Full wwPDB X-ray Structure Validation Report (i)

Feb 1, 2016 – 03:53 PM GMT

PDB ID	:	4DQY
Title	:	Structure of Human PARP-1 bound to a DNA double strand break
Authors	:	Langelier, M.F.; Pascal, J.M.
Deposited on	:	2012-02-16
Resolution	:	3.25 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:

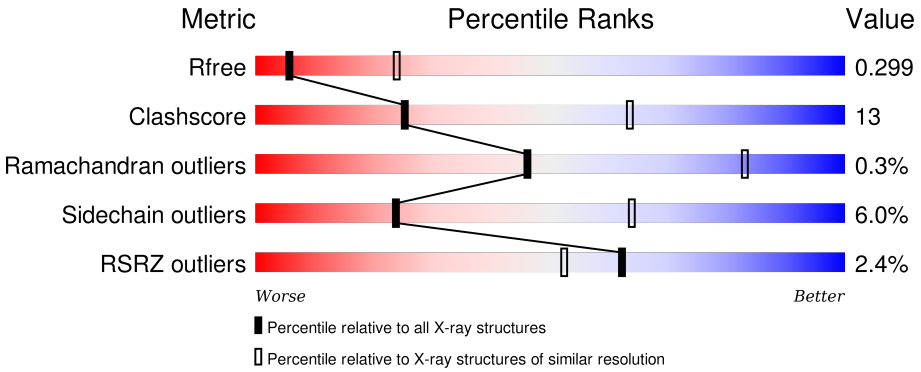
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	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 3.25 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	1624 (3.32-3.20)
Clashscore	102246	1806 (3.32-3.20)
Ramachandran outliers	100387	1773 (3.32-3.20)
Sidechain outliers	100360	1771 (3.32-3.20)
RSRZ outliers	91569	1632 (3.32-3.20)

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	116	57% 14% • 26%
1	D	116	2% 54% 16% • 26%
2	B	160	63% 20% • 15%
2	E	160	3% 66% 17% • 15%
3	C	506	% 64% 24% • 10%

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Mol	Chain	Length	Quality of chain
3	F	506	5% 65% 23% 10%
4	M	26	73% 23%
4	N	26	81% 19%

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
6	EDO	C	1101	-	-	-	X

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 11750 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 Poly [ADP-ribose] polymerase 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	86	Total	C	N	O	S	0	1	0
			712	452	128	126	6			
1	D	86	Total	C	N	O	S	0	1	0
			712	452	128	126	6			

There are 40 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-19	MET	-	EXPRESSION TAG	UNP P09874
A	-18	GLY	-	EXPRESSION TAG	UNP P09874
A	-17	SER	-	EXPRESSION TAG	UNP P09874
A	-16	SER	-	EXPRESSION TAG	UNP P09874
A	-15	HIS	-	EXPRESSION TAG	UNP P09874
A	-14	HIS	-	EXPRESSION TAG	UNP P09874
A	-13	HIS	-	EXPRESSION TAG	UNP P09874
A	-12	HIS	-	EXPRESSION TAG	UNP P09874
A	-11	HIS	-	EXPRESSION TAG	UNP P09874
A	-10	HIS	-	EXPRESSION TAG	UNP P09874
A	-9	SER	-	EXPRESSION TAG	UNP P09874
A	-8	SER	-	EXPRESSION TAG	UNP P09874
A	-7	GLY	-	EXPRESSION TAG	UNP P09874
A	-6	LEU	-	EXPRESSION TAG	UNP P09874
A	-5	VAL	-	EXPRESSION TAG	UNP P09874
A	-4	PRO	-	EXPRESSION TAG	UNP P09874
A	-3	ARG	-	EXPRESSION TAG	UNP P09874
A	-2	GLY	-	EXPRESSION TAG	UNP P09874
A	-1	SER	-	EXPRESSION TAG	UNP P09874
A	0	HIS	-	EXPRESSION TAG	UNP P09874
D	-19	MET	-	EXPRESSION TAG	UNP P09874
D	-18	GLY	-	EXPRESSION TAG	UNP P09874
D	-17	SER	-	EXPRESSION TAG	UNP P09874
D	-16	SER	-	EXPRESSION TAG	UNP P09874
D	-15	HIS	-	EXPRESSION TAG	UNP P09874

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Chain	Residue	Modelled	Actual	Comment	Reference
D	-14	HIS	-	EXPRESSION TAG	UNP P09874
D	-13	HIS	-	EXPRESSION TAG	UNP P09874
D	-12	HIS	-	EXPRESSION TAG	UNP P09874
D	-11	HIS	-	EXPRESSION TAG	UNP P09874
D	-10	HIS	-	EXPRESSION TAG	UNP P09874
D	-9	SER	-	EXPRESSION TAG	UNP P09874
D	-8	SER	-	EXPRESSION TAG	UNP P09874
D	-7	GLY	-	EXPRESSION TAG	UNP P09874
D	-6	LEU	-	EXPRESSION TAG	UNP P09874
D	-5	VAL	-	EXPRESSION TAG	UNP P09874
D	-4	PRO	-	EXPRESSION TAG	UNP P09874
D	-3	ARG	-	EXPRESSION TAG	UNP P09874
D	-2	GLY	-	EXPRESSION TAG	UNP P09874
D	-1	SER	-	EXPRESSION TAG	UNP P09874
D	0	HIS	-	EXPRESSION TAG	UNP P09874

- Molecule 2 is a protein called Poly [ADP-ribose] polymerase 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	136	Total	C	N	O	S	0	0	0
			1043	658	177	201	7			
2	E	136	Total	C	N	O	S	0	0	0
			1043	658	177	201	7			

There are 18 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	215	MET	-	INITIATING METHIONINE	UNP P09874
B	367	LEU	-	EXPRESSION TAG	UNP P09874
B	368	GLU	-	EXPRESSION TAG	UNP P09874
B	369	HIS	-	EXPRESSION TAG	UNP P09874
B	370	HIS	-	EXPRESSION TAG	UNP P09874
B	371	HIS	-	EXPRESSION TAG	UNP P09874
B	372	HIS	-	EXPRESSION TAG	UNP P09874
B	373	HIS	-	EXPRESSION TAG	UNP P09874
B	374	HIS	-	EXPRESSION TAG	UNP P09874
E	215	MET	-	INITIATING METHIONINE	UNP P09874
E	367	LEU	-	EXPRESSION TAG	UNP P09874
E	368	GLU	-	EXPRESSION TAG	UNP P09874
E	369	HIS	-	EXPRESSION TAG	UNP P09874
E	370	HIS	-	EXPRESSION TAG	UNP P09874
E	371	HIS	-	EXPRESSION TAG	UNP P09874

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Chain	Residue	Modelled	Actual	Comment	Reference
E	372	HIS	-	EXPRESSION TAG	UNP P09874
E	373	HIS	-	EXPRESSION TAG	UNP P09874
E	374	HIS	-	EXPRESSION TAG	UNP P09874

- Molecule 3 is a protein called Poly [ADP-ribose] polymerase 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	456	Total	C	N	O	S	0	0	0
			3586	2296	605	672	13			
3	F	456	Total	C	N	O	S	0	0	0
			3586	2296	605	672	13			

There are 20 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	517	MET	-	INITIATING METHIONINE	UNP P09874
C	762	ALA	VAL	SEE REMARK 999	UNP P09874
C	1015	LEU	-	EXPRESSION TAG	UNP P09874
C	1016	GLU	-	EXPRESSION TAG	UNP P09874
C	1017	HIS	-	EXPRESSION TAG	UNP P09874
C	1018	HIS	-	EXPRESSION TAG	UNP P09874
C	1019	HIS	-	EXPRESSION TAG	UNP P09874
C	1020	HIS	-	EXPRESSION TAG	UNP P09874
C	1021	HIS	-	EXPRESSION TAG	UNP P09874
C	1022	HIS	-	EXPRESSION TAG	UNP P09874
F	517	MET	-	INITIATING METHIONINE	UNP P09874
F	762	ALA	VAL	SEE REMARK 999	UNP P09874
F	1015	LEU	-	EXPRESSION TAG	UNP P09874
F	1016	GLU	-	EXPRESSION TAG	UNP P09874
F	1017	HIS	-	EXPRESSION TAG	UNP P09874
F	1018	HIS	-	EXPRESSION TAG	UNP P09874
F	1019	HIS	-	EXPRESSION TAG	UNP P09874
F	1020	HIS	-	EXPRESSION TAG	UNP P09874
F	1021	HIS	-	EXPRESSION TAG	UNP P09874
F	1022	HIS	-	EXPRESSION TAG	UNP P09874

- Molecule 4 is a DNA chain called DNA (26-MER).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	M	26	Total	C	N	O	P	0	0	0
			530	251	100	154	25			

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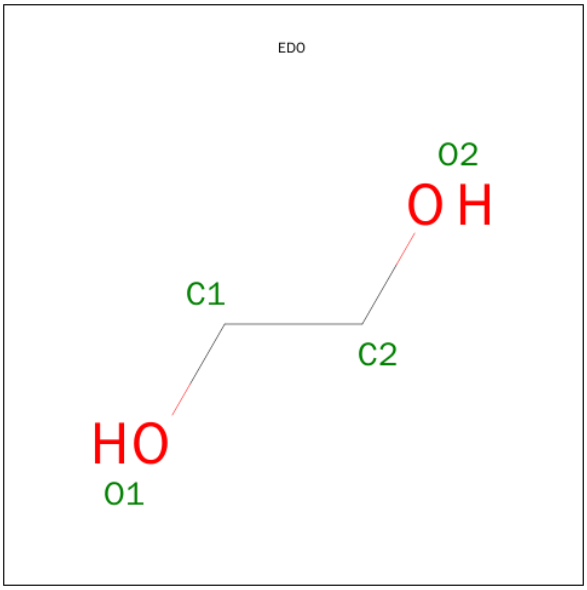
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	N	26	Total	C	N	O	P	0	0	0
			530	251	100	154	25			

- Molecule 5 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	B	1	Total	Zn	0	0
			1	1		
5	A	1	Total	Zn	0	0
			1	1		
5	D	1	Total	Zn	0	0
			1	1		
5	E	1	Total	Zn	0	0
			1	1		

- Molecule 6 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: $C_2H_6O_2$).



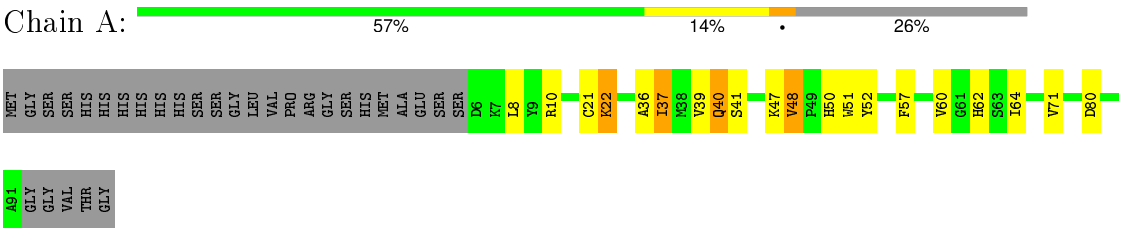
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	C	1	Total	C	O	0	0
			4	2	2		

3 Residue-property plots

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.

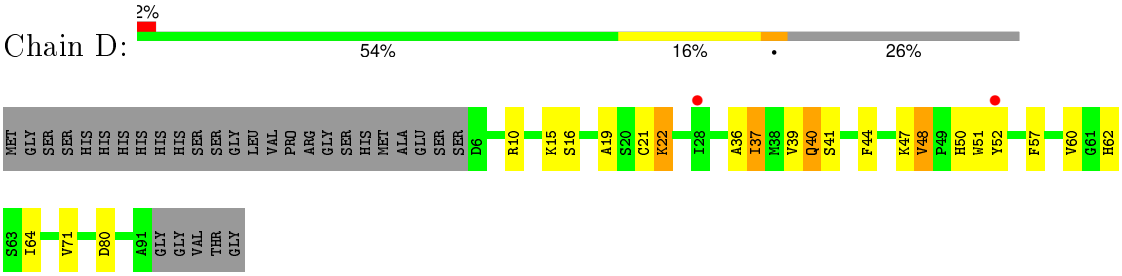
- Molecule 1: Poly [ADP-ribose] polymerase 1

Chain A:



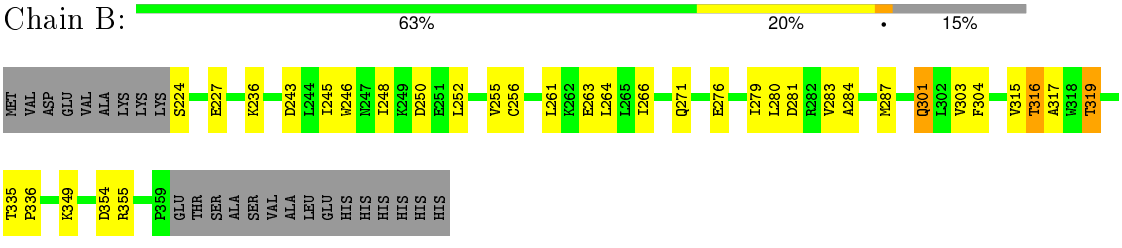
- Molecule 1: Poly [ADP-ribose] polymerase 1

Chain D:



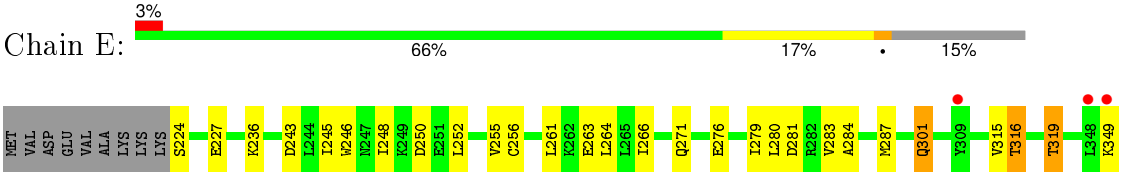
- Molecule 2: Poly [ADP-ribose] polymerase 1

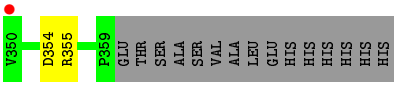
Chain B:



- Molecule 2: Poly [ADP-ribose] polymerase 1

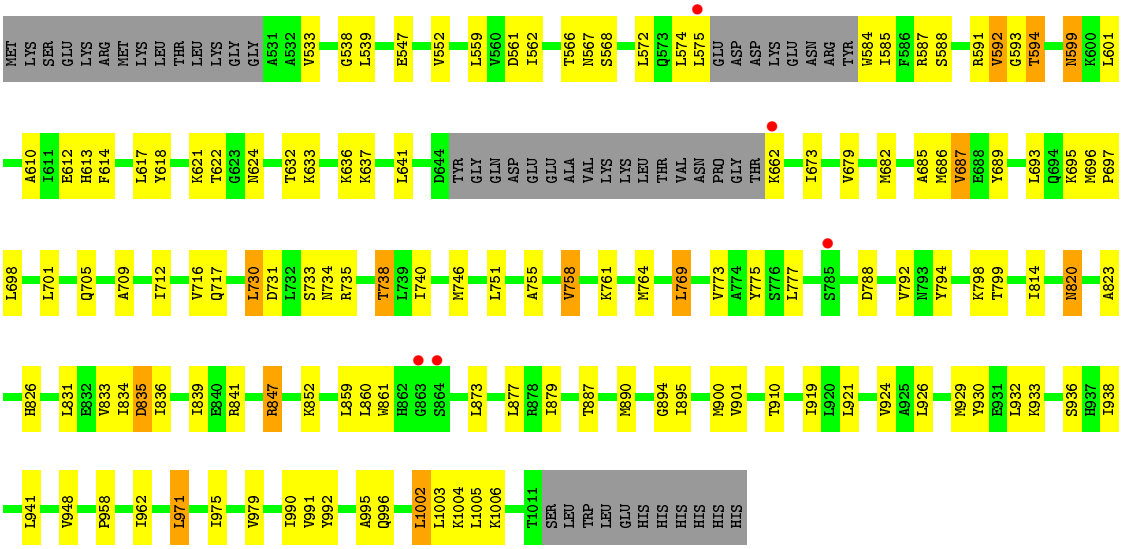
Chain E:





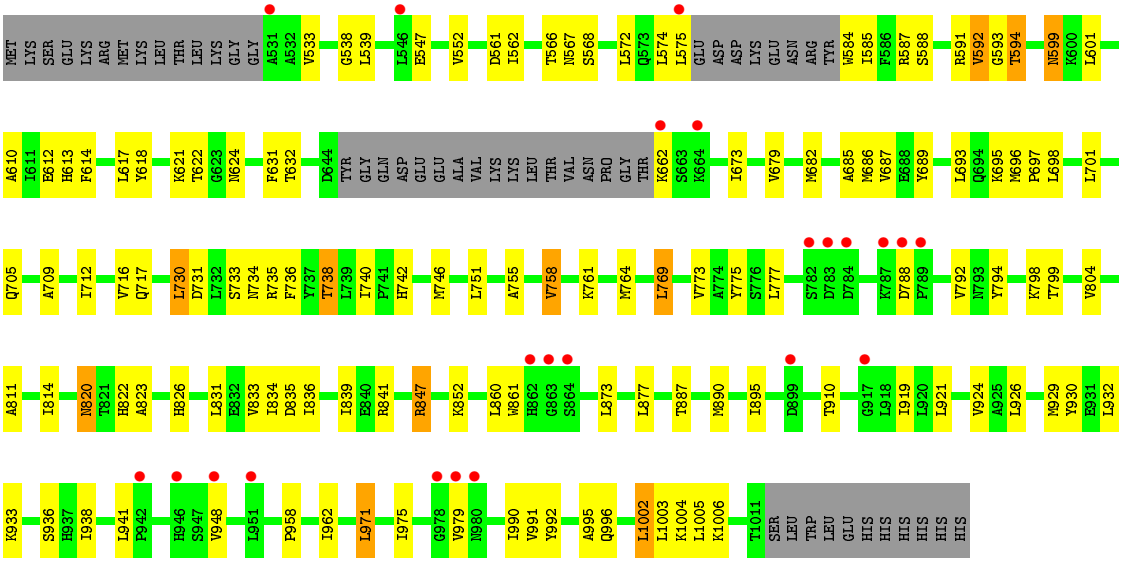
• Molecule 3: Poly [ADP-ribose] polymerase 1

Chain C:



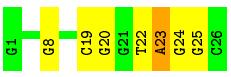
• Molecule 3: Poly [ADP-ribose] polymerase 1

Chain F:



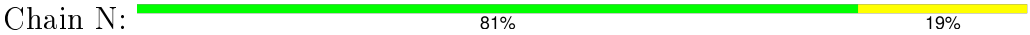
• Molecule 4: DNA (26-MER)

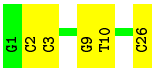
Chain M:



• Molecule 4: DNA (26-MER)

Chain N:





4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	65.09Å 112.97Å 294.72Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	20.00 – 3.25 32.06 – 3.24	Depositor EDS
% Data completeness (in resolution range)	94.4 (20.00-3.25) 94.1 (32.06-3.24)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.28 (at 3.24Å)	Xtriage
Refinement program	REFMAC 5.6.0119	Depositor
R, R_{free}	0.238 , 0.304 0.237 , 0.299	Depositor DCC
R_{free} test set	1681 reflections (5.33%)	DCC
Wilson B-factor (Å^2)	114.4	Xtriage
Anisotropy	0.428	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.24 , 97.8	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.46$, $< L^2 > = 0.29$	Xtriage
Outliers	1 of 33513 reflections (0.003%)	Xtriage
F_o,F_c correlation	0.93	EDS
Total number of atoms	11750	wwPDB-VP
Average B, all atoms (Å^2)	178.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 12.95% 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, EDO

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	0.57	0/735	0.56	0/986
1	D	0.55	0/735	0.52	0/986
2	B	0.44	0/1060	0.53	0/1430
2	E	0.43	0/1060	0.50	0/1430
3	C	0.43	0/3660	0.51	0/4940
3	F	0.41	0/3660	0.49	0/4940
4	M	0.33	0/594	0.88	2/915 (0.2%)
4	N	0.30	0/594	0.81	0/915
All	All	0.43	0/12098	0.56	2/16542 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	M	8	DG	P-O3'-C3'	7.75	129.01	119.70
4	M	23	DA	P-O3'-C3'	6.07	126.98	119.70

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	712	0	695	20	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	D	712	0	695	21	0
2	B	1043	0	1017	22	0
2	E	1043	0	1017	21	0
3	C	3586	0	3607	107	0
3	F	3586	0	3607	101	0
4	M	530	0	292	6	0
4	N	530	0	292	4	0
5	A	1	0	0	0	0
5	B	1	0	0	0	0
5	D	1	0	0	0	0
5	E	1	0	0	0	0
6	C	4	0	6	0	0
All	All	11750	0	11228	290	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 13.

All (290) 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)
3:C:926:LEU:HD13	3:C:929:MET:HE3	1.34	1.08
3:F:926:LEU:HD13	3:F:929:MET:HE3	1.40	1.02
3:F:574:LEU:HD11	3:F:610:ALA:HB1	1.43	0.99
3:C:574:LEU:HD11	3:C:610:ALA:HB1	1.45	0.98
2:E:319:THR:HG21	3:F:731:ASP:HA	1.47	0.95
3:F:594:THR:HG21	3:F:746:MET:HE3	1.65	0.79
3:C:679:VAL:HG11	3:C:775:TYR:CZ	2.21	0.76
3:C:831:LEU:HD12	3:C:1005:LEU:HD23	1.68	0.76
3:C:755:ALA:O	3:C:758:VAL:HG13	1.86	0.75
3:C:709:ALA:HB1	3:C:740:ILE:HD11	1.69	0.75
3:F:709:ALA:HB1	3:F:740:ILE:HD11	1.68	0.75
3:F:814:ILE:HG21	3:F:836:ILE:HD12	1.70	0.74
3:C:814:ILE:HG21	3:C:836:ILE:HD12	1.70	0.74
3:F:679:VAL:HG11	3:F:775:TYR:CZ	2.23	0.73
3:C:712:ILE:O	3:C:716:VAL:HG23	1.87	0.73
3:C:618:TYR:O	3:C:622:THR:HG22	1.88	0.73
3:F:712:ILE:O	3:F:716:VAL:HG23	1.89	0.73
3:C:926:LEU:HD13	3:C:929:MET:CE	2.17	0.72
3:F:618:TYR:O	3:F:622:THR:HG22	1.89	0.72
2:E:316:THR:HG21	3:F:731:ASP:OD1	1.89	0.72
3:F:755:ALA:O	3:F:758:VAL:HG13	1.90	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:64:ILE:HD13	1:A:71:VAL:CG2	2.20	0.70
3:F:831:LEU:HD12	3:F:1005:LEU:HD23	1.73	0.70
3:F:618:TYR:CE2	3:F:622:THR:HG21	2.27	0.70
3:C:539:LEU:HD11	3:C:601:LEU:HD21	1.74	0.70
3:F:926:LEU:HD13	3:F:929:MET:CE	2.21	0.70
1:D:64:ILE:HD13	1:D:71:VAL:CG2	2.22	0.69
3:C:730:LEU:HD12	3:C:734:ASN:ND2	2.08	0.69
3:C:682:MET:O	3:C:685:ALA:HB3	1.93	0.69
3:F:574:LEU:CD1	3:F:610:ALA:HB1	2.22	0.69
1:A:37:ILE:C	1:A:37:ILE:HD13	2.13	0.69
3:C:730:LEU:HD12	3:C:734:ASN:HD21	1.58	0.68
2:E:319:THR:CG2	3:F:731:ASP:HA	2.22	0.68
3:F:730:LEU:HD12	3:F:734:ASN:ND2	2.10	0.67
3:C:622:THR:HG23	3:C:624:ASN:H	1.60	0.67
3:F:622:THR:HG23	3:F:624:ASN:H	1.60	0.67
3:C:618:TYR:CE2	3:C:622:THR:HG21	2.30	0.67
2:E:319:THR:HG21	3:F:731:ASP:CA	2.23	0.66
3:C:709:ALA:CB	3:C:740:ILE:HD11	2.25	0.66
3:C:562:ILE:HD11	3:C:733:SER:HB3	1.77	0.66
3:F:539:LEU:HD11	3:F:601:LEU:HD21	1.77	0.66
3:F:709:ALA:CB	3:F:740:ILE:HD11	2.25	0.65
3:F:734:ASN:O	3:F:738:THR:OG1	2.14	0.65
2:B:319:THR:HG21	3:C:731:ASP:HA	1.79	0.65
3:C:574:LEU:CD1	3:C:610:ALA:HB1	2.24	0.65
3:F:682:MET:O	3:F:685:ALA:HB3	1.97	0.65
3:F:962:ILE:HD13	3:F:971:LEU:HD11	1.79	0.65
1:A:36:ALA:HB2	1:A:51:TRP:CZ3	2.32	0.64
1:D:36:ALA:HB2	1:D:51:TRP:CZ3	2.33	0.64
3:C:687:VAL:HG22	3:C:693:LEU:CD2	2.28	0.64
3:C:924:VAL:HG13	3:C:924:VAL:O	1.97	0.63
1:A:57:PHE:O	1:A:60:VAL:HG22	1.99	0.63
3:C:962:ILE:HD13	3:C:971:LEU:HD11	1.79	0.62
3:F:730:LEU:HD12	3:F:734:ASN:HD21	1.65	0.62
3:C:734:ASN:O	3:C:738:THR:OG1	2.17	0.62
3:F:591:ARG:HD3	3:F:746:MET:HE2	1.81	0.62
1:D:37:ILE:HD13	1:D:37:ILE:C	2.20	0.62
3:F:919:ILE:HG22	3:F:1005:LEU:HD11	1.81	0.62
3:C:686:MET:HA	3:C:686:MET:HE2	1.82	0.61
3:F:562:ILE:HD11	3:F:733:SER:HB3	1.82	0.61
3:C:591:ARG:HD3	3:C:746:MET:CE	2.31	0.61
3:F:587:ARG:HD3	3:F:617:LEU:HD13	1.83	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:57:PHE:O	1:D:60:VAL:HG22	2.01	0.61
3:C:769:LEU:O	3:C:773:VAL:HG23	2.02	0.60
3:C:990:ILE:HD12	3:C:990:ILE:N	2.16	0.60
3:F:701:LEU:HD11	3:F:705:GLN:HE21	1.67	0.60
2:B:319:THR:CG2	3:C:731:ASP:HA	2.32	0.59
3:F:769:LEU:O	3:F:773:VAL:HG23	2.02	0.59
3:F:938:ILE:HD11	3:F:992:TYR:CZ	2.38	0.58
3:F:687:VAL:HG22	3:F:693:LEU:CD2	2.33	0.58
3:F:861:TRP:CD2	3:F:921:LEU:HD21	2.39	0.58
3:C:938:ILE:HD11	3:C:992:TYR:CZ	2.39	0.58
3:F:686:MET:HA	3:F:686:MET:HE2	1.84	0.57
3:F:567:ASN:ND2	3:F:592:VAL:HG13	2.19	0.57
3:C:919:ILE:HG22	3:C:1005:LEU:HD11	1.86	0.57
2:E:245:ILE:HG23	2:E:284:ALA:HB1	1.87	0.57
3:F:839:ILE:HD13	3:F:1002:LEU:HB2	1.87	0.57
2:E:261:LEU:HA	2:E:264:LEU:HD12	1.87	0.56
3:C:701:LEU:HD11	3:C:705:GLN:HE21	1.70	0.56
3:F:624:ASN:HD21	3:F:632:THR:H	1.54	0.56
1:D:36:ALA:HB2	1:D:51:TRP:CE3	2.41	0.56
3:F:860:LEU:HD12	3:F:924:VAL:CG1	2.36	0.56
3:F:958:PRO:HD2	3:F:975:ILE:HD11	1.88	0.56
1:A:22:LYS:HD2	1:A:50:HIS:CG	2.41	0.55
1:D:22:LYS:HD2	1:D:50:HIS:CG	2.41	0.55
3:F:924:VAL:O	3:F:924:VAL:HG13	2.06	0.55
3:C:673:ILE:HD11	3:C:794:TYR:HB2	1.88	0.55
3:C:594:THR:HG21	3:C:746:MET:HE3	1.87	0.55
3:C:587:ARG:HD3	3:C:617:LEU:HD13	1.87	0.55
1:D:19:ALA:HB2	4:M:25:DG:H5"	1.88	0.55
2:B:261:LEU:HA	2:B:264:LEU:HD12	1.88	0.55
3:C:861:TRP:CD2	3:C:921:LEU:HD21	2.42	0.54
3:F:673:ILE:HD11	3:F:794:TYR:HB2	1.88	0.54
3:F:696:MET:N	3:F:697:PRO:HD2	2.22	0.54
3:C:633:LYS:NZ	3:C:637:LYS:O	2.28	0.54
3:F:990:ILE:HD12	3:F:990:ILE:N	2.23	0.54
3:F:687:VAL:HA	3:F:693:LEU:HD21	1.89	0.54
1:A:48:VAL:CG2	4:N:26:DC:C5	2.91	0.54
3:F:799:THR:HG22	3:F:841:ARG:HA	1.90	0.54
3:F:533:VAL:HG13	3:F:575:LEU:HD21	1.90	0.54
3:C:696:MET:N	3:C:697:PRO:HD2	2.22	0.53
3:F:562:ILE:CD1	3:F:733:SER:HB3	2.39	0.53
3:F:709:ALA:HB1	3:F:740:ILE:CD1	2.38	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:709:ALA:HB1	3:C:740:ILE:CD1	2.37	0.53
3:C:561:ASP:HB3	3:C:566:THR:CG2	2.38	0.53
2:E:248:ILE:CG2	2:E:287:MET:CE	2.86	0.53
4:M:22:DT:H2"	4:M:23:DA:C8	2.44	0.53
3:C:599:ASN:C	3:C:599:ASN:HD22	2.09	0.53
1:A:36:ALA:HB2	1:A:51:TRP:CE3	2.43	0.53
3:C:839:ILE:HD13	3:C:1002:LEU:HB2	1.90	0.53
3:F:761:LYS:HE2	3:F:764:MET:HE1	1.90	0.52
1:A:40:GLN:NE2	1:A:41:SER:O	2.42	0.52
3:C:641:LEU:HD21	3:C:738:THR:O	2.09	0.52
2:B:279:ILE:O	2:B:283:VAL:HG23	2.10	0.52
3:C:533:VAL:HG13	3:C:575:LEU:HD21	1.90	0.52
3:F:938:ILE:HD11	3:F:992:TYR:OH	2.09	0.52
3:C:958:PRO:HD2	3:C:975:ILE:HD11	1.90	0.52
3:F:599:ASN:HD22	3:F:599:ASN:C	2.12	0.52
3:C:539:LEU:CD1	3:C:601:LEU:HD21	2.38	0.52
3:C:687:VAL:HA	3:C:693:LEU:HD21	1.90	0.52
3:F:814:ILE:CG2	3:F:1003:LEU:HD21	2.40	0.52
2:E:315:VAL:HG13	2:E:316:THR:HG22	1.92	0.52
3:C:860:LEU:HD12	3:C:924:VAL:CG1	2.40	0.52
2:B:245:ILE:HG23	2:B:284:ALA:HB1	1.91	0.52
3:C:591:ARG:HD3	3:C:746:MET:HE2	1.91	0.51
3:C:788:ASP:O	3:C:792:VAL:HG23	2.10	0.51
3:C:1005:LEU:N	3:C:1005:LEU:HD12	2.26	0.51
1:D:10[A]:ARG:HB3	1:D:36:ALA:HB3	1.93	0.51
3:C:799:THR:HG22	3:C:841:ARG:HA	1.93	0.51
2:E:248:ILE:CG2	2:E:287:MET:HE1	2.40	0.51
3:C:773:VAL:O	3:C:777:LEU:HD23	2.11	0.51
3:F:788:ASP:O	3:F:792:VAL:HG23	2.10	0.51
3:F:1005:LEU:N	3:F:1005:LEU:HD12	2.25	0.50
3:C:933:LYS:NZ	3:C:979:VAL:HG11	2.26	0.50
3:C:562:ILE:CD1	3:C:733:SER:HB3	2.40	0.50
3:F:938:ILE:CD1	3:F:948:VAL:HG21	2.41	0.50
2:B:319:THR:HG21	3:C:731:ASP:CA	2.42	0.50
3:C:938:ILE:CD1	3:C:948:VAL:HG21	2.42	0.50
2:B:252:LEU:HA	2:B:255:VAL:HG22	1.93	0.50
2:E:248:ILE:HG21	2:E:287:MET:CE	2.42	0.50
3:C:567:ASN:ND2	3:C:592:VAL:HG13	2.27	0.50
3:F:561:ASP:HB3	3:F:566:THR:CG2	2.42	0.50
1:A:10[A]:ARG:HB3	1:A:36:ALA:HB3	1.93	0.50
3:C:561:ASP:HB3	3:C:566:THR:HG22	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:64:ILE:HD13	1:A:71:VAL:HG21	1.93	0.49
2:E:252:LEU:HA	2:E:255:VAL:HG22	1.93	0.49
3:C:624:ASN:HD21	3:C:632:THR:H	1.61	0.49
3:C:696:MET:N	3:C:697:PRO:CD	2.76	0.49
3:F:561:ASP:HB3	3:F:566:THR:HG22	1.94	0.49
3:F:696:MET:N	3:F:697:PRO:CD	2.75	0.49
3:C:814:ILE:CG2	3:C:1003:LEU:HD21	2.42	0.49
3:F:539:LEU:CD1	3:F:601:LEU:HD21	2.41	0.49
3:C:761:LYS:HE2	3:C:764:MET:HE1	1.95	0.49
3:C:591:ARG:HD3	3:C:746:MET:HE1	1.95	0.49
3:C:941:LEU:HD12	3:C:941:LEU:H	1.78	0.49
3:F:933:LYS:NZ	3:F:979:VAL:HG11	2.27	0.49
2:E:279:ILE:O	2:E:283:VAL:HG23	2.13	0.48
3:F:594:THR:HG21	3:F:746:MET:CE	2.42	0.48
3:C:547:GLU:OE2	3:C:552:VAL:HG22	2.13	0.48
3:F:823:ALA:HB3	3:F:826:HIS:HB2	1.96	0.48
3:F:547:GLU:OE2	3:F:552:VAL:HG22	2.14	0.48
4:N:9:DG:H2"	4:N:10:DT:C7	2.44	0.48
2:B:315:VAL:HG13	2:B:316:THR:HG22	1.95	0.48
2:E:276:GLU:O	2:E:280:LEU:HD23	2.14	0.47
3:C:687:VAL:HG22	3:C:693:LEU:HD22	1.96	0.47
3:F:773:VAL:O	3:F:777:LEU:HD23	2.14	0.47
3:F:834:ILE:HD11	3:F:1006:LYS:HB2	1.95	0.47
3:C:814:ILE:HG21	3:C:836:ILE:CD1	2.43	0.47
3:C:687:VAL:HG22	3:C:693:LEU:HD21	1.97	0.47
3:F:574:LEU:HD12	3:F:584:TRP:O	2.14	0.47
3:C:593:GLY:O	3:C:594:THR:HG23	2.14	0.47
3:F:814:ILE:HG21	3:F:836:ILE:CD1	2.42	0.47
3:C:938:ILE:HD11	3:C:992:TYR:OH	2.15	0.47
3:C:585:ILE:HG21	3:C:613:HIS:HD2	1.80	0.47
2:B:335:THR:HG22	2:B:336:PRO:O	2.15	0.46
2:E:316:THR:HG23	2:E:319:THR:H	1.80	0.46
3:F:833:VAL:HG11	3:F:836:ILE:HD11	1.97	0.46
1:A:39:VAL:HG22	1:A:48:VAL:HG12	1.97	0.46
3:C:834:ILE:HD11	3:C:1006:LYS:HB2	1.96	0.46
1:D:40:GLN:NE2	1:D:41:SER:O	2.49	0.46
3:C:574:LEU:HD12	3:C:584:TRP:O	2.14	0.46
3:C:712:ILE:HD13	3:C:735:ARG:HB3	1.98	0.46
3:C:861:TRP:CD2	3:C:901:VAL:HG23	2.50	0.46
2:B:248:ILE:CG2	2:B:287:MET:CE	2.94	0.46
1:D:10[B]:ARG:HB3	1:D:36:ALA:HB3	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:60:VAL:CG2	1:A:62:HIS:CD2	2.98	0.46
3:C:559:LEU:HD13	3:C:633:LYS:HZ1	1.79	0.46
3:C:585:ILE:HD11	3:C:614:PHE:HA	1.98	0.46
3:C:834:ILE:HG22	3:C:835:ASP:OD2	2.16	0.46
1:A:52:TYR:CZ	1:A:60:VAL:HG11	2.51	0.45
3:F:591:ARG:HD3	3:F:746:MET:CE	2.46	0.45
3:C:860:LEU:HD12	3:C:924:VAL:HG11	1.97	0.45
2:B:224:SER:HA	2:B:227:GLU:HB2	1.98	0.45
3:F:572:LEU:HD13	3:F:587:ARG:HG2	1.99	0.45
2:E:243:ASP:HA	2:E:246:TRP:HB2	1.99	0.45
2:B:236:LYS:HA	2:B:236:LYS:NZ	2.31	0.45
3:F:730:LEU:HD22	3:F:751:LEU:HD21	1.98	0.45
2:B:243:ASP:HA	2:B:246:TRP:HB2	1.99	0.45
2:B:263:GLU:HA	2:B:266:ILE:HD12	1.98	0.45
3:C:823:ALA:HB3	3:C:826:HIS:HB2	1.97	0.45
3:C:538:GLY:C	3:C:539:LEU:HD23	2.37	0.45
3:F:877:LEU:HD13	3:F:895:ILE:HG21	1.98	0.45
3:C:538:GLY:O	3:C:539:LEU:HD23	2.17	0.45
1:A:10[B]:ARG:HB3	1:A:36:ALA:HB3	1.97	0.45
1:D:19:ALA:HB2	4:M:25:DG:C5'	2.46	0.45
1:A:60:VAL:HG21	1:A:62:HIS:CD2	2.51	0.45
3:C:833:VAL:HG11	3:C:836:ILE:HD11	1.98	0.44
2:B:316:THR:HG23	2:B:319:THR:H	1.81	0.44
1:A:52:TYR:CE1	1:A:60:VAL:HG11	2.52	0.44
3:C:686:MET:O	3:C:689:TYR:N	2.48	0.44
3:F:574:LEU:HD11	3:F:610:ALA:CB	2.31	0.44
3:F:799:THR:HG21	3:F:873:LEU:HD12	2.00	0.44
3:F:820:ASN:N	3:F:820:ASN:HD22	2.15	0.44
3:F:686:MET:O	3:F:689:TYR:N	2.48	0.44
3:C:847:ARG:HD3	3:C:995:ALA:HA	1.98	0.44
3:F:736:PHE:CZ	3:F:740:ILE:HD12	2.53	0.44
3:C:991:VAL:HB	3:C:996:GLN:HE21	1.82	0.44
3:C:877:LEU:HD13	3:C:895:ILE:HG21	2.00	0.44
2:E:263:GLU:HA	2:E:266:ILE:HD12	2.00	0.44
3:F:585:ILE:HG21	3:F:613:HIS:HD2	1.83	0.44
3:F:593:GLY:O	3:F:594:THR:HG23	2.18	0.43
1:D:41:SER:HG	1:D:44:PHE:HD2	1.66	0.43
1:A:80:ASP:N	1:A:80:ASP:OD2	2.51	0.43
2:B:271:GLN:HB3	2:B:301:GLN:HG3	2.00	0.43
3:C:921:LEU:HD12	3:C:1003:LEU:HD11	2.00	0.43
3:C:533:VAL:HG13	3:C:575:LEU:CD2	2.48	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:F:742:HIS:NE2	3:F:764:MET:HE1	2.33	0.43
2:B:354:ASP:OD1	2:B:355:ARG:N	2.52	0.43
3:C:799:THR:HG21	3:C:873:LEU:HD12	2.00	0.43
3:F:936:SER:O	3:F:938:ILE:HG23	2.18	0.43
3:F:921:LEU:HD12	3:F:1003:LEU:HD11	2.01	0.43
3:F:847:ARG:HD3	3:F:995:ALA:HA	1.99	0.43
4:M:19:DC:H2"	4:M:20:DG:C8	2.53	0.43
3:C:859:LEU:HD13	3:C:921:LEU:HD22	2.01	0.43
1:D:60:VAL:HG21	1:D:62:HIS:CD2	2.54	0.43
3:F:533:VAL:HG13	3:F:575:LEU:CD2	2.48	0.43
3:C:730:LEU:HD22	3:C:751:LEU:HD21	2.00	0.43
2:B:255:VAL:HG23	2:B:256:CYS:SG	2.59	0.43
2:E:224:SER:HA	2:E:227:GLU:HB2	1.99	0.43
3:F:587:ARG:HD3	3:F:617:LEU:CD1	2.47	0.43
3:F:585:ILE:HD11	3:F:614:PHE:HA	1.99	0.43
3:C:861:TRP:CE3	3:C:901:VAL:HG23	2.54	0.42
3:C:572:LEU:HD13	3:C:587:ARG:HG2	2.00	0.42
3:C:717:GLN:HG3	3:C:887:THR:OG1	2.19	0.42
2:E:271:GLN:HB3	2:E:301:GLN:HG3	2.01	0.42
3:F:712:ILE:HD13	3:F:735:ARG:HB3	2.01	0.42
3:C:936:SER:O	3:C:938:ILE:HG23	2.19	0.42
2:E:255:VAL:HG23	2:E:256:CYS:SG	2.58	0.42
2:E:236:LYS:HA	2:E:236:LYS:NZ	2.34	0.42
3:F:822:HIS:ND1	3:F:831:LEU:HD23	2.34	0.42
1:D:60:VAL:CG2	1:D:62:HIS:CD2	3.03	0.42
1:D:15:LYS:HB3	4:M:24:DG:H5'	2.01	0.42
3:C:574:LEU:HD11	3:C:610:ALA:CB	2.33	0.42
1:D:22:LYS:HB3	1:D:52:TYR:CE1	2.55	0.42
3:F:860:LEU:HD12	3:F:924:VAL:HG11	2.00	0.42
2:E:354:ASP:OD1	2:E:355:ARG:N	2.53	0.42
3:C:1004:LYS:C	3:C:1005:LEU:HD12	2.40	0.42
1:D:39:VAL:HG22	1:D:48:VAL:HG12	2.01	0.42
3:F:717:GLN:HG3	3:F:887:THR:OG1	2.19	0.42
3:F:991:VAL:HB	3:F:996:GLN:HE21	1.84	0.42
1:D:52:TYR:CZ	1:D:60:VAL:HG11	2.55	0.42
3:F:930:TYR:CE2	3:F:932:LEU:HD21	2.55	0.42
3:C:930:TYR:CE2	3:C:932:LEU:HD21	2.55	0.41
3:F:1004:LYS:C	3:F:1005:LEU:HD12	2.39	0.41
3:F:799:THR:HG22	3:F:841:ARG:HG2	2.02	0.41
3:C:820:ASN:HD22	3:C:820:ASN:N	2.17	0.41
3:F:624:ASN:CG	3:F:631:PHE:CE1	2.93	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:N:9:DG:C2'	4:N:10:DT:H72	2.50	0.41
1:D:80:ASP:OD2	1:D:80:ASP:N	2.49	0.41
3:F:618:TYR:CD2	3:F:622:THR:HG21	2.54	0.41
3:F:804:VAL:HG12	3:F:811:ALA:HB2	2.01	0.41
3:C:861:TRP:CH2	3:C:921:LEU:HD11	2.56	0.41
3:F:538:GLY:C	3:F:539:LEU:HD23	2.41	0.41
3:C:587:ARG:HD3	3:C:617:LEU:CD1	2.50	0.41
3:F:941:LEU:HD12	3:F:941:LEU:H	1.85	0.41
2:B:316:THR:OG1	2:B:317:ALA:N	2.54	0.41
3:F:585:ILE:HD11	3:F:614:PHE:CA	2.51	0.41
2:B:276:GLU:O	2:B:280:LEU:HD23	2.20	0.41
4:N:2:DC:C2'	4:N:3:DC:O5'	2.69	0.41
1:D:52:TYR:CE1	1:D:60:VAL:HG11	2.56	0.41
1:D:16:SER:OG	4:M:25:DG:OP1	2.37	0.41
3:C:879:ILE:HG23	3:C:894:GLY:N	2.35	0.41
3:C:618:TYR:CD2	3:C:622:THR:HG21	2.56	0.40
1:A:22:LYS:HB3	1:A:52:TYR:CE1	2.56	0.40
3:C:585:ILE:HG21	3:C:613:HIS:CD2	2.56	0.40
2:B:303:VAL:HG12	2:B:304:PHE:O	2.21	0.40
3:C:859:LEU:CD1	3:C:921:LEU:HD22	2.51	0.40
1:A:37:ILE:C	1:A:37:ILE:CD1	2.84	0.40
2:B:248:ILE:HG21	2:B:287:MET:CE	2.51	0.40
1:A:8:LEU:HD12	1:A:8:LEU:O	2.21	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	85/116 (73%)	81 (95%)	4 (5%)	0	100	100
1	D	85/116 (73%)	82 (96%)	3 (4%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
2	B	134/160 (84%)	125 (93%)	8 (6%)	1 (1%)	26 70
2	E	134/160 (84%)	125 (93%)	8 (6%)	1 (1%)	26 70
3	C	450/506 (89%)	412 (92%)	36 (8%)	2 (0%)	39 78
3	F	450/506 (89%)	412 (92%)	38 (8%)	0	100 100
All	All	1338/1564 (86%)	1237 (92%)	97 (7%)	4 (0%)	46 83

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	C	636	LYS
2	B	349	LYS
2	E	349	LYS
3	C	687	VAL

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	78/100 (78%)	72 (92%)	6 (8%)	16 52
1	D	78/100 (78%)	72 (92%)	6 (8%)	16 52
2	B	111/145 (77%)	106 (96%)	5 (4%)	34 73
2	E	111/145 (77%)	106 (96%)	5 (4%)	34 73
3	C	391/443 (88%)	367 (94%)	24 (6%)	23 63
3	F	391/443 (88%)	368 (94%)	23 (6%)	24 64
All	All	1160/1376 (84%)	1091 (94%)	69 (6%)	24 64

All (69) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	21	CYS
1	A	22	LYS
1	A	37	ILE

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Mol	Chain	Res	Type
1	A	40	GLN
1	A	47	LYS
1	A	48	VAL
2	B	250	ASP
2	B	281	ASP
2	B	301	GLN
2	B	316	THR
2	B	319	THR
3	C	568	SER
3	C	588	SER
3	C	592	VAL
3	C	594	THR
3	C	599	ASN
3	C	612	GLU
3	C	621	LYS
3	C	662	LYS
3	C	695	LYS
3	C	698	LEU
3	C	730	LEU
3	C	738	THR
3	C	758	VAL
3	C	769	LEU
3	C	798	LYS
3	C	820	ASN
3	C	835	ASP
3	C	847	ARG
3	C	852	LYS
3	C	890	MET
3	C	900	MET
3	C	910	THR
3	C	971	LEU
3	C	1002	LEU
1	D	21	CYS
1	D	22	LYS
1	D	37	ILE
1	D	40	GLN
1	D	47	LYS
1	D	48	VAL
2	E	250	ASP
2	E	281	ASP
2	E	301	GLN
2	E	316	THR

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Mol	Chain	Res	Type
2	E	319	THR
3	F	568	SER
3	F	588	SER
3	F	592	VAL
3	F	594	THR
3	F	599	ASN
3	F	612	GLU
3	F	621	LYS
3	F	662	LYS
3	F	695	LYS
3	F	698	LEU
3	F	730	LEU
3	F	738	THR
3	F	758	VAL
3	F	769	LEU
3	F	798	LYS
3	F	820	ASN
3	F	835	ASP
3	F	847	ARG
3	F	852	LYS
3	F	890	MET
3	F	910	THR
3	F	971	LEU
3	F	1002	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (29) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	40	GLN
1	A	50	HIS
1	A	62	HIS
2	B	301	GLN
3	C	567	ASN
3	C	573	GLN
3	C	613	HIS
3	C	624	ASN
3	C	705	GLN
3	C	820	ASN
3	C	856	ASN
3	C	906	ASN
3	C	961	ASN
3	C	996	GLN

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Mol	Chain	Res	Type
1	D	40	GLN
1	D	50	HIS
1	D	62	HIS
2	E	301	GLN
3	F	567	ASN
3	F	573	GLN
3	F	599	ASN
3	F	613	HIS
3	F	705	GLN
3	F	820	ASN
3	F	856	ASN
3	F	862	HIS
3	F	906	ASN
3	F	961	ASN
3	F	996	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 5 ligands modelled in this entry, 4 are monoatomic - leaving 1 for Mogul analysis.

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	$\#\|Z\|>2$
6	EDO	C	1101	-	3,3,3	0.62	0	2,2,2	0.08	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
6	EDO	C	1101	-	-	0/1/1/1	0/0/0/0

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data

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	86/116 (74%)	-0.38	0 100 100	107, 140, 202, 238	0
1	D	86/116 (74%)	-0.15	2 (2%) 64 54	130, 193, 232, 239	0
2	B	136/160 (85%)	-0.38	0 100 100	96, 138, 237, 259	0
2	E	136/160 (85%)	-0.13	4 (2%) 55 46	168, 206, 267, 290	0
3	C	456/506 (90%)	-0.16	5 (1%) 82 75	90, 156, 230, 304	0
3	F	456/506 (90%)	0.15	23 (5%) 32 24	110, 207, 265, 326	0
4	M	26/26 (100%)	-0.80	0 100 100	119, 143, 192, 208	0
4	N	26/26 (100%)	-0.89	0 100 100	115, 155, 195, 223	0
All	All	1408/1616 (87%)	-0.12	34 (2%) 62 52	90, 180, 254, 326	0

All (34) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	E	349	LYS	5.9
3	F	863	GLY	5.0
3	F	662	LYS	5.0
3	F	978	GLY	4.5
3	F	782	SER	4.3
3	F	783	ASP	4.3
3	F	864	SER	4.0
2	E	309	TYR	3.7
3	F	862	HIS	3.7
3	F	946	HIS	3.6
3	F	575	LEU	3.6
3	F	789	PRO	3.5
3	C	785	SER	3.5
3	C	863	GLY	3.5
3	F	980	ASN	3.4
3	F	979	VAL	3.3

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Mol	Chain	Res	Type	RSRZ
3	C	662	LYS	3.2
3	F	784	ASP	3.2
3	F	948	VAL	3.1
3	C	575	LEU	2.9
2	E	348	LEU	2.7
3	F	951	LEU	2.6
1	D	52	TYR	2.5
3	F	788	ASP	2.5
3	F	787	LYS	2.5
3	C	864	SER	2.3
3	F	942	PRO	2.3
3	F	899	ASP	2.2
3	F	664	LYS	2.2
2	E	350	VAL	2.2
3	F	531	ALA	2.1
3	F	917	GLY	2.0
1	D	28	ILE	2.0
3	F	546	LEU	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
6	EDO	C	1101	4/4	0.97	0.75	4.19	83,89,95,95	0
5	ZN	B	400	1/1	0.99	0.09	-0.97	123,123,123,123	0
5	ZN	E	400	1/1	0.97	0.05	-1.68	201,201,201,201	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
5	ZN	A	200	1/1	0.99	0.11	-	165,165,165,165	0
5	ZN	D	200	1/1	0.98	0.07	-	204,204,204,204	0

6.5 Other polymers (i)

There are no such residues in this entry.