
1:C:300:MSE:HE3	1:C:322:MSE:HE1	1.94	0.48
1:E:239:ILE:HD13	1:E:305:ARG:HD3	1.95	0.48
1:B:88:ARG:HH22	1:B:306:HIS:HA	1.78	0.48
1:A:89:MSE:HE2	1:A:119:ASP:CA	2.35	0.48
1:F:219:VAL:HG11	1:F:284:ASP:HB3	1.96	0.48
1:F:36:GLU:H	1:F:36:GLU:CD	2.15	0.48
1:B:265:VAL:HG11	1:B:329:LEU:HD23	1.96	0.48
1:F:262:ILE:HD12	1:F:298:LEU:HD11	1.95	0.48
1:E:1:MSE:HE3	1:E:320:LEU:HD23	1.92	0.48
1:C:68:PHE:HB2	1:C:146:VAL:HB	1.96	0.48
1:E:262:ILE:CD1	1:E:298:LEU:HD11	2.41	0.47
1:B:35:LYS:NZ	1:B:182:HIS:O	2.48	0.47
1:E:68:PHE:HB2	1:E:146:VAL:HB	1.96	0.47
1:F:83:PRO:HD3	1:F:123:MSE:HE1	1.95	0.47
1:C:219:VAL:CG1	1:C:284:ASP:HB3	2.45	0.47
1:D:68:PHE:HB2	1:D:146:VAL:HB	1.96	0.47
1:F:62:HIS:CE1	1:F:167:ASP:HB2	2.50	0.47
1:E:157:HIS:ND1	3:E:1882:HOH:O	2.35	0.46
1:D:0:ALA:HB1	3:D:1808:HOH:O	2.13	0.46
1:E:36:GLU:HG3	1:E:38:ARG:HH12	1.80	0.46
1:D:284:ASP:N	1:D:284:ASP:OD2	2.44	0.46
1:A:36:GLU:H	1:A:36:GLU:CD	2.19	0.46
1:D:219:VAL:HG11	1:D:284:ASP:HB2	1.97	0.46
1:B:290:LEU:HD11	1:C:203:ARG:HG3	1.98	0.45
1:C:36:GLU:HG2	1:C:48:ARG:HB3	1.97	0.45
1:A:203:ARG:NH2	1:C:250:LYS:O	2.49	0.45
1:A:222:THR:CG2	1:A:304:THR:HG23	2.31	0.45
1:B:50:ASN:HD22	1:B:50:ASN:H	1.64	0.45
1:A:269:ILE:HD12	1:A:324:GLN:HG2	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:62:HIS:CG	1:D:198[A]:GLU:HG2	2.51	0.45
1:C:222:THR:HG22	1:C:223:ALA:N	2.31	0.45
1:D:342:THR:HB	3:D:1828:HOH:O	2.17	0.45
1:F:262:ILE:CD1	1:F:298:LEU:HD11	2.47	0.45
1:C:338:VAL:O	1:C:342:THR:HG22	2.17	0.45
1:F:116:GLN:HE21	1:F:116:GLN:HB3	1.69	0.45
1:C:62:HIS:CE1	1:C:167:ASP:HB2	2.52	0.45
1:E:250:LYS:HD2	1:E:250:LYS:HA	1.84	0.45
1:C:300:MSE:CE	1:C:322:MSE:HE1	2.47	0.44
1:A:345:ARG:CG	1:A:345:ARG:HH21	2.24	0.44
1:A:261:TRP:CH2	1:A:333:LEU:HD13	2.52	0.44
1:C:50:ASN:HD22	1:C:50:ASN:H	1.65	0.44
1:B:36:GLU:HG3	1:B:38:ARG:HH12	1.81	0.44
1:D:14:ALA:HB1	1:D:19:GLU:HA	1.98	0.44
1:F:252:LEU:HD13	1:F:289:HIS:CG	2.52	0.44
1:E:62:HIS:CE1	1:E:167:ASP:HB2	2.52	0.44
1:A:157:HIS:ND1	3:A:1507:HOH:O	2.36	0.44
1:F:88:ARG:NH2	3:F:2011:HOH:O	2.48	0.44
1:D:220:LEU:HA	1:D:300:MSE:O	2.17	0.44
1:D:50:ASN:H	1:D:50:ASN:HD22	1.66	0.43
1:B:1:MSE:HE2	1:B:172:TYR:OH	2.18	0.43
1:E:177:LEU:HD11	1:E:326:LEU:HD13	2.01	0.43
1:A:276:ASP:OD2	1:A:278:PHE:HE1	2.00	0.43
1:A:248:SER:OG	1:A:277:MSE:HG2	2.17	0.43
1:A:292:GLY:O	1:B:210:ARG:HD2	2.18	0.43
1:C:334:THR:O	1:C:338:VAL:HG13	2.19	0.43
1:C:35:LYS:HE2	1:C:49:LEU:O	2.18	0.43
1:A:48:ARG:HD3	1:A:191:TRP:CZ2	2.53	0.43
1:E:58:MSE:HE1	1:E:209:THR:OG1	2.19	0.42
1:B:62:HIS:CE1	1:B:167:ASP:HB2	2.54	0.42
1:A:68:PHE:HB2	1:A:146:VAL:HB	2.01	0.42
1:A:322:MSE:HE2	1:A:326:LEU:HG	2.00	0.42
1:B:255:PRO:HA	1:B:256:PRO:HD3	1.91	0.42
1:C:1:MSE:HA	1:C:1:MSE:HE2	2.01	0.42
1:D:250:LYS:O	1:E:203:ARG:NH2	2.52	0.42
1:B:248:SER:HB2	1:B:253:ILE:HD13	2.01	0.42
1:A:89:MSE:HE3	1:A:120:VAL:N	2.24	0.42
1:A:166:ASP:HA	1:A:167:ASP:HA	1.87	0.42
1:F:89:MSE:HE3	1:F:119:ASP:OD1	2.20	0.42
1:B:157:HIS:ND1	3:B:1568:HOH:O	2.35	0.42
1:E:289:HIS:NE2	1:E:290:LEU:HD13	2.35	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:71:ARG:HD3	3:E:1905:HOH:O	2.19	0.41
1:C:88:ARG:NE	1:C:307:GLY:O	2.53	0.41
1:F:289:HIS:CD2	1:F:290:LEU:HD13	2.55	0.41
1:D:276:ASP:OD2	1:D:278:PHE:HE1	2.03	0.41
1:C:322:MSE:HE2	1:C:326:LEU:HG	2.02	0.41
1:E:50:ASN:H	1:E:50:ASN:HD22	1.67	0.41
1:E:219:VAL:CG1	1:E:284:ASP:HB3	2.49	0.41
1:B:89:MSE:SE	1:B:120:VAL:H	2.53	0.41
1:B:198[B]:GLU:OE1	1:B:205:GLY:N	2.54	0.41
1:B:118:ASN:C	1:B:118:ASN:ND2	2.74	0.41
1:D:116:GLN:HB3	1:D:116:GLN:HE21	1.65	0.41
1:C:218:ILE:CG2	1:C:300:MSE:HE2	2.51	0.41
1:F:68:PHE:HB2	1:F:146:VAL:HB	2.03	0.41
1:E:261:TRP:CH2	1:E:333:LEU:HD13	2.56	0.41
1:A:251:SER:CB	1:A:286:GLY:HA3	2.42	0.41
1:F:62:HIS:NE2	1:F:167:ASP:HB2	2.37	0.41
1:F:334:THR:O	1:F:338:VAL:HG13	2.22	0.40
1:E:36:GLU:CD	1:E:36:GLU:H	2.25	0.40
1:D:334:THR:O	1:D:338:VAL:HG13	2.21	0.40
1:A:14:ALA:HB1	1:A:19:GLU:HA	2.03	0.40
1:C:261:TRP:CH2	1:C:333:LEU:HD13	2.56	0.40
1:A:62:HIS:HB3	1:A:198[A]:GLU:HG3	2.04	0.40
1:F:289:HIS:NE2	1:F:290:LEU:HD13	2.36	0.40
1:D:322:MSE:HE2	1:D:326:LEU:HG	2.03	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	348/348 (100%)	340 (98%)	8 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	B	348/348 (100%)	342 (98%)	6 (2%)	0	100	100
1	C	348/348 (100%)	343 (99%)	5 (1%)	0	100	100
1	D	348/348 (100%)	342 (98%)	6 (2%)	0	100	100
1	E	348/348 (100%)	340 (98%)	8 (2%)	0	100	100
1	F	348/348 (100%)	342 (98%)	5 (1%)	1 (0%)	46	42
All	All	2088/2088 (100%)	2049 (98%)	38 (2%)	1 (0%)	100	100

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	F	203	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	286/272 (105%)	267 (93%)	19 (7%)	21	14
1	B	286/272 (105%)	267 (93%)	19 (7%)	21	14
1	C	286/272 (105%)	269 (94%)	17 (6%)	24	18
1	D	286/272 (105%)	269 (94%)	17 (6%)	24	18
1	E	286/272 (105%)	268 (94%)	18 (6%)	22	16
1	F	286/272 (105%)	272 (95%)	14 (5%)	31	26
All	All	1716/1632 (105%)	1612 (94%)	104 (6%)	24	17

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

Mol	Chain	Res	Type
1	A	24	GLN
1	A	26	LEU
1	A	27	LEU
1	A	35	LYS
1	A	46	LEU

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Mol	Chain	Res	Type
1	A	49	LEU
1	A	50	ASN
1	A	123	MSE
1	A	155	LEU
1	A	177	LEU
1	A	183	ASP
1	A	186	LEU
1	A	227	LYS
1	A	247	LEU
1	A	290	LEU
1	A	333	LEU
1	A	338	VAL
1	A	340	GLN
1	A	345	ARG
1	B	24	GLN
1	B	26	LEU
1	B	27	LEU
1	B	35	LYS
1	B	46	LEU
1	B	49	LEU
1	B	50	ASN
1	B	111	LEU
1	B	118	ASN
1	B	155	LEU
1	B	181	LEU
1	B	186	LEU
1	B	202	LEU
1	B	247	LEU
1	B	280	ASN
1	B	290	LEU
1	B	298	LEU
1	B	333	LEU
1	B	340	GLN
1	C	26	LEU
1	C	27	LEU
1	C	35	LYS
1	C	46	LEU
1	C	49	LEU
1	C	50	ASN
1	C	116	GLN
1	C	183	ASP
1	C	186	LEU

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Mol	Chain	Res	Type
1	C	203	ARG
1	C	247	LEU
1	C	284	ASP
1	C	290	LEU
1	C	298	LEU
1	C	333	LEU
1	C	338	VAL
1	C	340	GLN
1	D	26	LEU
1	D	27	LEU
1	D	35	LYS
1	D	46	LEU
1	D	49	LEU
1	D	50	ASN
1	D	186	LEU
1	D	198[A]	GLU
1	D	198[B]	GLU
1	D	203	ARG
1	D	247	LEU
1	D	284	ASP
1	D	290	LEU
1	D	298	LEU
1	D	300	MSE
1	D	333	LEU
1	D	338	VAL
1	E	26	LEU
1	E	27	LEU
1	E	35	LYS
1	E	36	GLU
1	E	46	LEU
1	E	49	LEU
1	E	50	ASN
1	E	186	LEU
1	E	198[A]	GLU
1	E	198[B]	GLU
1	E	202	LEU
1	E	247	LEU
1	E	290	LEU
1	E	298	LEU
1	E	300	MSE
1	E	333	LEU
1	E	338	VAL

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Mol	Chain	Res	Type
1	E	340	GLN
1	F	26	LEU
1	F	27	LEU
1	F	35	LYS
1	F	46	LEU
1	F	49	LEU
1	F	50	ASN
1	F	88	ARG
1	F	118	ASN
1	F	186	LEU
1	F	202	LEU
1	F	247	LEU
1	F	290	LEU
1	F	333	LEU
1	F	338	VAL

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (34) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	24	GLN
1	A	50	ASN
1	A	95	GLN
1	A	137	GLN
1	A	182	HIS
1	B	50	ASN
1	B	95	GLN
1	B	116	GLN
1	B	118	ASN
1	B	137	GLN
1	B	182	HIS
1	B	206	GLN
1	C	50	ASN
1	C	95	GLN
1	C	116	GLN
1	C	137	GLN
1	C	206	GLN
1	D	50	ASN
1	D	95	GLN
1	D	116	GLN
1	D	137	GLN
1	D	182	HIS
1	D	206	GLN

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Mol	Chain	Res	Type
1	D	340	GLN
1	E	50	ASN
1	E	95	GLN
1	E	137	GLN
1	E	182	HIS
1	E	206	GLN
1	F	50	ASN
1	F	95	GLN
1	F	116	GLN
1	F	182	HIS
1	F	206	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

Of 12 ligands modelled in this entry, 12 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers

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	334/348 (95%)	0.77	25 (7%)	17	23	25, 33, 54, 64	2 (0%)
1	B	334/348 (95%)	0.76	23 (6%)	20	27	24, 33, 54, 65	1 (0%)
1	C	334/348 (95%)	0.74	24 (7%)	18	25	24, 33, 54, 65	1 (0%)
1	D	334/348 (95%)	0.78	31 (9%)	11	17	25, 33, 53, 65	1 (0%)
1	E	334/348 (95%)	0.75	21 (6%)	23	32	25, 33, 54, 65	1 (0%)
1	F	334/348 (95%)	0.79	19 (5%)	27	37	25, 33, 54, 65	1 (0%)
All	All	2004/2088 (95%)	0.77	143 (7%)	19	26	24, 33, 54, 65	7 (0%)

All (143) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	286	GLY	7.2
1	C	118	ASN	6.6
1	F	282	GLY	6.2
1	F	202	LEU	5.8
1	C	282	GLY	5.8
1	A	341	LEU	5.3
1	A	278	PHE	5.2
1	E	341	LEU	5.2
1	E	282	GLY	4.9
1	E	183	ASP	4.7
1	F	280	ASN	4.7
1	A	117	GLY	4.7
1	E	121	SER	4.6
1	F	281	GLY	4.4
1	B	204	GLY	4.4
1	B	282	GLY	4.3
1	B	202	LEU	4.3
1	D	118	ASN	4.1
1	B	280	ASN	4.1

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Mol	Chain	Res	Type	RSRZ
1	B	284	ASP	4.0
1	E	278	PHE	3.9
1	F	284	ASP	3.9
1	C	278	PHE	3.8
1	E	284	ASP	3.7
1	D	26	LEU	3.6
1	D	281	GLY	3.5
1	D	202	LEU	3.5
1	A	36	GLU	3.5
1	F	183	ASP	3.4
1	D	177	LEU	3.4
1	F	47	ILE	3.4
1	C	281	GLY	3.3
1	E	36	GLU	3.3
1	B	121	SER	3.3
1	A	204	GLY	3.3
1	C	202	LEU	3.3
1	C	183	ASP	3.3
1	E	116	GLN	3.2
1	C	345	ARG	3.2
1	D	286	GLY	3.2
1	D	183	ASP	3.1
1	E	118	ASN	3.1
1	F	75	ARG	3.1
1	F	283	THR	3.1
1	A	118	ASN	3.1
1	C	286	GLY	3.1
1	B	278	PHE	3.0
1	F	46	LEU	3.0
1	B	116	GLN	3.0
1	A	120	VAL	3.0
1	A	226	ALA	3.0
1	F	342	THR	2.9
1	C	26	LEU	2.9
1	E	122	ALA	2.9
1	A	75	ARG	2.9
1	B	118	ASN	2.9
1	D	42	LEU	2.8
1	F	118	ASN	2.8
1	B	47	ILE	2.8
1	C	341	LEU	2.8
1	C	86	ASN	2.8

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Mol	Chain	Res	Type	RSRZ
1	E	286	GLY	2.8
1	F	114	ASP	2.8
1	F	115	ARG	2.7
1	A	183	ASP	2.7
1	E	345	ARG	2.7
1	A	59	ILE	2.6
1	C	284	ASP	2.6
1	D	114	ASP	2.6
1	B	201	GLY	2.6
1	F	286	GLY	2.6
1	A	222	THR	2.6
1	D	284	ASP	2.6
1	E	233	ALA	2.6
1	E	47	ILE	2.6
1	D	0	ALA	2.5
1	B	120	VAL	2.5
1	D	338	VAL	2.5
1	D	203	ARG	2.5
1	C	30	ALA	2.5
1	B	112	ASP	2.5
1	D	46	LEU	2.5
1	A	119	ASP	2.5
1	D	280	ASN	2.5
1	A	205	GLY	2.5
1	A	282	GLY	2.5
1	C	231	TYR	2.4
1	E	177	LEU	2.4
1	C	280	ASN	2.4
1	F	333	LEU	2.4
1	C	47	ILE	2.4
1	D	75	ARG	2.4
1	C	181	LEU	2.3
1	B	184	ALA	2.3
1	A	345	ARG	2.3
1	B	283	THR	2.3
1	B	341	LEU	2.3
1	C	27	LEU	2.3
1	E	307	GLY	2.3
1	F	171	CYS	2.3
1	D	253	ILE	2.3
1	B	75	ARG	2.3
1	D	170	SER	2.2

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Mol	Chain	Res	Type	RSRZ
1	D	282	GLY	2.2
1	D	341	LEU	2.2
1	B	342	THR	2.2
1	A	203	ARG	2.2
1	A	42	LEU	2.2
1	A	340	GLN	2.2
1	E	317	ARG	2.2
1	B	111	LEU	2.2
1	C	177	LEU	2.2
1	E	3	LEU	2.2
1	D	279	SER	2.2
1	E	336	GLU	2.2
1	B	286	GLY	2.1
1	D	105	CYS	2.1
1	D	181	LEU	2.1
1	D	287	ALA	2.1
1	D	262	ILE	2.1
1	D	119	ASP	2.1
1	F	297	THR	2.1
1	C	37	VAL	2.1
1	D	157	HIS	2.1
1	A	86	ASN	2.1
1	D	137	GLN	2.1
1	B	178	LEU	2.1
1	D	103[A]	GLU	2.1
1	D	121	SER	2.1
1	A	295	VAL	2.1
1	C	298	LEU	2.1
1	A	122	ALA	2.1
1	B	60	CYS	2.1
1	A	218	ILE	2.0
1	E	127	ILE	2.0
1	A	192	LEU	2.0
1	C	203	ARG	2.0
1	E	280	ASN	2.0
1	F	240	GLY	2.0
1	B	37	VAL	2.0
1	C	125	VAL	2.0
1	D	224	CYS	2.0
1	C	279	SER	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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95^{th} 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	LLDF	B-factors(Å^2)	Q<0.9
2	ZN	C	1647	1/1	0.82	0.10	-1.28	47,47,47,47	1
2	ZN	B	1546	1/1	0.74	0.09	-1.43	36,36,36,36	1
2	ZN	F	1947	1/1	0.76	0.08	-1.57	49,49,49,49	1
2	ZN	D	1747	1/1	0.57	0.10	-1.65	48,48,48,48	1
2	ZN	B	1547	1/1	0.82	0.07	-1.74	49,49,49,49	1
2	ZN	A	1446	1/1	0.88	0.06	-1.78	37,37,37,37	1
2	ZN	F	1946	1/1	0.79	0.07	-2.24	36,36,36,36	1
2	ZN	D	1746	1/1	0.89	0.06	-2.40	37,37,37,37	1
2	ZN	C	1646	1/1	0.98	0.03	-3.29	38,38,38,38	1
2	ZN	E	1846	1/1	0.81	0.07	-4.05	36,36,36,36	1
2	ZN	A	1447	1/1	0.87	0.08	-	47,47,47,47	1
2	ZN	E	1847	1/1	0.96	0.10	-	49,49,49,49	1

6.5 Other polymers (i)

There are no such residues in this entry.