Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 09:16 AM GMT

PDB ID	:	3HST
Title	:	N-Terminal RNASE H domain of rv2228c from mycobacterium tuberculosis as a fusion protein with maltose binding protein
Authors	:	Watkins, H.A.; Baker, E.N.
Deposited on	:	2009-06-10
Resolution	:	2.25 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 ⓘ symbol.

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

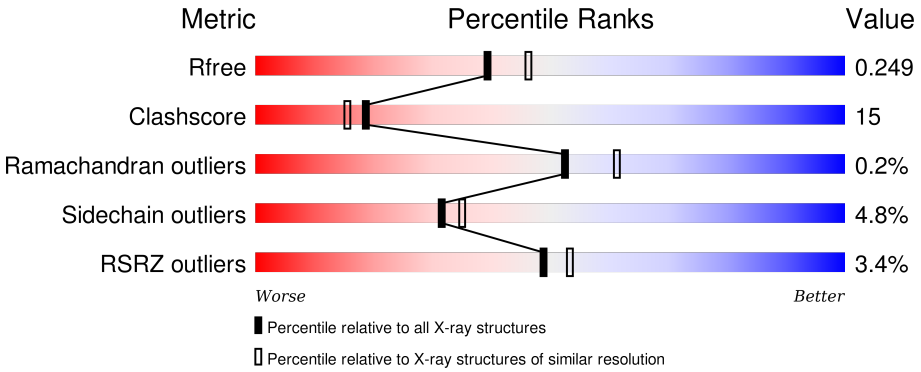
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	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 2.25 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	1640 (2.28-2.24)
Clashscore	102246	1095 (2.26-2.26)
Ramachandran outliers	100387	1063 (2.26-2.26)
Sidechain outliers	100360	1063 (2.26-2.26)
RSRZ outliers	91569	1647 (2.28-2.24)

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	387	3% 77% 16% • 6%
1	C	387	2% 73% 20% • 5%
2	B	141	4% 59% 33% 6% ••
2	D	141	8% 66% 25% • 7%

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
4	EDO	A	2	-	-	X	-
4	EDO	C	3	-	-	X	X
4	EDO	C	396	-	-	-	X
5	TAR	C	395	X	-	-	X

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 8127 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 Maltose-binding periplasmic protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	365	Total	C	N	O	S	0	0	0
			2829	1820	460	543	6			
1	C	369	Total	C	N	O	S	0	0	0
			2859	1838	464	551	6			

There are 42 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	8	MET	-	EXPRESSION TAG	UNP P0AEX9
A	375	ASN	-	EXPRESSION TAG	UNP P0AEX9
A	376	SER	-	EXPRESSION TAG	UNP P0AEX9
A	377	SER	-	EXPRESSION TAG	UNP P0AEX9
A	378	SER	-	EXPRESSION TAG	UNP P0AEX9
A	379	ASN	-	EXPRESSION TAG	UNP P0AEX9
A	380	ASN	-	EXPRESSION TAG	UNP P0AEX9
A	381	ASN	-	EXPRESSION TAG	UNP P0AEX9
A	382	ASN	-	EXPRESSION TAG	UNP P0AEX9
A	383	ASN	-	EXPRESSION TAG	UNP P0AEX9
A	384	ASN	-	EXPRESSION TAG	UNP P0AEX9
A	385	ASN	-	EXPRESSION TAG	UNP P0AEX9
A	386	ASN	-	EXPRESSION TAG	UNP P0AEX9
A	387	ASN	-	EXPRESSION TAG	UNP P0AEX9
A	388	ASN	-	EXPRESSION TAG	UNP P0AEX9
A	389	LEU	-	EXPRESSION TAG	UNP P0AEX9
A	390	GLY	-	EXPRESSION TAG	UNP P0AEX9
A	391	ILE	-	EXPRESSION TAG	UNP P0AEX9
A	392	GLU	-	EXPRESSION TAG	UNP P0AEX9
A	393	GLY	-	EXPRESSION TAG	UNP P0AEX9
A	394	ARG	-	EXPRESSION TAG	UNP P0AEX9
C	8	MET	-	EXPRESSION TAG	UNP P0AEX9
C	375	ASN	-	EXPRESSION TAG	UNP P0AEX9
C	376	SER	-	EXPRESSION TAG	UNP P0AEX9
C	377	SER	-	EXPRESSION TAG	UNP P0AEX9

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Chain	Residue	Modelled	Actual	Comment	Reference
C	378	SER	-	EXPRESSION TAG	UNP P0AEX9
C	379	ASN	-	EXPRESSION TAG	UNP P0AEX9
C	380	ASN	-	EXPRESSION TAG	UNP P0AEX9
C	381	ASN	-	EXPRESSION TAG	UNP P0AEX9
C	382	ASN	-	EXPRESSION TAG	UNP P0AEX9
C	383	ASN	-	EXPRESSION TAG	UNP P0AEX9
C	384	ASN	-	EXPRESSION TAG	UNP P0AEX9
C	385	ASN	-	EXPRESSION TAG	UNP P0AEX9
C	386	ASN	-	EXPRESSION TAG	UNP P0AEX9
C	387	ASN	-	EXPRESSION TAG	UNP P0AEX9
C	388	ASN	-	EXPRESSION TAG	UNP P0AEX9
C	389	LEU	-	EXPRESSION TAG	UNP P0AEX9
C	390	GLY	-	EXPRESSION TAG	UNP P0AEX9
C	391	ILE	-	EXPRESSION TAG	UNP P0AEX9
C	392	GLU	-	EXPRESSION TAG	UNP P0AEX9
C	393	GLY	-	EXPRESSION TAG	UNP P0AEX9
C	394	ARG	-	EXPRESSION TAG	UNP P0AEX9

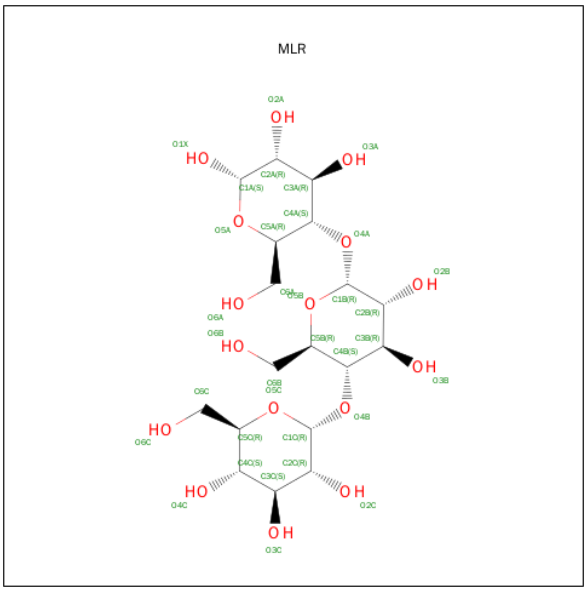
- Molecule 2 is a protein called Protein Rv2228c/MT2287.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	139	Total	C	N	O	S	0	0	0
			1045	651	192	199	3			
2	D	131	Total	C	N	O	S	0	0	0
			999	625	183	188	3			

There are 4 discrepancies between the modelled and reference sequences:

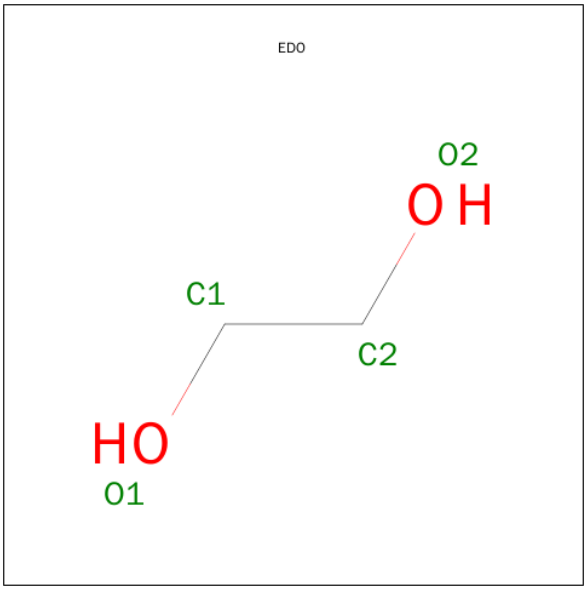
Chain	Residue	Modelled	Actual	Comment	Reference
B	0	SER	-	EXPRESSION TAG	UNP P64955
B	1	VAL	-	EXPRESSION TAG	UNP P64955
D	0	SER	-	EXPRESSION TAG	UNP P64955
D	1	VAL	-	EXPRESSION TAG	UNP P64955

- Molecule 3 is MALTOTRIOSE (three-letter code: MLR) (formula: $C_{18}H_{32}O_{16}$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total C O 34 18 16	0	0
3	C	1	Total C O 34 18 16	0	0

- Molecule 4 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: $C_2H_6O_2$).



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

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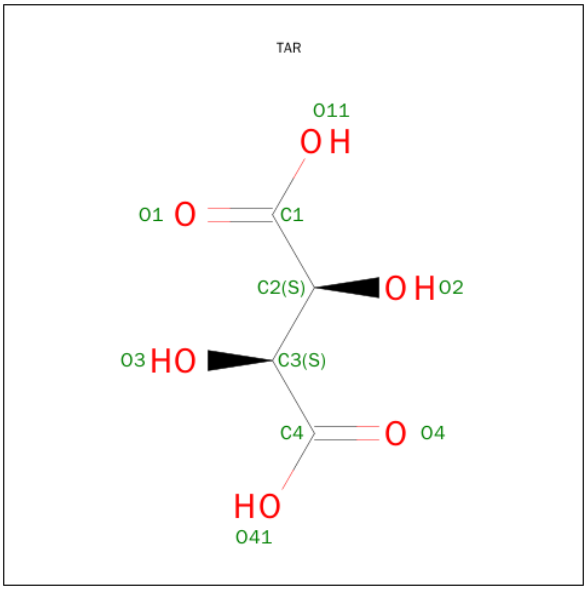
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	C	1	Total C O 4 2 2	0	0

- Molecule 5 is D(-)-TARTARIC ACID (three-letter code: TAR) (formula: $C_4H_6O_6$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	C	1	Total C O 10 4 6	0	0

- Molecule 6 is water.

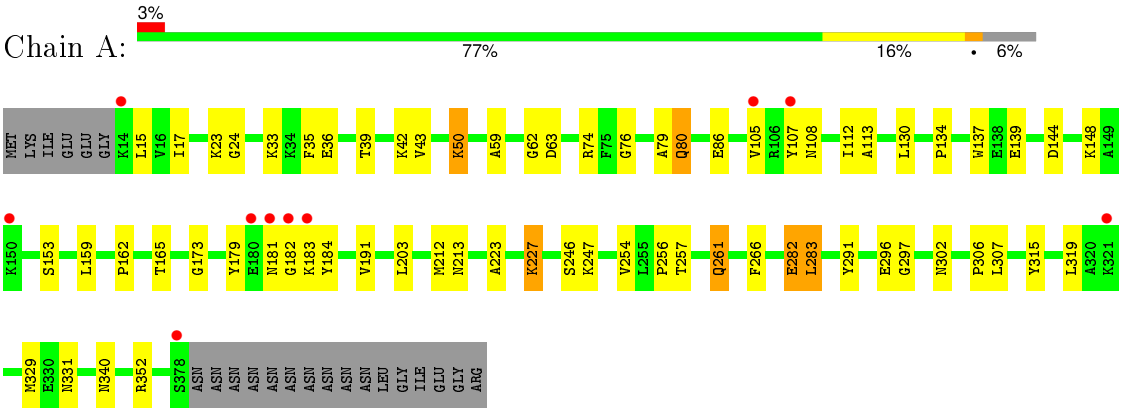
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	130	Total O 130 130	0	0
6	B	30	Total O 30 30	0	0
6	C	134	Total O 134 134	0	0
6	D	11	Total O 11 11	0	0

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.

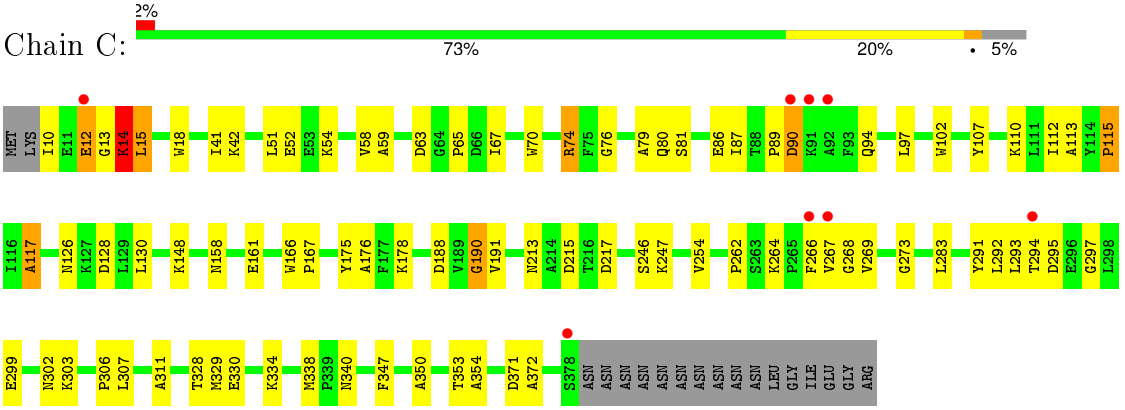
- Molecule 1: Maltose-binding periplasmic protein

Chain A:



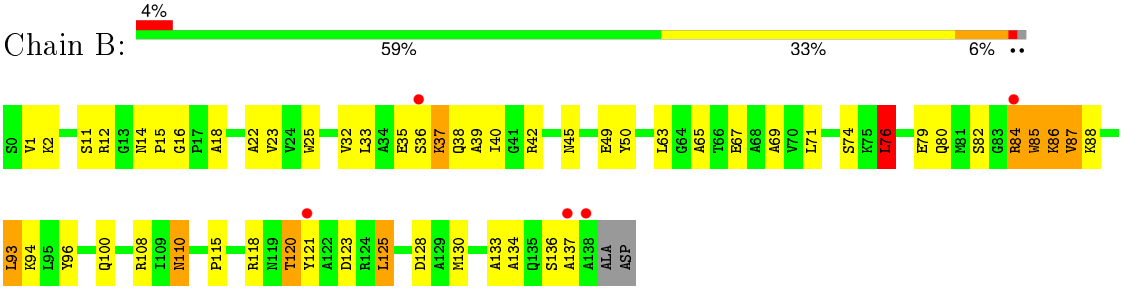
- Molecule 1: Maltose-binding periplasmic protein

Chain C:



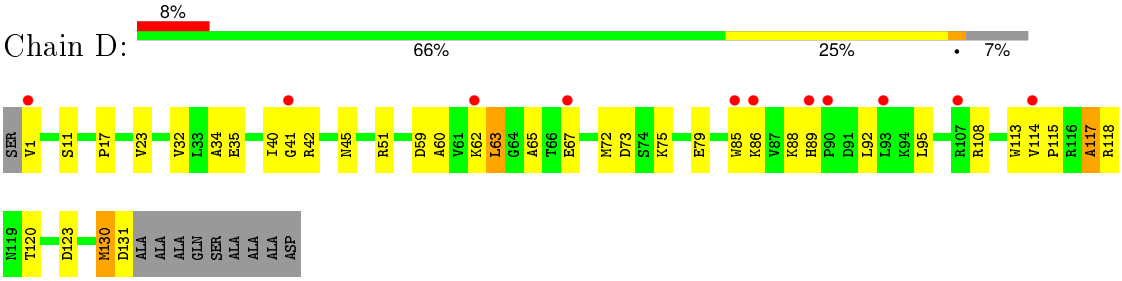
- Molecule 2: Protein Rv2228c/MT2287

Chain B:



• Molecule 2: Protein Rv2228c/MT2287

Chain D:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	73.63Å 101.38Å 76.09Å 90.00° 109.01° 90.00°	Depositor
Resolution (Å)	41.45 – 2.25 41.44 – 2.25	Depositor EDS
% Data completeness (in resolution range)	100.0 (41.45-2.25) 100.0 (41.44-2.25)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.89 (at 2.24Å)	Xtriage
Refinement program	REFMAC 5.3.0037	Depositor
R, R_{free}	0.183 , 0.239 0.210 , 0.249	Depositor DCC
R_{free} test set	2576 reflections (5.41%)	DCC
Wilson B-factor (Å^2)	25.8	Xtriage
Anisotropy	0.261	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.32 , 37.5	EDS
Estimated twinning fraction	0.022 for l,-k,h	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.33$	Xtriage
Outliers	2 of 50198 reflections (0.004%)	Xtriage
F_o,F_c correlation	0.93	EDS
Total number of atoms	8127	wwPDB-VP
Average B, all atoms (Å^2)	18.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.97% 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: MLR, EDO, TAR

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	1.02	1/2898 (0.0%)	0.88	5/3936 (0.1%)
1	C	1.09	1/2928 (0.0%)	0.92	7/3976 (0.2%)
2	B	1.00	0/1062	0.99	4/1441 (0.3%)
2	D	0.90	0/1016	0.85	3/1378 (0.2%)
All	All	1.03	2/7904 (0.0%)	0.91	19/10731 (0.2%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	86	GLU	CB-CG	5.39	1.62	1.52
1	C	190	GLY	C-O	-5.01	1.15	1.23

All (19) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	120	THR	CB-CA-C	-7.97	90.08	111.60
1	C	117	ALA	CB-CA-C	7.06	120.69	110.10
1	C	115	PRO	CB-CA-C	-7.03	94.43	112.00
2	B	120	THR	N-CA-C	6.91	129.66	111.00
2	B	85	TRP	N-CA-C	-5.80	95.33	111.00
1	C	15	LEU	CA-CB-CG	5.57	128.12	115.30
2	D	51	ARG	NE-CZ-NH1	-5.56	117.52	120.30
1	A	181	ASN	N-CA-CB	5.54	120.57	110.60
1	A	181	ASN	C-N-CA	-5.53	110.69	122.30
2	D	51	ARG	NE-CZ-NH2	5.49	123.04	120.30
1	C	74	ARG	NE-CZ-NH1	5.48	123.04	120.30
2	B	76	LEU	CA-CB-CG	5.41	127.75	115.30
1	C	90	ASP	N-CA-CB	-5.37	100.94	110.60
1	A	74	ARG	NE-CZ-NH2	-5.25	117.67	120.30
1	A	227	LYS	CD-CE-NZ	-5.14	99.88	111.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	130	LEU	CA-CB-CG	5.08	127.00	115.30
2	D	123	ASP	CB-CG-OD1	5.08	122.88	118.30
1	C	15	LEU	CB-CG-CD1	5.08	119.64	111.00
1	C	14	LYS	CB-CA-C	-5.08	100.24	110.40

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	2829	0	2794	67	0
1	C	2859	0	2820	87	0
2	B	1045	0	1043	56	0
2	D	999	0	1000	35	0
3	A	34	0	32	1	0
3	C	34	0	32	1	0
4	A	4	0	6	4	0
4	C	8	0	12	8	0
5	C	10	0	4	0	0
6	A	130	0	0	5	0
6	B	30	0	0	3	0
6	C	134	0	0	3	0
6	D	11	0	0	1	0
All	All	8127	0	7743	240	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 15.

All (240) 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:B:84:ARG:O	2:B:85:TRP:HD1	1.12	1.23
1:A:80:GLN:HB3	1:A:107:TYR:OH	1.36	1.20
2:B:84:ARG:O	2:B:85:TRP:CD1	1.97	1.18

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:114:VAL:HB	2:D:115:PRO:HD2	1.26	1.11
1:A:179:TYR:OH	1:A:182:GLY:HA2	1.56	1.05
2:B:87:VAL:HG22	2:B:93:LEU:HD13	1.32	1.03
2:B:12:ARG:NE	2:B:130:MET:HE2	1.77	0.98
1:A:246:SER:O	1:A:247:LYS:HG2	1.65	0.97
1:A:165:THR:HG23	6:A:414:HOH:O	1.70	0.90
1:C:293:LEU:O	1:C:294:THR:HG23	1.70	0.88
2:D:114:VAL:HB	2:D:115:PRO:CD	2.05	0.84
1:A:179:TYR:CD1	1:A:183:LYS:O	2.31	0.83
1:A:80:GLN:CB	1:A:107:TYR:OH	2.22	0.83
2:B:79:GLU:OE1	2:B:84:ARG:HG3	1.80	0.82
1:C:262:PRO:HB3	1:C:334:LYS:HD3	1.60	0.81
1:A:62:GLY:O	2:B:94:LYS:HG2	1.84	0.78
2:D:67:GLU:CG	2:D:108:ARG:HB3	2.13	0.78
1:A:246:SER:O	1:A:247:LYS:CG	2.32	0.77
1:C:13:GLY:O	1:C:41:ILE:HG23	1.85	0.77
1:C:293:LEU:O	1:C:294:THR:CG2	2.33	0.76
1:C:59:ALA:HA	1:C:63:ASP:O	1.86	0.75
2:B:2:LYS:HE2	6:B:166:HOH:O	1.86	0.75
2:D:59:ASP:O	2:D:63:LEU:HD23	1.87	0.75
2:D:60:ALA:HA	2:D:63:LEU:HD23	1.69	0.74
1:C:12:GLU:C	1:C:14:LYS:H	1.90	0.74
2:B:25:TRP:CZ2	2:B:121:TYR:CZ	2.76	0.73
2:D:79:GLU:HB3	2:D:85:TRP:CG	2.24	0.73
1:A:179:TYR:HH	1:A:182:GLY:HA2	1.53	0.72
1:A:247:LYS:HB3	1:C:247:LYS:HB3	1.71	0.72
2:D:40:ILE:HG13	2:D:40:ILE:O	1.89	0.71
1:A:79:ALA:HB3	1:A:107:TYR:CD2	2.26	0.71
2:B:115:PRO:HD2	2:B:118:ARG:HD3	1.74	0.70
2:B:37:LYS:O	2:D:34:ALA:HA	1.92	0.70
2:D:60:ALA:HA	2:D:63:LEU:CD2	2.21	0.70
1:C:302:ASN:HD22	1:C:307:LEU:H	1.40	0.70
1:C:76:GLY:HA3	1:C:340:ASN:O	1.91	0.69
1:A:80:GLN:HB3	1:A:107:TYR:CZ	2.27	0.69
1:A:179:TYR:HD1	1:A:183:LYS:O	1.75	0.69
1:A:79:ALA:CB	1:A:107:TYR:CD2	2.77	0.68
2:D:67:GLU:HG2	2:D:108:ARG:HB3	1.74	0.68
1:C:213:ASN:HB2	6:C:449:HOH:O	1.94	0.68
2:B:32:VAL:HG22	2:B:32:VAL:O	1.93	0.67
1:C:14:LYS:HE3	1:C:42:LYS:HD3	1.76	0.67
1:A:76:GLY:HA3	1:A:340:ASN:O	1.94	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:82:SER:HB3	2:B:84:ARG:HD3	1.77	0.67
2:B:1:VAL:HG13	2:B:65:ALA:HA	1.76	0.66
1:C:158:ASN:OD1	1:C:217:ASP:HA	1.95	0.66
1:A:80:GLN:HB3	1:A:107:TYR:HH	1.57	0.65
2:D:1:VAL:HG13	2:D:65:ALA:HA	1.79	0.65
2:B:25:TRP:CZ2	2:B:121:TYR:CE2	2.84	0.65
1:A:105:VAL:CG2	1:A:113:ALA:HB3	2.28	0.64
1:C:215:ASP:HB2	6:C:502:HOH:O	1.97	0.64
1:C:246:SER:O	1:C:247:LYS:HG2	1.97	0.64
1:C:63:ASP:HB3	6:C:437:HOH:O	1.98	0.64
2:B:12:ARG:CZ	2:B:130:MET:HE2	2.28	0.63
2:B:134:ALA:O	2:B:137:ALA:N	2.30	0.63
1:C:12:GLU:C	1:C:14:LYS:N	2.48	0.63
1:A:329:MET:HA	1:A:329:MET:CE	2.28	0.62
2:D:130:MET:HA	6:D:143:HOH:O	2.00	0.62
2:B:32:VAL:HG22	6:B:170:HOH:O	1.99	0.62
1:C:254:VAL:HG11	1:C:334:LYS:NZ	2.15	0.61
1:A:50:LYS:HA	6:A:397:HOH:O	2.01	0.61
2:D:40:ILE:CG1	2:D:40:ILE:O	2.49	0.61
1:C:302:ASN:ND2	1:C:306:PRO:HA	2.15	0.60
2:B:32:VAL:O	2:B:32:VAL:CG2	2.48	0.60
2:B:96:TYR:O	2:B:100:GLN:HG2	2.00	0.60
1:C:175:TYR:O	1:C:190:GLY:CA	2.50	0.59
1:C:158:ASN:ND2	1:C:161:GLU:HB2	2.17	0.59
2:B:69:ALA:HA	2:B:110:ASN:ND2	2.16	0.59
1:C:293:LEU:C	1:C:294:THR:HG23	2.22	0.59
1:C:371:ASP:HB3	4:C:3:EDO:H21	1.85	0.59
1:C:254:VAL:HG22	1:C:330:GLU:CD	2.23	0.58
1:C:294:THR:O	1:C:297:GLY:N	2.36	0.58
2:B:23:VAL:HG21	2:B:121:TYR:HB3	1.85	0.58
1:A:79:ALA:HB3	1:A:107:TYR:CE2	2.38	0.58
2:B:12:ARG:CD	2:B:130:MET:HE2	2.33	0.58
1:C:12:GLU:O	1:C:14:LYS:N	2.37	0.58
1:C:115:PRO:O	1:C:311:ALA:CB	2.52	0.57
1:A:35:PHE:CZ	1:A:39:THR:HG21	2.40	0.57
2:B:25:TRP:CH2	2:B:121:TYR:CZ	2.92	0.57
1:C:291:TYR:O	1:C:294:THR:OG1	2.21	0.57
2:D:72:MET:O	2:D:113:TRP:HA	2.04	0.57
1:C:175:TYR:O	1:C:190:GLY:HA3	2.05	0.57
2:B:12:ARG:CZ	2:B:130:MET:CE	2.82	0.57
2:B:37:LYS:NZ	2:B:128:ASP:HB2	2.20	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:105:VAL:HG21	1:A:113:ALA:HB3	1.86	0.56
2:B:33:LEU:HB3	2:B:63:LEU:HD22	1.87	0.56
2:B:87:VAL:CG2	2:B:93:LEU:HD13	2.21	0.56
1:A:246:SER:O	1:A:247:LYS:CB	2.49	0.56
1:C:115:PRO:O	1:C:311:ALA:HB3	2.06	0.56
1:A:179:TYR:CZ	1:A:182:GLY:HA2	2.41	0.56
1:A:105:VAL:HG21	1:A:113:ALA:N	2.21	0.55
1:A:223:ALA:O	1:A:227:LYS:HG3	2.06	0.55
2:B:25:TRP:HZ2	2:B:121:TYR:CZ	2.21	0.55
1:A:329:MET:HA	1:A:329:MET:HE2	1.86	0.55
1:C:178:LYS:HG2	1:C:188:ASP:OD2	2.07	0.55
1:C:294:THR:O	1:C:295:ASP:C	2.44	0.55
2:B:25:TRP:HZ2	2:B:121:TYR:CE2	2.23	0.55
2:B:11:SER:C	2:B:130:MET:HE3	2.26	0.55
2:B:67:GLU:HG3	2:B:108:ARG:HB3	1.88	0.55
1:C:18:TRP:CD2	1:C:65:PRO:HG3	2.41	0.54
1:C:51:LEU:HD12	1:C:51:LEU:C	2.28	0.54
2:B:49:GLU:HG2	2:B:74:SER:CB	2.38	0.54
2:D:114:VAL:HG12	2:D:118:ARG:NH1	2.23	0.54
1:C:158:ASN:HD22	1:C:161:GLU:HB2	1.71	0.54
1:A:137:TRP:CD1	1:A:256:PRO:HB2	2.42	0.54
2:B:82:SER:CB	2:B:84:ARG:HD3	2.37	0.53
1:C:268:GLY:HA2	1:C:338:MET:HE3	1.89	0.53
1:A:134:PRO:HB3	1:A:139:GLU:HG3	1.90	0.53
1:C:371:ASP:CB	4:C:3:EDO:H21	2.39	0.53
1:A:15:LEU:HB3	1:A:43:VAL:HG22	1.90	0.53
2:D:23:VAL:HG23	2:D:32:VAL:HG13	1.90	0.53
1:A:302:ASN:ND2	1:A:307:LEU:H	2.06	0.52
1:C:264:LYS:HG2	1:C:334:LYS:O	2.09	0.52
1:C:89:PRO:HB2	1:C:94:GLN:HG3	1.91	0.52
2:D:73:ASP:O	2:D:113:TRP:NE1	2.42	0.52
1:C:70:TRP:CD1	1:C:74:ARG:HG2	2.44	0.52
1:C:353:THR:HB	4:C:3:EDO:H11	1.92	0.52
1:C:18:TRP:CG	1:C:65:PRO:HG3	2.44	0.52
2:D:17:PRO:HA	2:D:41:GLY:O	2.10	0.52
1:C:246:SER:O	1:C:247:LYS:CB	2.57	0.51
2:D:79:GLU:HB3	2:D:85:TRP:CD1	2.45	0.51
1:C:350:ALA:O	4:C:3:EDO:C1	2.58	0.51
2:B:37:LYS:NZ	2:B:128:ASP:CB	2.74	0.51
1:A:105:VAL:HG23	1:A:113:ALA:HB3	1.92	0.51
1:C:328:THR:HG22	1:C:329:MET:HE2	1.92	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:254:VAL:HG11	1:C:334:LYS:HZ1	1.76	0.50
1:A:79:ALA:HB1	1:A:107:TYR:HD2	1.76	0.50
1:A:306:PRO:O	4:A:2:EDO:H11	2.11	0.50
1:C:97:LEU:HA	1:C:311:ALA:O	2.11	0.49
1:A:203:LEU:HD12	1:A:212:MET:HE1	1.94	0.49
1:A:282:GLU:HG2	1:A:283:LEU:N	2.26	0.49
2:B:22:ALA:HB3	2:B:36:SER:OG	2.12	0.49
1:A:105:VAL:HG22	1:A:112:ILE:HG13	1.95	0.49
1:A:79:ALA:HB1	1:A:107:TYR:CD2	2.46	0.49
1:C:372:ALA:HB2	4:C:3:EDO:H12	1.95	0.49
1:C:74:ARG:HD3	3:C:2:MLR:O2C	2.13	0.49
2:B:25:TRP:CZ2	2:B:121:TYR:CE1	3.01	0.48
1:A:105:VAL:HG21	1:A:113:ALA:O	2.13	0.48
2:B:12:ARG:NE	2:B:130:MET:CE	2.64	0.48
1:A:247:LYS:HA	6:A:438:HOH:O	2.13	0.48
1:C:246:SER:O	1:C:247:LYS:CG	2.61	0.48
1:C:354:ALA:N	4:C:3:EDO:H11	2.28	0.48
2:B:11:SER:H	2:B:45:ASN:ND2	2.11	0.48
1:A:179:TYR:CD1	1:A:184:TYR:CE1	3.01	0.48
1:C:302:ASN:ND2	1:C:307:LEU:H	2.10	0.48
2:B:49:GLU:HG2	2:B:74:SER:HB2	1.95	0.48
1:C:87:ILE:HD12	1:C:89:PRO:HD3	1.95	0.48
1:A:315:TYR:CE2	1:A:319:LEU:HD11	2.49	0.48
2:B:39:ALA:HB1	2:B:133:ALA:HB2	1.96	0.48
1:C:262:PRO:HB3	1:C:334:LYS:CD	2.40	0.48
1:C:268:GLY:CA	1:C:338:MET:CE	2.92	0.48
1:C:166:TRP:NE1	1:C:266:PHE:CE2	2.82	0.48
1:C:58:VAL:O	1:C:63:ASP:HB2	2.14	0.47
1:A:257:THR:HB	1:A:261:GLN:O	2.13	0.47
1:A:105:VAL:CG2	1:A:113:ALA:N	2.78	0.47
1:A:307:LEU:HD23	4:A:2:EDO:H22	1.96	0.47
1:A:59:ALA:HA	1:A:63:ASP:O	2.14	0.47
2:D:114:VAL:C	2:D:115:PRO:O	2.51	0.47
2:D:114:VAL:HG12	2:D:118:ARG:CZ	2.45	0.47
1:C:268:GLY:HA2	1:C:338:MET:CE	2.44	0.47
1:A:302:ASN:HD22	1:A:307:LEU:H	1.63	0.47
1:C:86:GLU:HG3	1:C:110:LYS:HB3	1.97	0.47
2:D:114:VAL:CB	2:D:115:PRO:CD	2.76	0.46
2:B:14:ASN:HA	2:B:15:PRO:HA	1.67	0.46
2:B:37:LYS:CE	2:B:128:ASP:HB2	2.46	0.46
1:C:117:ALA:O	1:C:269:VAL:HG13	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:14:LYS:HG3	1:C:42:LYS:HB3	1.97	0.46
1:A:105:VAL:HG21	1:A:113:ALA:CA	2.46	0.46
1:C:254:VAL:HG21	1:C:330:GLU:OE2	2.16	0.46
2:D:60:ALA:HA	2:D:63:LEU:HD21	1.98	0.46
2:B:25:TRP:HZ2	2:B:121:TYR:CE1	2.33	0.45
1:A:144:ASP:O	1:A:148:LYS:HG2	2.16	0.45
2:D:75:LYS:HE3	2:D:75:LYS:HB2	1.56	0.45
1:A:162:PRO:HD3	1:A:352:ARG:HG3	1.98	0.45
2:D:11:SER:H	2:D:45:ASN:ND2	2.15	0.45
1:C:176:ALA:HB2	1:C:347:PHE:CE1	2.51	0.45
1:C:254:VAL:CG2	1:C:330:GLU:OE2	2.65	0.44
2:B:123:ASP:HB2	6:B:165:HOH:O	2.16	0.44
1:A:296:GLU:HB2	6:A:445:HOH:O	2.18	0.44
2:B:37:LYS:HB2	2:B:125:LEU:HG	1.98	0.44
2:B:25:TRP:HZ2	2:B:121:TYR:CD2	2.35	0.44
1:C:166:TRP:CD1	1:C:266:PHE:CD2	3.06	0.44
1:C:97:LEU:HD22	1:C:102:TRP:CZ2	2.52	0.44
2:B:18:ALA:HB3	2:B:40:ILE:HG12	2.00	0.44
1:C:67:ILE:HA	1:C:273:GLY:O	2.18	0.44
2:B:50:TYR:OH	2:B:80:GLN:NE2	2.42	0.44
1:C:262:PRO:CB	1:C:334:LYS:HD3	2.40	0.43
2:D:108:ARG:HB2	2:D:108:ARG:HE	1.62	0.43
1:C:299:GLU:O	1:C:303:LYS:HB2	2.18	0.43
2:D:117:ALA:HA	2:D:120:THR:HG22	1.99	0.43
2:D:130:MET:O	2:D:131:ASP:C	2.56	0.43
1:C:166:TRP:CD1	1:C:266:PHE:CE2	3.07	0.43
1:A:36:GLU:OE2	1:A:42:LYS:HG2	2.18	0.43
1:C:191:VAL:O	1:C:191:VAL:HG12	2.18	0.43
2:B:79:GLU:O	2:B:84:ARG:HG2	2.18	0.43
1:C:80:GLN:NE2	1:C:107:TYR:OH	2.51	0.43
2:B:37:LYS:HZ1	2:B:128:ASP:HB2	1.82	0.43
2:D:79:GLU:CB	2:D:85:TRP:CG	2.97	0.43
1:C:354:ALA:HB2	1:C:372:ALA:HB2	2.01	0.43
1:A:79:ALA:CB	1:A:107:TYR:HD2	2.27	0.43
1:C:292:LEU:O	1:C:294:THR:N	2.52	0.43
1:A:159:LEU:HD12	1:A:213:ASN:O	2.19	0.42
2:D:115:PRO:O	2:D:115:PRO:CD	2.65	0.42
1:C:58:VAL:O	1:C:63:ASP:N	2.50	0.42
1:C:79:ALA:HB2	1:C:112:ILE:HD13	2.00	0.42
1:C:112:ILE:O	1:C:113:ALA:HB2	2.18	0.42
1:A:254:VAL:HA	1:A:331:ASN:HD21	1.85	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:12:ARG:HG2	2:B:130:MET:CE	2.50	0.42
1:C:350:ALA:O	4:C:3:EDO:H11	2.20	0.42
2:B:38:GLN:HG3	2:B:39:ALA:O	2.20	0.42
1:A:15:LEU:O	1:A:43:VAL:HA	2.19	0.42
1:C:126:ASN:OD1	1:C:128:ASP:HB2	2.19	0.42
2:B:76:LEU:C	2:B:76:LEU:HD13	2.40	0.42
1:A:33:LYS:HE2	1:C:215:ASP:OD2	2.20	0.42
1:C:51:LEU:HD12	1:C:52:GLU:N	2.34	0.42
1:A:173:GLY:HA2	6:A:417:HOH:O	2.18	0.42
1:C:176:ALA:CB	1:C:347:PHE:CE1	3.03	0.42
2:D:79:GLU:CB	2:D:85:TRP:CD2	3.03	0.41
2:B:16:GLY:O	2:B:42:ARG:HA	2.19	0.41
1:A:80:GLN:N	1:A:107:TYR:HE2	2.18	0.41
1:C:354:ALA:HB2	4:C:3:EDO:H12	2.03	0.41
2:B:38:GLN:NE2	2:D:59:ASP:O	2.51	0.41
1:A:352:ARG:HD2	3:A:1:MLR:C6C	2.50	0.41
1:C:54:LYS:O	1:C:58:VAL:HG22	2.21	0.41
1:A:105:VAL:HG21	1:A:113:ALA:CB	2.49	0.41
1:A:17:ILE:HD12	1:A:43:VAL:CG1	2.51	0.41
2:D:130:MET:H	2:D:130:MET:HG2	1.43	0.41
2:D:73:ASP:C	2:D:113:TRP:CD1	2.94	0.41
1:A:148:LYS:HZ3	1:A:153:SER:HB3	1.86	0.41
1:A:291:TYR:O	1:A:297:GLY:HA3	2.21	0.41
1:C:267:VAL:HG12	1:C:267:VAL:O	2.20	0.41
1:C:175:TYR:CD1	1:C:190:GLY:HA3	2.56	0.41
1:A:24:GLY:H	4:A:2:EDO:C2	2.34	0.41
1:A:107:TYR:O	1:A:108:ASN:HB2	2.20	0.40
2:D:67:GLU:HG2	2:D:108:ARG:CB	2.49	0.40
1:A:23:LYS:HB3	4:A:2:EDO:H21	2.04	0.40
2:B:86:LYS:HD3	2:B:86:LYS:HA	1.29	0.40
1:C:254:VAL:HG11	1:C:334:LYS:HZ2	1.84	0.40
1:C:166:TRP:N	1:C:167:PRO:CD	2.84	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	363/387 (94%)	355 (98%)	8 (2%)	0	100 100
1	C	367/387 (95%)	354 (96%)	13 (4%)	0	100 100
2	B	137/141 (97%)	132 (96%)	4 (3%)	1 (1%)	26 26
2	D	129/141 (92%)	124 (96%)	4 (3%)	1 (1%)	24 21
All	All	996/1056 (94%)	965 (97%)	29 (3%)	2 (0%)	52 61

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	120	THR
2	D	117	ALA

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	293/312 (94%)	286 (98%)	7 (2%)	57 67
1	C	296/312 (95%)	287 (97%)	9 (3%)	48 59
2	B	103/104 (99%)	91 (88%)	12 (12%)	7 4
2	D	100/104 (96%)	90 (90%)	10 (10%)	9 7
All	All	792/832 (95%)	754 (95%)	38 (5%)	31 35

All (38) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	50	LYS
1	A	80	GLN
1	A	191	VAL
1	A	261	GLN

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Mol	Chain	Res	Type
1	A	266	PHE
1	A	282	GLU
1	A	283	LEU
2	B	35	GLU
2	B	37	LYS
2	B	71	LEU
2	B	76	LEU
2	B	84	ARG
2	B	86	LYS
2	B	87	VAL
2	B	88	LYS
2	B	93	LEU
2	B	110	ASN
2	B	125	LEU
2	B	136	SER
1	C	10	ILE
1	C	12	GLU
1	C	14	LYS
1	C	15	LEU
1	C	81	SER
1	C	90	ASP
1	C	130	LEU
1	C	148	LYS
1	C	283	LEU
2	D	35	GLU
2	D	42	ARG
2	D	62	LYS
2	D	63	LEU
2	D	86	LYS
2	D	88	LYS
2	D	89	HIS
2	D	92	LEU
2	D	95	LEU
2	D	130	MET

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (21) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	20	ASN
1	A	57	GLN
1	A	80	GLN
1	A	302	ASN

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Mol	Chain	Res	Type
1	A	373	GLN
1	A	375	ASN
2	B	45	ASN
2	B	80	GLN
2	B	110	ASN
2	B	127	ASN
2	B	135	GLN
1	C	20	ASN
1	C	57	GLN
1	C	80	GLN
1	C	261	GLN
1	C	280	ASN
1	C	302	ASN
1	C	375	ASN
2	D	45	ASN
2	D	80	GLN
2	D	98	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

6 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	$\#\|Z\|>2$
3	MLR	A	1	-	36,36,36	0.82	1 (2%)	53,53,53	1.38	8 (15%)
4	EDO	A	2	-	3,3,3	0.31	0	2,2,2	1.02	0
3	MLR	C	2	-	36,36,36	0.77	0	53,53,53	1.40	7 (13%)
4	EDO	C	3	-	3,3,3	0.35	0	2,2,2	0.34	0
5	TAR	C	395	-	3,9,9	1.21	0	6,12,12	1.33	1 (16%)
4	EDO	C	396	-	3,3,3	0.48	0	2,2,2	0.26	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
3	MLR	A	1	-	-	0/14/74/74	0/3/3/3
4	EDO	A	2	-	-	0/1/1/1	0/0/0/0
3	MLR	C	2	-	-	0/14/74/74	0/3/3/3
4	EDO	C	3	-	-	0/1/1/1	0/0/0/0
5	TAR	C	395	-	1/1/4/4	0/4/12/12	0/0/0/0
4	EDO	C	396	-	-	0/1/1/1	0/0/0/0

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	1	MLR	O5C-C1C	2.25	1.47	1.41

All (16) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	C	2	MLR	C1B-O4A-C4A	-4.20	107.03	118.01
3	A	1	MLR	O5B-C5B-C6B	-2.66	99.63	106.36
3	A	1	MLR	O6A-C6A-C5A	-2.59	102.78	111.33
3	C	2	MLR	O4A-C1B-C2B	-2.55	101.89	108.10
3	A	1	MLR	C3B-C4B-C5B	-2.46	105.27	110.84
5	C	395	TAR	O2-C2-C1	-2.43	105.07	111.21
3	A	1	MLR	C1B-C2B-C3B	-2.30	105.44	109.97
3	C	2	MLR	O2A-C2A-C1A	-2.30	104.76	109.82
3	A	1	MLR	C3A-C4A-C5A	-2.06	106.18	110.84
3	C	2	MLR	O5C-C5C-C4C	2.20	113.82	109.68
3	A	1	MLR	O4C-C4C-C5C	2.22	115.13	109.24
3	C	2	MLR	O3C-C3C-C4C	2.37	115.68	110.34
3	C	2	MLR	C1A-C2A-C3A	2.92	114.77	110.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	A	1	MLR	C1B-O5B-C5B	3.02	119.60	113.75
3	C	2	MLR	C1C-O5C-C5C	3.73	120.99	113.75
3	A	1	MLR	C1A-O5A-C5A	3.90	120.68	113.47

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
5	C	395	TAR	C2

There are no torsion outliers.

There are no ring outliers.

4 monomers are involved in 14 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	1	MLR	1	0
4	A	2	EDO	4	0
3	C	2	MLR	1	0
4	C	3	EDO	8	0

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	365/387 (94%)	-0.14	10 (2%) 58 62	6, 15, 25, 34	0
1	C	369/387 (95%)	-0.18	8 (2%) 65 70	8, 14, 25, 37	0
2	B	139/141 (98%)	0.05	5 (3%) 46 50	14, 20, 30, 38	0
2	D	131/141 (92%)	0.25	11 (8%) 14 15	15, 21, 30, 32	0
All	All	1004/1056 (95%)	-0.08	34 (3%) 49 53	6, 17, 28, 38	0

All (34) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	378	SER	6.6
1	C	91	LYS	6.2
2	B	121	TYR	6.0
1	C	378	SER	4.9
1	C	92	ALA	4.0
1	A	321	LYS	3.8
2	D	89	HIS	3.8
2	D	1	VAL	3.7
2	B	84	ARG	3.6
1	A	180	GLU	3.5
1	A	14	LYS	3.5
1	A	105	VAL	3.2
1	C	267	VAL	3.2
2	D	107	ARG	3.0
2	D	41	GLY	2.9
2	D	114	VAL	2.8
1	A	183	LYS	2.8
1	A	182	GLY	2.8
1	C	90	ASP	2.8
2	B	36	SER	2.7
1	A	107	TYR	2.6

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Mol	Chain	Res	Type	RSRZ
2	D	67	GLU	2.5
1	C	294	THR	2.5
2	D	93	LEU	2.4
2	B	137	ALA	2.3
2	D	90	PRO	2.3
2	D	86	LYS	2.3
1	C	12	GLU	2.3
1	A	150	LYS	2.3
2	B	138	ALA	2.2
1	A	181	ASN	2.1
1	C	266	PHE	2.0
2	D	62	LYS	2.0
2	D	85	TRP	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
4	EDO	C	3	4/4	0.92	0.38	14.77	29,29,32,33	0
4	EDO	C	396	4/4	0.87	0.18	2.92	40,44,45,48	0
5	TAR	C	395	10/10	0.85	0.20	2.12	39,45,47,49	0
3	MLR	A	1	34/34	0.94	0.12	-0.03	14,23,30,31	0
3	MLR	C	2	34/34	0.94	0.11	-0.49	10,17,31,32	0
4	EDO	A	2	4/4	0.96	0.11	-1.12	21,21,25,26	0

6.5 Other polymers (i)

There are no such residues in this entry.