



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 07:42 AM GMT

PDB ID : 3BSM  
Title : Crystal structure of D-mannonate dehydratase from Chromohalobacter salexigens  
Authors : Fedorov, A.A.; Fedorov, E.V.; Toro, R.; Sauder, J.M.; Burley, S.K.; Almo, S.C.; New York SGX Research Center for Structural Genomics (NYSGXRC)  
Deposited on : 2007-12-25  
Resolution : 2.20 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](mailto: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.

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The following versions of software and data (see [references ⓘ](#)) 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

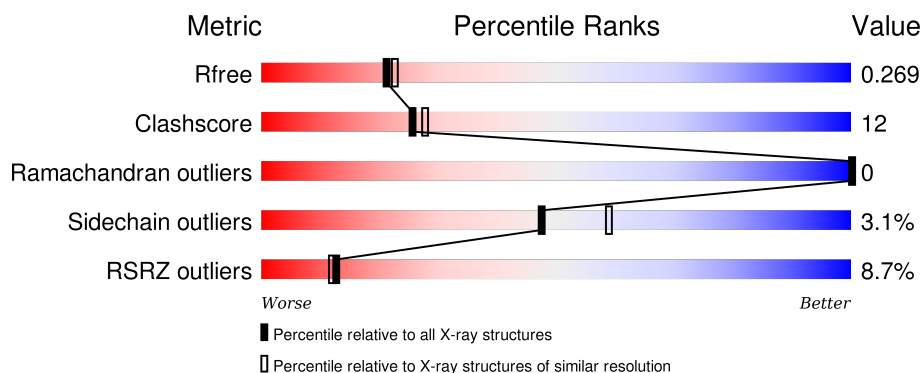
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.20 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	3774 (2.20-2.20)
Clashscore	102246	4477 (2.20-2.20)
Ramachandran outliers	100387	4404 (2.20-2.20)
Sidechain outliers	100360	4405 (2.20-2.20)
RSRZ outliers	91569	3781 (2.20-2.20)

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  $\geq 3$ , 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  $\leq 5\%$ . The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	413	<div> <div>4%</div> <div>64% 21% • 13%</div> </div>
1	B	413	<div> <div>5%</div> <div>66% 19% • 13%</div> </div>
1	C	413	<div> <div>10%</div> <div>65% 20% • 13%</div> </div>
1	D	413	<div> <div>11%</div> <div>63% 22% • 13%</div> </div>

## 2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 11512 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 Mandelate racemase/muconate lactonizing enzyme.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	358	Total	C	N	O	S	0	0	0
			2825	1789	505	517	14			
1	B	358	Total	C	N	O	S	0	0	0
			2825	1789	505	517	14			
1	C	358	Total	C	N	O	S	0	0	0
			2825	1789	505	517	14			
1	D	358	Total	C	N	O	S	0	0	0
			2825	1789	505	517	14			

There are 44 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1	MET	-	EXPRESSION TAG	UNP Q1QT89
A	2	SER	-	EXPRESSION TAG	UNP Q1QT89
A	3	LEU	-	EXPRESSION TAG	UNP Q1QT89
A	406	GLU	-	EXPRESSION TAG	UNP Q1QT89
A	407	GLY	-	EXPRESSION TAG	UNP Q1QT89
A	408	HIS	-	EXPRESSION TAG	UNP Q1QT89
A	409	HIS	-	EXPRESSION TAG	UNP Q1QT89
A	410	HIS	-	EXPRESSION TAG	UNP Q1QT89
A	411	HIS	-	EXPRESSION TAG	UNP Q1QT89
A	412	HIS	-	EXPRESSION TAG	UNP Q1QT89
A	413	HIS	-	EXPRESSION TAG	UNP Q1QT89
B	1	MET	-	EXPRESSION TAG	UNP Q1QT89
B	2	SER	-	EXPRESSION TAG	UNP Q1QT89
B	3	LEU	-	EXPRESSION TAG	UNP Q1QT89
B	406	GLU	-	EXPRESSION TAG	UNP Q1QT89
B	407	GLY	-	EXPRESSION TAG	UNP Q1QT89
B	408	HIS	-	EXPRESSION TAG	UNP Q1QT89
B	409	HIS	-	EXPRESSION TAG	UNP Q1QT89
B	410	HIS	-	EXPRESSION TAG	UNP Q1QT89
B	411	HIS	-	EXPRESSION TAG	UNP Q1QT89
B	412	HIS	-	EXPRESSION TAG	UNP Q1QT89

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Chain	Residue	Modelled	Actual	Comment	Reference
B	413	HIS	-	EXPRESSION TAG	UNP Q1QT89
C	1	MET	-	EXPRESSION TAG	UNP Q1QT89
C	2	SER	-	EXPRESSION TAG	UNP Q1QT89
C	3	LEU	-	EXPRESSION TAG	UNP Q1QT89
C	406	GLU	-	EXPRESSION TAG	UNP Q1QT89
C	407	GLY	-	EXPRESSION TAG	UNP Q1QT89
C	408	HIS	-	EXPRESSION TAG	UNP Q1QT89
C	409	HIS	-	EXPRESSION TAG	UNP Q1QT89
C	410	HIS	-	EXPRESSION TAG	UNP Q1QT89
C	411	HIS	-	EXPRESSION TAG	UNP Q1QT89
C	412	HIS	-	EXPRESSION TAG	UNP Q1QT89
C	413	HIS	-	EXPRESSION TAG	UNP Q1QT89
D	1	MET	-	EXPRESSION TAG	UNP Q1QT89
D	2	SER	-	EXPRESSION TAG	UNP Q1QT89
D	3	LEU	-	EXPRESSION TAG	UNP Q1QT89
D	406	GLU	-	EXPRESSION TAG	UNP Q1QT89
D	407	GLY	-	EXPRESSION TAG	UNP Q1QT89
D	408	HIS	-	EXPRESSION TAG	UNP Q1QT89
D	409	HIS	-	EXPRESSION TAG	UNP Q1QT89
D	410	HIS	-	EXPRESSION TAG	UNP Q1QT89
D	411	HIS	-	EXPRESSION TAG	UNP Q1QT89
D	412	HIS	-	EXPRESSION TAG	UNP Q1QT89
D	413	HIS	-	EXPRESSION TAG	UNP Q1QT89

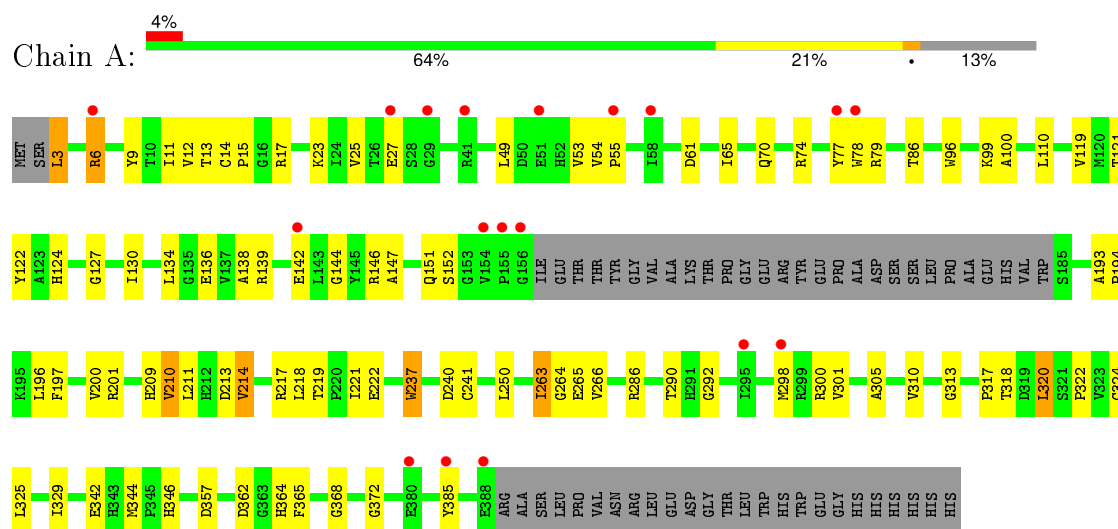
- Molecule 2 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	67	Total O 67 67	0	0
2	B	60	Total O 60 60	0	0
2	C	46	Total O 46 46	0	0
2	D	39	Total O 39 39	0	0

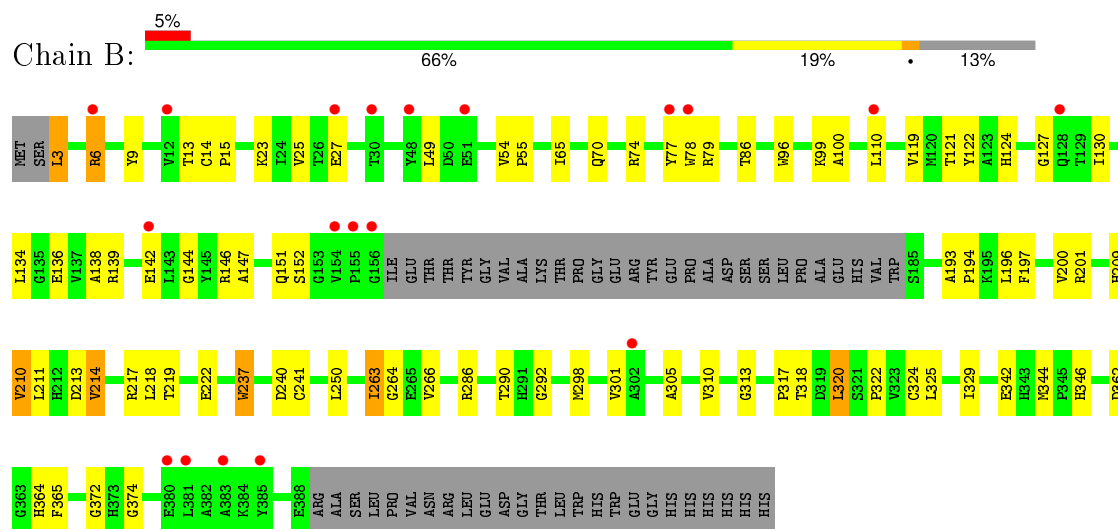
### 3 Residue-property plots [i](#)

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: Mandelate racemase/muconate lactonizing enzyme

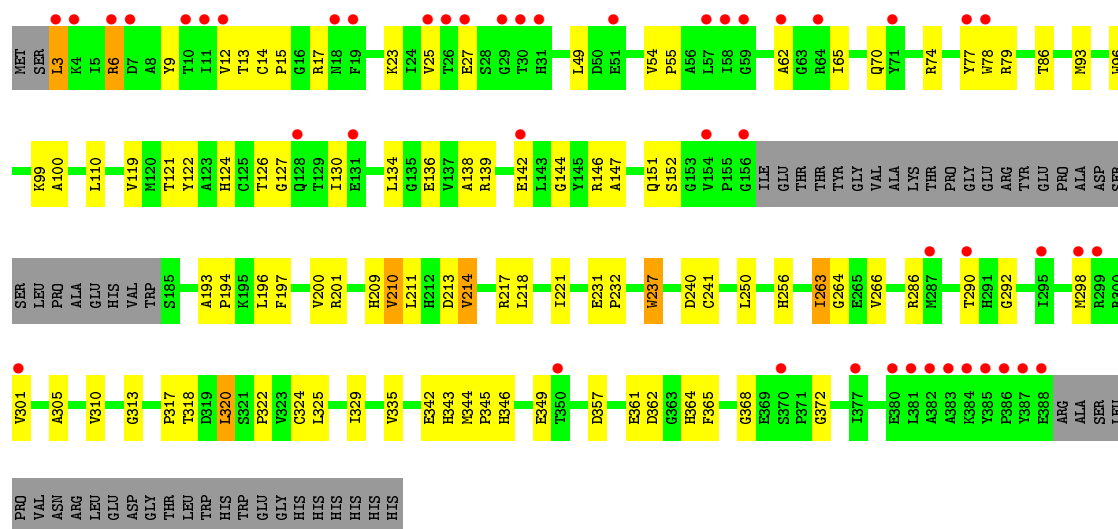


- Molecule 1: Mandelate racemase/muconate lactonizing enzyme



- Molecule 1: Mandelate racemase/muconate lactonizing enzyme





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	110.12Å 163.07Å 84.55Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	24.93 – 2.20 39.47 – 1.99	Depositor EDS
% Data completeness (in resolution range)	99.5 (24.93-2.20) 96.8 (39.47-1.99)	Depositor EDS
$R_{merge}$	0.08	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.42 (at 2.00Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, $R_{free}$	0.243 , 0.268 0.243 , 0.269	Depositor DCC
$R_{free}$ test set	3849 reflections (4.97%)	DCC
Wilson B-factor (Å <sup>2</sup> )	34.7	Xtriage
Anisotropy	0.600	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.38 , 55.3	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.33$	Xtriage
Outliers	1 of 101553 reflections (0.001%)	Xtriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	11512	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	44.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.33% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical values of  $\langle |L| \rangle$ ,  $\langle L^2 \rangle$  for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 0.2 for perfectly twinned datasets.

## 5 Model quality [i](#)

### 5.1 Standard geometry [i](#)

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	0.37	0/2900	0.62	0/3945
1	B	0.37	0/2900	0.62	0/3945
1	C	0.37	0/2900	0.62	0/3945
1	D	0.36	0/2900	0.62	0/3945
All	All	0.37	0/11600	0.62	0/15780

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

### 5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2825	0	2733	76	1
1	B	2825	0	2733	67	0
1	C	2825	0	2733	71	0
1	D	2825	0	2733	76	1
2	A	67	0	0	6	1
2	B	60	0	0	2	0
2	C	46	0	0	2	0
2	D	39	0	0	1	1
All	All	11512	0	10932	278	2

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 12.



All (278) 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:C:292:GLY:HA3	1:C:298:MET:HE1	1.43	0.99
1:A:292:GLY:HA3	1:A:298:MET:HE1	1.44	0.98
1:D:292:GLY:HA3	1:D:298:MET:HE1	1.45	0.96
1:B:292:GLY:HA3	1:B:298:MET:HE1	1.46	0.95
1:A:265:GLU:OE1	2:A:480:HOH:O	1.89	0.89
1:C:151:GLN:HE22	1:C:213:ASP:H	1.22	0.88
1:D:151:GLN:HE22	1:D:213:ASP:H	1.22	0.87
1:B:151:GLN:HE22	1:B:213:ASP:H	1.23	0.86
1:A:151:GLN:HE22	1:A:213:ASP:H	1.20	0.85
1:A:99:LYS:HG2	1:A:110:LEU:HD21	1.65	0.79
1:B:99:LYS:HG2	1:B:110:LEU:HD21	1.64	0.77
1:D:99:LYS:HG2	1:D:110:LEU:HD21	1.65	0.77
1:C:99:LYS:HG2	1:C:110:LEU:HD21	1.64	0.76
1:C:119:VAL:HG22	1:C:365:PHE:HB2	1.67	0.76
1:B:119:VAL:HG22	1:B:365:PHE:HB2	1.68	0.76
1:D:119:VAL:HG22	1:D:365:PHE:HB2	1.67	0.75
1:A:119:VAL:HG22	1:A:365:PHE:HB2	1.69	0.74
1:A:266:VAL:HG13	1:C:79:ARG:HD3	1.72	0.72
1:D:197:PHE:O	1:D:200:VAL:HG22	1.91	0.71
1:A:197:PHE:O	1:A:200:VAL:HG22	1.91	0.70
1:B:290:THR:HG23	1:B:324:CYS:SG	2.30	0.70
1:D:298:MET:HA	1:D:301:VAL:HG22	1.74	0.70
1:A:317:PRO:HD2	1:A:320:LEU:HD22	1.74	0.70
1:C:317:PRO:HD2	1:C:320:LEU:HD22	1.74	0.69
1:B:317:PRO:HD2	1:B:320:LEU:HD22	1.74	0.69
1:B:266:VAL:HG13	1:D:79:ARG:HD3	1.74	0.69
1:C:197:PHE:O	1:C:200:VAL:HG22	1.92	0.69
1:D:263:ILE:HD13	1:D:264:GLY:H	1.57	0.69
1:B:197:PHE:O	1:B:200:VAL:HG22	1.93	0.68
1:C:290:THR:HG23	1:C:324:CYS:SG	2.35	0.67
1:D:317:PRO:HD2	1:D:320:LEU:HD22	1.75	0.67
1:B:263:ILE:HD13	1:B:264:GLY:H	1.58	0.67
1:C:263:ILE:HD13	1:C:264:GLY:H	1.59	0.66
1:A:263:ILE:HD13	1:A:264:GLY:H	1.61	0.65
1:A:290:THR:HG23	1:A:324:CYS:SG	2.36	0.65
1:A:298:MET:HA	1:A:301:VAL:HG22	1.77	0.65
1:D:100:ALA:HB3	1:D:372:GLY:HA2	1.77	0.65
1:D:290:THR:HG23	1:D:324:CYS:SG	2.37	0.65
1:A:138:ALA:O	1:A:142:GLU:HG2	1.97	0.65
1:C:298:MET:HA	1:C:301:VAL:HG22	1.77	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:138:ALA:O	1:C:142:GLU:HG2	1.97	0.64
1:C:100:ALA:HB3	1:C:372:GLY:HA2	1.79	0.64
1:B:100:ALA:HB3	1:B:372:GLY:HA2	1.77	0.64
1:D:138:ALA:O	1:D:142:GLU:HG2	1.97	0.64
1:A:100:ALA:HB3	1:A:372:GLY:HA2	1.78	0.64
1:C:271:HIS:HD2	2:C:441:HOH:O	1.80	0.63
1:B:138:ALA:O	1:B:142:GLU:HG2	1.97	0.63
1:D:74:ARG:HG3	1:D:78:TRP:CZ2	2.34	0.63
1:D:193:ALA:HB3	1:D:194:PRO:HD3	1.80	0.63
1:D:217:ARG:HH11	1:D:217:ARG:HG3	1.65	0.62
1:B:79:ARG:HD3	1:D:266:VAL:HG13	1.82	0.62
1:B:74:ARG:HG3	1:B:78:TRP:CZ2	2.35	0.62
1:A:79:ARG:HD3	1:C:266:VAL:HG13	1.81	0.61
1:A:217:ARG:HH11	1:A:217:ARG:HG3	1.64	0.61
1:B:298:MET:HA	1:B:301:VAL:HG22	1.80	0.61
1:A:193:ALA:HB3	1:A:194:PRO:HD3	1.83	0.61
1:D:292:GLY:CA	1:D:298:MET:HE1	2.27	0.61
1:B:193:ALA:HB3	1:B:194:PRO:HD3	1.83	0.61
1:A:74:ARG:HG3	1:A:78:TRP:CZ2	2.35	0.61
1:B:217:ARG:HG3	1:B:217:ARG:HH11	1.65	0.61
1:A:121:THR:CG2	1:A:122:TYR:N	2.64	0.61
1:C:74:ARG:HG3	1:C:78:TRP:CZ2	2.35	0.61
1:C:121:THR:CG2	1:C:122:TYR:N	2.64	0.60
1:A:241:CYS:SG	2:A:446:HOH:O	2.56	0.60
1:C:193:ALA:HB3	1:C:194:PRO:HD3	1.82	0.60
1:C:217:ARG:HG3	1:C:217:ARG:HH11	1.66	0.59
1:A:121:THR:HG22	1:A:122:TYR:N	2.17	0.59
1:D:121:THR:CG2	1:D:122:TYR:N	2.66	0.59
1:B:121:THR:CG2	1:B:122:TYR:N	2.66	0.58
1:C:121:THR:HG22	1:C:122:TYR:N	2.18	0.58
1:D:121:THR:HG22	1:D:122:TYR:N	2.19	0.58
1:D:256:HIS:HD2	2:D:417:HOH:O	1.87	0.58
1:A:325:LEU:O	1:A:329:ILE:HG13	2.04	0.57
1:C:292:GLY:CA	1:C:298:MET:HE1	2.26	0.57
1:B:374:GLY:HA3	2:B:436:HOH:O	2.05	0.57
1:B:13:THR:OG1	1:B:15:PRO:HD3	2.04	0.57
1:A:292:GLY:CA	1:A:298:MET:HE1	2.28	0.56
1:B:121:THR:HG22	1:B:122:TYR:N	2.20	0.56
1:C:325:LEU:O	1:C:329:ILE:HG13	2.06	0.56
1:B:292:GLY:CA	1:B:298:MET:HE1	2.28	0.56
1:C:3:LEU:HD13	1:C:3:LEU:N	2.21	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:70:GLN:O	1:A:74:ARG:HD3	2.06	0.56
1:D:325:LEU:O	1:D:329:ILE:HG13	2.05	0.56
1:A:266:VAL:HG21	1:C:77:TYR:HB3	1.88	0.55
1:D:74:ARG:HG3	1:D:78:TRP:CH2	2.41	0.55
1:B:74:ARG:HG3	1:B:78:TRP:CH2	2.42	0.55
1:A:61:ASP:OD2	2:A:441:HOH:O	2.18	0.55
1:D:70:GLN:O	1:D:74:ARG:HD3	2.06	0.55
1:A:74:ARG:HG3	1:A:78:TRP:CH2	2.42	0.55
1:C:19:PHE:O	2:C:456:HOH:O	2.18	0.55
1:C:74:ARG:HG3	1:C:78:TRP:CH2	2.42	0.54
1:D:119:VAL:CG2	1:D:365:PHE:HB2	2.37	0.54
1:C:9:TYR:OH	1:C:23:LYS:HD3	2.08	0.54
1:B:119:VAL:CG2	1:B:365:PHE:HB2	2.37	0.54
1:C:70:GLN:O	1:C:74:ARG:HD3	2.08	0.54
1:A:13:THR:OG1	1:A:15:PRO:HD3	2.07	0.54
1:C:13:THR:OG1	1:C:15:PRO:HD3	2.07	0.54
1:C:49:LEU:O	1:C:54:VAL:HG23	2.08	0.54
1:B:49:LEU:O	1:B:54:VAL:HG23	2.08	0.54
1:B:70:GLN:O	1:B:74:ARG:HD3	2.08	0.53
1:A:3:LEU:HD13	1:A:3:LEU:N	2.23	0.53
1:B:325:LEU:O	1:B:329:ILE:HG13	2.09	0.53
1:A:11:ILE:O	2:A:442:HOH:O	2.19	0.53
1:C:119:VAL:CG2	1:C:365:PHE:HB2	2.36	0.53
1:C:298:MET:O	1:C:301:VAL:HG22	2.09	0.53
1:B:298:MET:O	1:B:301:VAL:HG22	2.09	0.53
1:B:139:ARG:O	1:B:142:GLU:HB2	2.09	0.53
1:D:13:THR:OG1	1:D:15:PRO:HD3	2.09	0.53
1:D:263:ILE:CD1	1:D:264:GLY:H	2.23	0.52
1:C:286:ARG:HD2	1:C:313:GLY:O	2.09	0.52
1:C:298:MET:SD	1:C:301:VAL:HG21	2.50	0.52
1:A:298:MET:SD	1:A:301:VAL:HG21	2.50	0.52
1:B:3:LEU:N	1:B:3:LEU:HD13	2.24	0.52
1:A:286:ARG:HD2	1:A:313:GLY:O	2.10	0.52
1:D:49:LEU:O	1:D:54:VAL:HG23	2.09	0.52
1:D:9:TYR:OH	1:D:23:LYS:HD3	2.10	0.52
1:D:139:ARG:O	1:D:142:GLU:HB2	2.09	0.52
1:D:3:LEU:HD13	1:D:3:LEU:N	2.25	0.52
1:C:139:ARG:O	1:C:142:GLU:HB2	2.11	0.51
1:D:298:MET:SD	1:D:301:VAL:HG21	2.50	0.51
1:B:298:MET:SD	1:B:301:VAL:HG21	2.50	0.51
1:B:266:VAL:HG21	1:D:77:TYR:HB3	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:286:ARG:HD2	1:D:313:GLY:O	2.11	0.51
1:C:211:LEU:HD12	1:C:211:LEU:N	2.26	0.51
1:D:54:VAL:HB	1:D:55:PRO:HD3	1.93	0.51
1:D:211:LEU:HD12	1:D:211:LEU:N	2.26	0.51
1:D:196:LEU:O	1:D:200:VAL:HG13	2.11	0.50
1:A:147:ALA:CB	1:A:209:HIS:HB2	2.41	0.50
1:B:211:LEU:N	1:B:211:LEU:HD12	2.25	0.50
1:B:54:VAL:HB	1:B:55:PRO:HD3	1.93	0.50
1:D:298:MET:O	1:D:301:VAL:HG22	2.12	0.50
1:A:263:ILE:CD1	1:A:264:GLY:H	2.25	0.50
1:C:54:VAL:HB	1:C:55:PRO:HD3	1.94	0.50
1:D:151:GLN:NE2	1:D:213:ASP:H	2.02	0.50
1:C:196:LEU:O	1:C:200:VAL:HG13	2.12	0.50
1:B:9:TYR:OH	1:B:23:LYS:HD3	2.12	0.49
1:A:49:LEU:O	1:A:54:VAL:HG23	2.12	0.49
1:A:77:TYR:HB3	1:C:266:VAL:HG21	1.93	0.49
1:B:286:ARG:HD2	1:B:313:GLY:O	2.12	0.49
1:A:211:LEU:HD12	1:A:211:LEU:N	2.27	0.49
1:B:196:LEU:O	1:B:200:VAL:HG13	2.13	0.49
1:A:54:VAL:HB	1:A:55:PRO:HD3	1.94	0.49
1:A:196:LEU:O	1:A:200:VAL:HG13	2.11	0.49
1:A:119:VAL:CG2	1:A:365:PHE:HB2	2.40	0.49
1:B:263:ILE:CD1	1:B:264:GLY:H	2.26	0.49
1:A:214:VAL:HG23	1:A:214:VAL:O	2.12	0.49
1:D:214:VAL:O	1:D:214:VAL:HG23	2.11	0.49
1:B:214:VAL:O	1:B:214:VAL:HG23	2.11	0.49
1:A:298:MET:O	1:A:301:VAL:HG22	2.13	0.48
1:C:263:ILE:CD1	1:C:264:GLY:H	2.25	0.48
1:C:147:ALA:CB	1:C:209:HIS:HB2	2.43	0.48
1:A:139:ARG:O	1:A:142:GLU:HB2	2.13	0.48
1:B:147:ALA:CB	1:B:209:HIS:HB2	2.44	0.48
1:A:214:VAL:HG22	1:A:240:ASP:O	2.13	0.48
1:C:214:VAL:O	1:C:214:VAL:HG23	2.12	0.48
1:D:147:ALA:CB	1:D:209:HIS:HB2	2.43	0.48
1:C:362:ASP:O	1:C:364:HIS:HD2	1.97	0.48
1:D:6:ARG:HG3	1:D:25:VAL:O	2.14	0.48
1:A:362:ASP:O	1:A:364:HIS:HD2	1.95	0.48
1:C:119:VAL:HG23	1:C:119:VAL:O	2.13	0.48
1:C:136:GLU:OE2	1:C:139:ARG:HD3	2.14	0.48
1:B:214:VAL:HG22	1:B:240:ASP:O	2.14	0.48
1:B:362:ASP:O	1:B:364:HIS:HD2	1.96	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:362:ASP:O	1:D:364:HIS:HD2	1.97	0.47
1:A:305:ALA:HB1	1:A:310:VAL:HB	1.95	0.47
1:C:127:GLY:O	1:C:152:SER:HA	2.15	0.47
1:D:214:VAL:HG22	1:D:240:ASP:O	2.14	0.47
1:D:298:MET:CA	1:D:301:VAL:HG22	2.43	0.47
1:A:136:GLU:OE2	1:A:139:ARG:HD3	2.15	0.47
1:A:147:ALA:HB2	1:A:209:HIS:HB2	1.96	0.47
1:A:9:TYR:OH	1:A:23:LYS:HD3	2.14	0.47
1:D:136:GLU:OE2	1:D:139:ARG:HD3	2.15	0.47
1:C:6:ARG:HG3	1:C:25:VAL:O	2.14	0.47
1:B:119:VAL:O	1:B:119:VAL:HG23	2.14	0.47
1:D:201:ARG:NH2	1:D:210:VAL:HG13	2.30	0.47
1:D:119:VAL:HG23	1:D:119:VAL:O	2.13	0.46
1:C:322:PRO:HG3	1:C:346:HIS:CD2	2.51	0.46
1:D:237:TRP:CD1	1:D:237:TRP:C	2.89	0.46
1:B:266:VAL:CG1	1:D:79:ARG:HD3	2.45	0.46
1:B:136:GLU:OE2	1:B:139:ARG:HD3	2.15	0.46
1:C:214:VAL:HG22	1:C:240:ASP:O	2.15	0.46
1:C:237:TRP:C	1:C:237:TRP:CD1	2.89	0.46
1:A:119:VAL:O	1:A:119:VAL:HG23	2.13	0.46
1:B:77:TYR:HB3	1:D:266:VAL:HG21	1.97	0.46
1:A:219:THR:OG1	1:A:222:GLU:HG3	2.16	0.46
1:A:127:GLY:O	1:A:152:SER:HA	2.15	0.46
1:A:266:VAL:CG1	1:C:79:ARG:HD3	2.43	0.46
1:D:322:PRO:HG3	1:D:346:HIS:CD2	2.51	0.46
1:A:237:TRP:CD1	1:A:237:TRP:C	2.88	0.46
1:B:201:ARG:NH2	1:B:210:VAL:HG13	2.31	0.46
1:D:147:ALA:HB2	1:D:209:HIS:HB2	1.98	0.46
1:A:201:ARG:NH2	1:A:210:VAL:HG13	2.31	0.46
1:A:322:PRO:HG3	1:A:346:HIS:CD2	2.51	0.46
1:B:292:GLY:HA3	1:B:298:MET:CE	2.32	0.46
1:B:127:GLY:O	1:B:152:SER:HA	2.15	0.46
1:A:6:ARG:HG3	1:A:25:VAL:O	2.16	0.45
1:B:237:TRP:C	1:B:237:TRP:CD1	2.89	0.45
1:C:219:THR:OG1	1:C:222:GLU:HG3	2.16	0.45
1:D:305:ALA:HB1	1:D:310:VAL:HB	1.98	0.45
1:D:127:GLY:O	1:D:152:SER:HA	2.16	0.45
1:B:322:PRO:HG3	1:B:346:HIS:CD2	2.52	0.45
1:A:298:MET:CA	1:A:301:VAL:HG22	2.46	0.44
1:A:346:HIS:HD2	2:A:456:HOH:O	1.99	0.44
1:C:298:MET:CA	1:C:301:VAL:HG22	2.46	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:147:ALA:HB2	1:C:209:HIS:HB2	1.99	0.44
1:C:119:VAL:CG2	1:C:119:VAL:O	2.66	0.44
1:C:305:ALA:HB1	1:C:310:VAL:HB	1.99	0.44
1:C:130:ILE:O	1:C:134:LEU:HG	2.18	0.44
1:B:6:ARG:HG3	1:B:25:VAL:O	2.17	0.44
1:C:201:ARG:NH2	1:C:210:VAL:HG13	2.33	0.43
1:C:144:GLY:O	1:C:146:ARG:NH1	2.51	0.43
1:B:124:HIS:HE1	1:B:342:GLU:OE2	2.01	0.43
1:D:119:VAL:O	1:D:119:VAL:CG2	2.66	0.43
1:D:86:THR:HA	1:D:290:THR:O	2.19	0.43
1:A:318:THR:N	1:A:344:MET:HE2	2.33	0.43
1:C:214:VAL:CG2	1:C:241:CYS:HA	2.49	0.43
1:D:130:ILE:O	1:D:134:LEU:HG	2.19	0.43
1:B:147:ALA:HB2	1:B:209:HIS:HB2	2.00	0.43
1:B:130:ILE:O	1:B:134:LEU:HG	2.19	0.43
1:A:119:VAL:O	1:A:119:VAL:CG2	2.66	0.42
1:B:305:ALA:HB1	1:B:310:VAL:HB	2.00	0.42
1:D:144:GLY:O	1:D:146:ARG:NH1	2.52	0.42
1:B:119:VAL:O	1:B:119:VAL:CG2	2.67	0.42
1:B:3:LEU:HA	1:B:27:GLU:OE2	2.20	0.42
1:C:12:VAL:O	1:C:12:VAL:HG13	2.19	0.42
1:B:374:GLY:CA	2:B:436:HOH:O	2.67	0.42
1:C:124:HIS:HE1	1:C:342:GLU:OE2	2.03	0.42
1:A:86:THR:HA	1:A:290:THR:O	2.20	0.42
1:C:86:THR:HA	1:C:290:THR:O	2.20	0.42
1:A:214:VAL:CG2	1:A:241:CYS:HA	2.50	0.42
1:D:121:THR:CG2	1:D:343:HIS:HB3	2.50	0.42
1:B:86:THR:HA	1:B:290:THR:O	2.19	0.42
1:D:214:VAL:CG2	1:D:241:CYS:HA	2.50	0.42
1:D:357:ASP:CG	1:D:368:GLY:HA3	2.40	0.42
1:A:318:THR:H	1:A:344:MET:HE2	1.85	0.42
1:C:65:ILE:HG21	1:C:96:TRP:NE1	2.35	0.42
1:D:126:THR:HG22	1:D:151:GLN:HB2	2.02	0.41
1:A:79:ARG:HD3	1:C:266:VAL:HG22	2.02	0.41
1:B:214:VAL:CG2	1:B:241:CYS:HA	2.50	0.41
1:A:130:ILE:O	1:A:134:LEU:HG	2.20	0.41
1:D:12:VAL:HG13	1:D:12:VAL:O	2.20	0.41
1:D:3:LEU:HA	1:D:27:GLU:OE2	2.20	0.41
1:A:124:HIS:HE1	1:A:342:GLU:OE2	2.04	0.41
1:C:126:THR:HG22	1:C:151:GLN:HB2	2.02	0.41
1:D:231:GLU:N	1:D:232:PRO:CD	2.84	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:231:GLU:N	1:C:232:PRO:CD	2.84	0.41
1:B:79:ARG:HD3	1:D:266:VAL:CG1	2.49	0.41
1:D:3:LEU:HD23	1:D:62:ALA:HB3	2.02	0.41
1:D:221:ILE:HD12	1:D:221:ILE:HA	1.96	0.41
1:B:318:THR:N	1:B:344:MET:HE2	2.35	0.41
1:B:200:VAL:HG23	1:B:201:ARG:N	2.36	0.41
1:A:12:VAL:O	1:A:12:VAL:HG13	2.21	0.41
1:C:335:VAL:HG13	1:C:335:VAL:O	2.20	0.41
1:D:93:MET:CE	1:D:290:THR:HG22	2.50	0.41
1:C:3:LEU:HA	1:C:27:GLU:OE2	2.21	0.41
1:A:49:LEU:HA	1:A:53:VAL:HB	2.03	0.41
1:A:3:LEU:HA	1:A:27:GLU:OE2	2.20	0.41
1:B:144:GLY:O	1:B:146:ARG:NH1	2.53	0.41
1:A:221:ILE:HA	1:A:221:ILE:HD12	1.95	0.41
1:D:349:GLU:CD	1:D:349:GLU:H	2.25	0.41
1:A:144:GLY:O	1:A:146:ARG:NH1	2.53	0.41
1:C:93:MET:CE	1:C:290:THR:HG22	2.50	0.40
1:A:65:ILE:HG21	1:A:96:TRP:NE1	2.35	0.40
1:D:343:HIS:NE2	1:D:345:PRO:HG3	2.37	0.40
1:C:3:LEU:HD23	1:C:62:ALA:HB3	2.03	0.40
1:D:14:CYS:HA	1:D:17:ARG:O	2.21	0.40
1:B:65:ILE:HG21	1:B:96:TRP:NE1	2.36	0.40
1:B:219:THR:OG1	1:B:222:GLU:HG3	2.21	0.40
1:D:65:ILE:HG21	1:D:96:TRP:NE1	2.35	0.40
1:A:357:ASP:CG	1:A:368:GLY:HA3	2.42	0.40
1:D:318:THR:HG23	1:D:344:MET:CE	2.52	0.40
1:B:14:CYS:O	1:B:14:CYS:SG	2.80	0.40
1:A:300:ARG:NH1	2:A:450:HOH:O	2.41	0.40
1:D:124:HIS:HE1	1:D:342:GLU:OE2	2.04	0.40
1:A:217:ARG:HG3	1:A:217:ARG:NH1	2.35	0.40
1:C:14:CYS:HA	1:C:17:ARG:O	2.22	0.40
1:D:335:VAL:O	1:D:335:VAL:HG13	2.21	0.40
1:A:14:CYS:HA	1:A:17:ARG:O	2.21	0.40

All (2) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:385:TYR:OH	1:D:361:GLU:OE2[3_556]	2.05	0.15
2:A:478:HOH:O	2:D:447:HOH:O[2_655]	2.13	0.07

## 5.3 Torsion angles

### 5.3.1 Protein backbone

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	354/413 (86%)	343 (97%)	11 (3%)	0	100	100
1	B	354/413 (86%)	341 (96%)	13 (4%)	0	100	100
1	C	354/413 (86%)	342 (97%)	12 (3%)	0	100	100
1	D	354/413 (86%)	339 (96%)	15 (4%)	0	100	100
All	All	1416/1652 (86%)	1365 (96%)	51 (4%)	0	100	100

There are no Ramachandran outliers to report.

### 5.3.2 Protein sidechains

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	292/339 (86%)	283 (97%)	9 (3%)	47	59
1	B	292/339 (86%)	283 (97%)	9 (3%)	47	59
1	C	292/339 (86%)	283 (97%)	9 (3%)	47	59
1	D	292/339 (86%)	283 (97%)	9 (3%)	47	59
All	All	1168/1356 (86%)	1132 (97%)	36 (3%)	47	59

All (36) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	3	LEU
1	A	6	ARG

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Mol	Chain	Res	Type
1	A	210	VAL
1	A	214	VAL
1	A	218	LEU
1	A	237	TRP
1	A	250	LEU
1	A	263	ILE
1	A	320	LEU
1	B	3	LEU
1	B	6	ARG
1	B	210	VAL
1	B	214	VAL
1	B	218	LEU
1	B	237	TRP
1	B	250	LEU
1	B	263	ILE
1	B	320	LEU
1	C	3	LEU
1	C	6	ARG
1	C	210	VAL
1	C	214	VAL
1	C	218	LEU
1	C	237	TRP
1	C	250	LEU
1	C	263	ILE
1	C	320	LEU
1	D	3	LEU
1	D	6	ARG
1	D	210	VAL
1	D	214	VAL
1	D	218	LEU
1	D	237	TRP
1	D	250	LEU
1	D	263	ILE
1	D	320	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (39) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	124	HIS
1	A	128	GLN
1	A	140	HIS
1	A	151	GLN

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Mol	Chain	Res	Type
1	A	278	GLN
1	A	291	HIS
1	A	341	GLN
1	A	343	HIS
1	A	346	HIS
1	A	364	HIS
1	B	124	HIS
1	B	128	GLN
1	B	140	HIS
1	B	151	GLN
1	B	278	GLN
1	B	291	HIS
1	B	341	GLN
1	B	343	HIS
1	B	346	HIS
1	B	364	HIS
1	C	124	HIS
1	C	128	GLN
1	C	140	HIS
1	C	151	GLN
1	C	271	HIS
1	C	291	HIS
1	C	341	GLN
1	C	343	HIS
1	C	346	HIS
1	C	364	HIS
1	D	124	HIS
1	D	128	GLN
1	D	140	HIS
1	D	151	GLN
1	D	291	HIS
1	D	341	GLN
1	D	343	HIS
1	D	346	HIS
1	D	364	HIS

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

There are no ligands in this entry.

## 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<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	358/413 (86%)	0.26	18 (5%)	32 32	25, 39, 62, 75	0
1	B	358/413 (86%)	0.28	19 (5%)	30 29	25, 41, 61, 76	0
1	C	358/413 (86%)	0.64	40 (11%)	7 6	26, 47, 64, 76	0
1	D	358/413 (86%)	0.76	47 (13%)	5 4	26, 48, 65, 76	0
All	All	1432/1652 (86%)	0.48	124 (8%)	13 12	25, 44, 63, 76	0

All (124) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	6	ARG	6.6
1	D	78	TRP	6.4
1	D	29	GLY	6.3
1	D	383	ALA	6.2
1	C	27	GLU	6.0
1	B	154	VAL	5.9
1	C	29	GLY	5.9
1	D	27	GLU	5.8
1	D	384	LYS	5.7
1	D	385	TYR	5.4
1	D	156	GLY	4.9
1	A	154	VAL	4.8
1	D	26	THR	4.7
1	A	78	TRP	4.7
1	D	142	GLU	4.6
1	C	78	TRP	4.6
1	D	6	ARG	4.5
1	A	6	ARG	4.3
1	D	380	GLU	4.3
1	B	142	GLU	4.3
1	D	387	TYR	4.2

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Mol	Chain	Res	Type	RSRZ
1	D	25	VAL	4.2
1	C	44	ALA	4.2
1	B	155	PRO	4.2
1	D	388	GLU	4.1
1	C	128	GLN	4.0
1	B	156	GLY	4.0
1	C	289	LEU	3.9
1	D	58	ILE	3.8
1	D	386	PRO	3.8
1	D	57	LEU	3.7
1	C	51	GLU	3.7
1	B	128	GLN	3.6
1	C	4	LYS	3.6
1	A	155	PRO	3.6
1	D	382	ALA	3.5
1	A	58	ILE	3.4
1	D	19	PHE	3.3
1	A	29	GLY	3.3
1	C	142	GLU	3.3
1	A	142	GLU	3.3
1	B	78	TRP	3.3
1	D	381	LEU	3.3
1	C	62	ALA	3.2
1	D	154	VAL	3.2
1	A	156	GLY	3.2
1	C	154	VAL	3.2
1	C	298	MET	3.1
1	C	25	VAL	3.0
1	D	77	TYR	3.0
1	D	377	ILE	3.0
1	D	3	LEU	3.0
1	D	350	THR	3.0
1	C	383	ALA	3.0
1	C	13	THR	3.0
1	C	26	THR	3.0
1	B	51	GLU	2.9
1	C	102	ALA	2.9
1	D	30	THR	2.9
1	A	41	ARG	2.8
1	C	380	GLU	2.7
1	B	48	TYR	2.7
1	D	4	LYS	2.7

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Mol	Chain	Res	Type	RSRZ
1	B	385	TYR	2.7
1	C	385	TYR	2.7
1	D	7	ASP	2.7
1	C	64	ARG	2.6
1	D	10	THR	2.6
1	C	31	HIS	2.6
1	C	387	TYR	2.6
1	B	27	GLU	2.6
1	B	77	TYR	2.5
1	C	290	THR	2.5
1	D	290	THR	2.5
1	D	301	VAL	2.5
1	C	207	ASP	2.5
1	D	128	GLN	2.5
1	D	298	MET	2.5
1	C	384	LYS	2.5
1	A	51	GLU	2.5
1	D	31	HIS	2.5
1	A	55	PRO	2.4
1	C	155	PRO	2.4
1	C	5	ILE	2.4
1	C	58	ILE	2.4
1	D	62	ALA	2.4
1	C	50	ASP	2.4
1	A	295	ILE	2.4
1	B	380	GLU	2.4
1	D	370	SER	2.4
1	C	301	VAL	2.4
1	C	30	THR	2.4
1	C	386	PRO	2.4
1	D	12	VAL	2.4
1	B	6	ARG	2.4
1	D	64	ARG	2.4
1	C	14	CYS	2.3
1	D	295	ILE	2.3
1	C	359	ARG	2.3
1	C	16	GLY	2.3
1	D	59	GLY	2.3
1	A	298	MET	2.3
1	A	77	TYR	2.2
1	A	385	TYR	2.2
1	B	381	LEU	2.2

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Mol	Chain	Res	Type	RSRZ
1	C	295	ILE	2.2
1	D	287	MET	2.2
1	B	30	THR	2.2
1	A	388	GLU	2.2
1	B	302	ALA	2.2
1	D	11	ILE	2.2
1	A	27	GLU	2.1
1	B	110	LEU	2.1
1	D	71	TYR	2.1
1	B	383	ALA	2.1
1	B	12	VAL	2.1
1	D	51	GLU	2.1
1	D	18	ASN	2.1
1	D	299	ARG	2.1
1	C	10	THR	2.1
1	C	18	ASN	2.1
1	D	131	GLU	2.1
1	C	12	VAL	2.0
1	A	380	GLU	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](#)

There are no ligands in this entry.

## 6.5 Other polymers [i](#)

There are no such residues in this entry.