



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 14, 2017 – 06:54 am GMT

PDB ID : 3HDI  
Title : Crystal structure of Bacillus halodurans metallo peptidase  
Authors : Aleshin, A.; Gramatikova, S.; Strongin, A.Y.; Stec, B.; Liddington, R.C.;  
Smith, J.W.  
Deposited on : 2009-05-07  
Resolution : 2.70 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 : 1.7.2 (RC1), CSD as538be (2017)  
Xtriage (Phenix) : 1.9-1692  
EDS : trunk28620  
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)  
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) : recalc28949

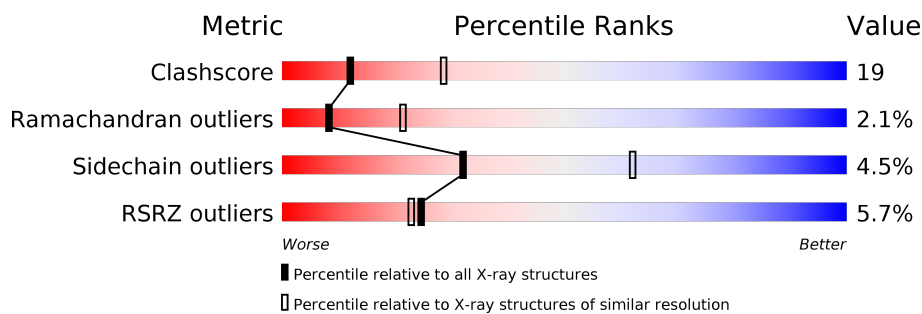
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.70 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))
Clashscore	112137	2590 (2.70-2.70)
Ramachandran outliers	110173	2550 (2.70-2.70)
Sidechain outliers	110143	2550 (2.70-2.70)
RSRZ outliers	101464	2275 (2.70-2.70)

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	421	<div> <div>2%</div> <div>59%</div> <div>37%</div> <div>..</div> </div>
1	B	421	<div> <div>2%</div> <div>59%</div> <div>36%</div> <div>..</div> </div>
2	C	17	<div> <div>82%</div> <div>59%</div> <div>24%</div> <div>18%</div> </div>
2	D	17	<div> <div>100%</div> <div>59%</div> <div>24%</div> <div>18%</div> </div>

## 2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 6988 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 Processing protease.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	414	Total	C	N	O	S	0	0	0
			3271	2059	552	644	16			
1	B	414	Total	C	N	O	S	0	0	0
			3271	2059	552	644	16			

There are 16 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	414	LEU	-	EXPRESSION TAG	UNP Q9KA85
A	415	GLU	-	EXPRESSION TAG	UNP Q9KA85
A	416	HIS	-	EXPRESSION TAG	UNP Q9KA85
A	417	HIS	-	EXPRESSION TAG	UNP Q9KA85
A	418	HIS	-	EXPRESSION TAG	UNP Q9KA85
A	419	HIS	-	EXPRESSION TAG	UNP Q9KA85
A	420	HIS	-	EXPRESSION TAG	UNP Q9KA85
A	421	HIS	-	EXPRESSION TAG	UNP Q9KA85
B	414	LEU	-	EXPRESSION TAG	UNP Q9KA85
B	415	GLU	-	EXPRESSION TAG	UNP Q9KA85
B	416	HIS	-	EXPRESSION TAG	UNP Q9KA85
B	417	HIS	-	EXPRESSION TAG	UNP Q9KA85
B	418	HIS	-	EXPRESSION TAG	UNP Q9KA85
B	419	HIS	-	EXPRESSION TAG	UNP Q9KA85
B	420	HIS	-	EXPRESSION TAG	UNP Q9KA85
B	421	HIS	-	EXPRESSION TAG	UNP Q9KA85

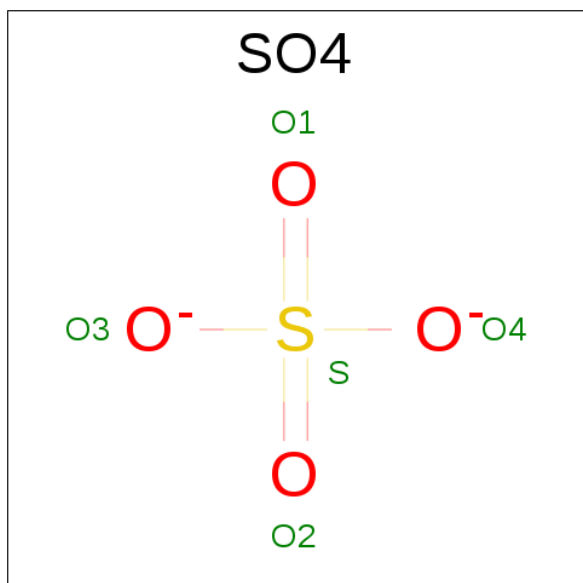
- Molecule 2 is a protein called Synthetic peptide.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	C	14	Total	C	N	O	0	0	0
			70	42	14	14			
2	D	17	Total	C	N	O	0	0	0
			85	51	17	17			

- Molecule 3 is COBALT (II) ION (three-letter code: CO) (formula: Co).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	B	1	Total	Co	0	0
			1	1		
3	A	1	Total	Co	0	0
			1	1		

- Molecule 4 is SULFATE ION (three-letter code: SO4) (formula: O<sub>4</sub>S).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	O	S	0	0
			5	4	1		
4	A	1	Total	O	S	0	0
			5	4	1		
4	A	1	Total	O	S	0	0
			5	4	1		
4	A	1	Total	O	S	0	0
			5	4	1		
4	B	1	Total	O	S	0	0
			5	4	1		
4	B	1	Total	O	S	0	0
			5	4	1		

- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	136	Total	O	0	0
			136	136		

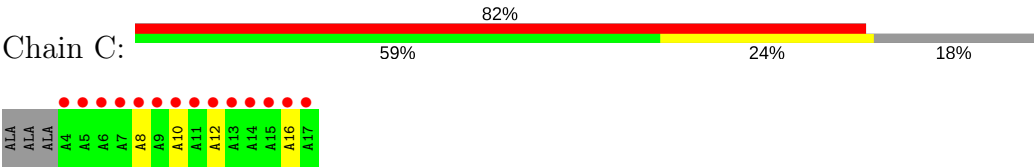
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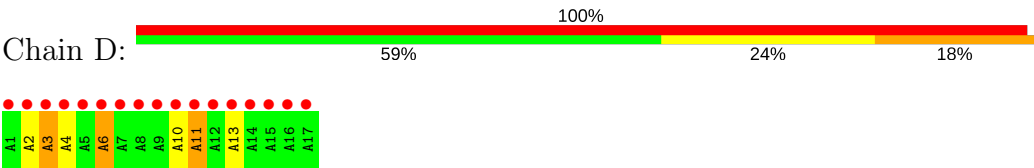
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	B	119	Total 119	O 119	0	0
5	C	2	Total 2	O 2	0	0
5	D	2	Total 2	O 2	0	0



● Molecule 2: Synthetic peptide



● Molecule 2: Synthetic peptide



## 4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	91.14Å 193.98Å 125.57Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	40.00 – 2.70 39.19 – 2.70	Depositor EDS
% Data completeness (in resolution range)	89.0 (40.00-2.70) 82.9 (39.19-2.70)	Depositor EDS
$R_{merge}$	0.08	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.77 (at 2.69Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, $R_{free}$	0.196 , 0.269 0.202 , (Not available)	Depositor DCC
$R_{free}$ test set	No test flags present.	DCC
Wilson B-factor (Å <sup>2</sup> )	63.0	Xtriage
Anisotropy	0.309	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.36 , 61.8	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	6988	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	63.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.54% 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, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.



## 5 Model quality [i](#)

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

Bond lengths and bond angles in the following residue types are not validated in this section: CO, SO4

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	0.38	0/3328	0.62	0/4485
1	B	0.38	0/3328	0.60	0/4485
2	C	0.30	0/69	0.33	0/95
2	D	0.26	0/84	0.37	0/116
All	All	0.38	0/6809	0.61	0/9181

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	3271	0	3231	131	0
1	B	3271	0	3231	131	0
2	C	70	0	69	2	0
2	D	85	0	87	6	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
4	A	20	0	0	0	0
4	B	10	0	0	0	0
5	A	136	0	0	4	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	B	119	0	0	2	0
5	C	2	0	0	0	0
5	D	2	0	0	0	0
All	All	6988	0	6618	255	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 19.

All (255) 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:B:246:ILE:HD12	1:B:247:GLY:H	1.13	1.09
1:B:409:LYS:H	1:B:409:LYS:HD2	1.15	1.05
1:B:246:ILE:HD12	1:B:247:GLY:N	1.78	0.96
1:A:20:THR:HB	1:B:20:THR:HB	1.46	0.95
1:A:260:VAL:HG21	1:A:326:LEU:HD21	1.50	0.89
1:B:11:VAL:HG11	1:B:207:VAL:HG11	1.54	0.88
1:B:246:ILE:HG13	1:B:291:ARG:HA	1.59	0.83
1:A:145:ALA:HB2	1:A:226:ILE:HG13	1.60	0.82
1:A:149:LYS:HA	1:A:149:LYS:HE2	1.62	0.82
1:A:71:ILE:HD13	1:A:90:VAL:HG12	1.60	0.82
1:B:409:LYS:H	1:B:409:LYS:CD	1.95	0.79
1:B:274:ARG:HH22	2:C:16:ALA:HA	1.49	0.78
1:A:225:ARG:HH22	1:A:411:LEU:HD23	1.49	0.78
1:A:409:LYS:HD2	1:A:409:LYS:N	1.99	0.76
1:A:408:PRO:C	1:A:409:LYS:HD2	2.06	0.76
1:B:408:PRO:HG2	1:B:411:LEU:HB2	1.68	0.76
1:B:136:ASP:HA	2:D:10:ALA:HB1	1.69	0.74
1:B:409:LYS:N	1:B:409:LYS:HD2	1.99	0.74
1:A:142:LEU:HD22	1:A:238:CYS:HB3	1.68	0.74
1:B:280:CYS:HB2	1:B:283:VAL:HG23	1.68	0.73
1:A:60:SER:OG	1:A:63:GLU:HG3	1.89	0.73
1:B:105:MET:O	1:B:109:SER:HB2	1.90	0.72
1:A:348:SER:HB3	1:A:351:SER:HB2	1.72	0.72
1:B:60:SER:OG	1:B:63:GLU:HG3	1.89	0.72
1:B:71:ILE:HD12	1:B:90:VAL:HG11	1.71	0.72
1:B:315:GLN:HE22	1:B:414:LEU:HG	1.57	0.70
1:B:44:ILE:HD11	1:B:171:LEU:HD23	1.72	0.70
1:B:93:ASP:HA	5:B:507:HOH:O	1.90	0.70
1:B:246:ILE:CG1	1:B:291:ARG:HA	2.23	0.68
1:B:270:PHE:CZ	1:B:274:ARG:HD3	2.28	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:280:CYS:HB2	1:B:283:VAL:CG2	2.23	0.67
1:B:315:GLN:HE22	1:B:414:LEU:CG	2.08	0.67
1:B:173:HIS:O	1:B:177:ARG:HG3	1.96	0.66
1:B:119:GLU:O	1:B:122:VAL:HG22	1.96	0.65
1:B:116:LEU:HD23	1:B:116:LEU:O	1.98	0.63
1:B:71:ILE:HD12	1:B:90:VAL:CG1	2.28	0.63
1:B:229:LYS:HB2	1:B:405:GLY:HA3	1.79	0.63
1:A:280:CYS:CB	1:A:283:VAL:HG13	2.29	0.63
1:A:260:VAL:CG2	1:A:326:LEU:HD21	2.27	0.63
1:A:237:LEU:HD13	1:A:400:LEU:HD13	1.81	0.62
1:A:227:VAL:HG21	1:A:407:LEU:HG	1.82	0.62
1:B:371:GLU:O	1:B:375:GLN:HG2	1.99	0.62
1:B:239:LEU:HD22	1:B:398:ILE:HG13	1.81	0.61
1:A:407:LEU:H	1:A:407:LEU:HD12	1.64	0.61
1:B:256:LEU:HD12	1:B:379:VAL:HG11	1.82	0.61
1:A:89:LYS:HD2	1:A:350:ASN:ND2	2.17	0.60
1:A:369:LEU:O	1:A:373:ILE:HG12	2.02	0.60
1:A:275:GLU:HG3	1:B:54:LYS:NZ	2.16	0.59
1:A:136:ASP:OD1	2:C:10:ALA:HB3	2.02	0.59
1:A:404:ASN:HD22	1:A:404:ASN:N	1.98	0.59
1:A:308:ASP:OD2	1:A:409:LYS:HB2	2.01	0.59
1:A:218:LYS:HD2	1:A:218:LYS:N	2.17	0.59
1:A:342:LEU:HD21	1:A:369:LEU:HD12	1.85	0.59
1:B:350:ASN:HB3	2:D:4:ALA:O	2.02	0.58
1:A:243:GLY:N	1:A:295:MET:HA	2.18	0.58
1:A:71:ILE:HD13	1:A:90:VAL:CG1	2.33	0.57
1:A:89:LYS:HD2	1:A:350:ASN:HD21	1.68	0.57
1:A:14:ILE:HD13	1:A:356:ASN:HB3	1.85	0.57
1:A:42:ASN:HD22	1:A:43:GLY:N	2.01	0.57
1:B:339:LYS:O	1:B:343:MET:HG2	2.04	0.57
1:B:246:ILE:CD1	1:B:247:GLY:N	2.62	0.57
1:A:332:GLU:O	1:A:336:GLU:HG2	2.03	0.57
1:B:346:LEU:HD11	1:B:369:LEU:HD13	1.87	0.57
1:B:123:VAL:O	1:B:127:ILE:HG13	2.04	0.57
1:A:124:PHE:O	1:A:128:LYS:HG3	2.05	0.56
1:B:44:ILE:CD1	1:B:171:LEU:HD23	2.34	0.56
1:A:272:ASP:O	1:A:277:ARG:HG2	2.04	0.56
1:A:404:ASN:HD22	1:A:405:GLY:N	2.03	0.56
1:B:2:ILE:N	5:B:470:HOH:O	2.38	0.56
1:A:134:PRO:HD3	1:A:230:LYS:NZ	2.21	0.56
1:B:310:LEU:HD11	1:B:314:ILE:HD11	1.88	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:251:VAL:O	1:A:255:VAL:HG23	2.07	0.55
1:B:398:ILE:HG21	1:B:411:LEU:HD21	1.89	0.55
1:B:402:ASN:OD1	1:B:405:GLY:N	2.36	0.54
1:A:404:ASN:N	1:A:404:ASN:ND2	2.55	0.54
1:A:103:SER:OG	1:A:203:THR:HG21	2.07	0.54
1:B:142:LEU:HD22	1:B:238:CYS:HB3	1.89	0.54
1:A:104:ASP:OD1	1:A:108:HIS:HB2	2.08	0.54
1:A:280:CYS:HB2	1:A:283:VAL:HG13	1.90	0.54
1:B:17:LYS:HE3	1:B:192:VAL:O	2.07	0.54
1:B:75:VAL:HG22	1:B:76:ASN:N	2.23	0.54
1:B:238:CYS:HB2	1:B:399:SER:OG	2.08	0.54
1:A:18:MET:HG2	1:A:352:ARG:NH2	2.23	0.53
1:A:331:LEU:HD22	1:A:381:LYS:HA	1.90	0.53
1:A:404:ASN:HD22	1:A:405:GLY:H	1.56	0.53
1:B:14:ILE:HD12	1:B:356:ASN:HB3	1.91	0.53
1:B:35:ARG:HG3	1:B:152:LEU:HD13	1.91	0.53
1:A:412:ILE:HD13	1:A:414:LEU:HD12	1.91	0.53
1:A:134:PRO:HB2	1:A:236:HIS:CD2	2.44	0.53
1:A:368:SER:HB3	1:A:371:GLU:HG3	1.91	0.52
1:B:147:TYR:CD2	1:B:152:LEU:HB3	2.45	0.52
1:A:20:THR:HB	1:B:20:THR:CB	2.31	0.52
1:A:2:ILE:HD13	1:A:356:ASN:OD1	2.10	0.52
1:A:255:VAL:HG13	5:A:456:HOH:O	2.09	0.52
1:B:163:LEU:HD23	1:B:166:PHE:CD1	2.44	0.52
1:A:22:ARG:HG3	1:A:92:ASP:OD2	2.10	0.52
1:B:197:ILE:HG22	1:B:201:LYS:HE2	1.91	0.52
1:A:116:LEU:C	1:A:116:LEU:HD23	2.30	0.52
1:A:404:ASN:H	1:A:404:ASN:ND2	2.07	0.52
1:B:404:ASN:OD1	1:B:406:GLU:HG2	2.09	0.52
1:B:369:LEU:O	1:B:373:ILE:HG13	2.10	0.52
1:A:339:LYS:O	1:A:343:MET:HG2	2.09	0.51
1:A:331:LEU:HD22	1:A:381:LYS:CA	2.40	0.51
1:B:270:PHE:CE2	1:B:274:ARG:HD3	2.45	0.51
1:B:114:GLU:HG2	1:B:115:GLU:OE1	2.10	0.51
1:B:312:TYR:O	1:B:315:GLN:HB2	2.10	0.51
1:A:38:SER:O	1:A:39:ALA:C	2.48	0.51
1:B:125:GLU:OE2	1:B:125:GLU:HA	2.09	0.51
1:A:342:LEU:HD22	1:A:373:ILE:HD11	1.91	0.51
1:B:239:LEU:CD2	1:B:398:ILE:HG13	2.41	0.51
1:B:368:SER:O	1:B:372:MET:HG3	2.11	0.51
1:B:225:ARG:HA	1:B:398:ILE:O	2.10	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:344:LEU:HD13	1:B:74:GLN:HG3	1.94	0.50
1:B:219:PRO:HG2	1:B:293:SER:HB2	1.94	0.50
1:A:9:ASN:ND2	1:A:207:VAL:HB	2.27	0.50
1:A:62:GLN:HE21	1:B:271:GLN:HG3	1.76	0.50
1:A:368:SER:O	1:A:372:MET:HG3	2.11	0.50
1:A:78:PHE:CD1	1:A:85:CYS:HB3	2.47	0.50
1:A:11:VAL:HG22	1:A:184:VAL:HB	1.94	0.49
1:A:225:ARG:HG3	1:A:398:ILE:HB	1.94	0.49
1:B:139:HIS:CD2	2:D:10:ALA:HB3	2.47	0.49
1:A:221:PHE:O	1:A:222:LEU:HD23	2.13	0.49
1:A:26:ILE:HG21	1:A:99:ILE:HD12	1.95	0.49
1:B:112:GLN:HB3	1:B:114:GLU:OE1	2.13	0.49
1:B:246:ILE:HG12	1:B:291:ARG:HG3	1.94	0.49
1:A:18:MET:SD	1:A:352:ARG:HD2	2.53	0.49
1:A:322:ALA:HB2	1:A:392:LEU:HB2	1.94	0.49
1:A:386:ARG:O	1:A:390:ILE:HG13	2.13	0.49
1:A:229:LYS:HB2	1:A:405:GLY:HA3	1.95	0.49
1:B:408:PRO:HD2	1:B:411:LEU:HD22	1.95	0.49
1:A:238:CYS:HB2	1:A:399:SER:HB3	1.95	0.48
1:B:315:GLN:O	1:B:319:SER:HB2	2.13	0.48
1:A:38:SER:H	1:A:41:GLU:HG3	1.78	0.48
1:A:225:ARG:NH2	1:A:411:LEU:HD23	2.22	0.48
1:A:257:LEU:HD12	1:A:257:LEU:O	2.13	0.48
1:B:168:GLU:CD	1:B:172:ARG:HE	2.17	0.48
1:A:219:PRO:HG2	1:A:293:SER:HB2	1.93	0.48
1:A:40:GLU:CD	1:A:40:GLU:H	2.17	0.48
1:A:119:GLU:HA	1:A:119:GLU:OE1	2.13	0.48
1:B:46:HIS:CE1	1:B:50:HIS:CD2	3.01	0.48
1:A:217:GLU:HG2	1:A:218:LYS:N	2.28	0.48
1:B:127:ILE:O	1:B:130:VAL:HG22	2.14	0.48
1:A:336:GLU:HA	1:A:336:GLU:OE2	2.13	0.48
1:B:38:SER:O	1:B:39:ALA:C	2.52	0.47
1:B:411:LEU:O	1:B:412:ILE:HD13	2.14	0.47
1:B:5:MET:CE	1:B:201:LYS:HD3	2.44	0.47
1:B:315:GLN:NE2	1:B:414:LEU:HG	2.26	0.47
1:B:365:LYS:HG2	1:B:366:HIS:N	2.30	0.47
1:A:101:THR:O	1:A:105:MET:HG3	2.15	0.47
1:A:277:ARG:HG2	1:A:277:ARG:HH21	1.80	0.47
1:B:407:LEU:HD22	1:B:411:LEU:HD23	1.96	0.47
1:A:5:MET:O	1:A:12:ARG:HA	2.16	0.46
1:A:285:SER:HA	1:A:297:THR:O	2.14	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:52:PHE:CE1	1:A:106:PHE:HA	2.50	0.46
1:A:270:PHE:CE1	1:A:274:ARG:HD3	2.50	0.46
1:B:5:MET:HE1	1:B:201:LYS:HD3	1.97	0.46
1:B:119:GLU:OE2	1:B:122:VAL:HG21	2.15	0.46
1:B:40:GLU:H	1:B:40:GLU:CD	2.19	0.46
1:B:204:PHE:O	1:B:207:VAL:HG12	2.16	0.46
1:B:268:ARG:HB3	1:B:317:THR:CG2	2.46	0.46
1:B:11:VAL:HG12	1:B:184:VAL:HB	1.98	0.46
1:B:103:SER:OG	1:B:203:THR:HG21	2.16	0.46
1:A:365:LYS:HG3	1:A:366:HIS:N	2.31	0.46
1:B:409:LYS:N	1:B:409:LYS:CD	2.71	0.45
1:A:370:ASP:O	1:A:374:GLU:HG3	2.16	0.45
1:A:409:LYS:CD	1:A:409:LYS:N	2.75	0.45
1:B:11:VAL:HG12	1:B:181:GLY:HA2	1.98	0.45
1:A:302:THR:HG23	1:A:303:GLY:O	2.16	0.45
2:D:10:ALA:O	2:D:11:ALA:HB2	2.17	0.45
1:A:326:LEU:CD1	1:A:384:VAL:HG11	2.46	0.45
1:B:24:VAL:HG11	1:B:95:ALA:HB2	1.99	0.45
1:A:54:LYS:HE3	1:A:115:GLU:OE1	2.16	0.45
1:B:326:LEU:O	1:B:381:LYS:HD2	2.16	0.45
1:A:99:ILE:HG21	1:A:199:LYS:CD	2.47	0.45
1:B:124:PHE:CE2	1:B:160:VAL:HG13	2.52	0.45
1:A:38:SER:HA	5:A:541:HOH:O	2.17	0.44
1:B:9:ASN:ND2	1:B:207:VAL:HG13	2.32	0.44
1:A:264:SER:HB2	1:B:69:ASP:OD1	2.18	0.44
1:B:208:LYS:HA	1:B:209:PRO:HD3	1.89	0.44
1:B:315:GLN:HE22	1:B:414:LEU:CB	2.31	0.44
1:B:78:PHE:CE1	1:B:85:CYS:HB3	2.53	0.44
1:A:225:ARG:NH1	1:A:225:ARG:HG2	2.33	0.44
1:A:29:TRP:HZ2	1:A:354:SER:HA	1.83	0.44
1:A:188:VAL:HG12	1:A:192:VAL:HG21	1.99	0.44
1:A:38:SER:OG	1:A:41:GLU:HG2	2.18	0.44
1:B:172:ARG:HH21	1:B:172:ARG:HG2	1.83	0.43
1:A:116:LEU:O	1:A:116:LEU:HD23	2.18	0.43
1:B:94:HIS:ND1	1:B:97:GLN:NE2	2.67	0.43
1:A:134:PRO:HD3	1:A:230:LYS:HZ3	1.82	0.43
1:B:277:ARG:HG3	1:B:277:ARG:HH21	1.83	0.43
1:B:412:ILE:HG22	1:B:413:HIS:N	2.34	0.43
1:A:232:THR:O	1:A:304:HIS:CE1	2.72	0.43
1:A:296:LEU:HD23	1:A:392:LEU:HD21	1.99	0.43
1:B:111:PHE:HB2	1:B:168:GLU:HG3	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:237:LEU:HD11	1:B:239:LEU:HD21	2.00	0.43
1:A:103:SER:OG	1:A:203:THR:CG2	2.67	0.42
1:A:375:GLN:O	1:A:379:VAL:HG23	2.18	0.42
1:A:388:ALA:O	1:A:392:LEU:HB2	2.19	0.42
1:A:62:GLN:O	1:A:66:GLU:HG3	2.18	0.42
1:A:92:ASP:OD1	1:A:93:ASP:N	2.52	0.42
1:A:78:PHE:CE1	1:A:85:CYS:HB3	2.54	0.42
1:B:326:LEU:H	1:B:326:LEU:HD23	1.83	0.42
1:B:29:TRP:CZ2	1:B:354:SER:HA	2.54	0.42
1:B:38:SER:H	1:B:41:GLU:HG3	1.84	0.42
1:A:96:GLY:O	1:A:99:ILE:HG22	2.19	0.42
1:A:306:GLN:HE22	1:B:121:LYS:NZ	2.17	0.42
1:B:134:PRO:HB2	1:B:236:HIS:CD2	2.55	0.42
1:B:346:LEU:CD1	1:B:369:LEU:HD22	2.50	0.42
1:A:99:ILE:CG2	1:A:100:ASP:N	2.83	0.42
1:B:397:SER:C	1:B:398:ILE:HD12	2.41	0.42
1:A:124:PHE:CE2	1:A:160:VAL:HA	2.55	0.42
1:A:270:PHE:CZ	1:A:274:ARG:HD3	2.55	0.41
1:A:196:LEU:O	1:A:200:ILE:HG13	2.20	0.41
1:A:272:ASP:HA	1:A:276:LYS:HD2	2.01	0.41
1:B:218:LYS:HD2	1:B:292:ASP:OD1	2.20	0.41
1:B:285:SER:HA	1:B:297:THR:O	2.20	0.41
1:B:350:ASN:HD22	1:B:350:ASN:HA	1.62	0.41
1:A:308:ASP:OD1	1:A:409:LYS:HD3	2.20	0.41
1:B:164:ASN:HA	1:B:164:ASN:HD22	1.60	0.41
1:B:178:PHE:O	1:B:183:TYR:HB2	2.20	0.41
1:B:348:SER:HB3	1:B:351:SER:HB2	2.03	0.41
1:A:252:TYR:CD2	1:A:375:GLN:HB3	2.56	0.41
1:A:265:MET:CB	1:B:65:ALA:HB1	2.50	0.41
1:A:304:HIS:CE1	1:A:403:ALA:HB2	2.56	0.41
1:B:80:SER:OG	1:B:81:LYS:N	2.51	0.41
1:A:145:ALA:O	1:A:224:ASN:HB2	2.21	0.41
1:B:363:LEU:O	1:B:364:LYS:HB2	2.21	0.41
1:B:400:LEU:HD21	1:B:402:ASN:ND2	2.36	0.41
1:B:81:LYS:HD2	1:B:290:PHE:CE2	2.56	0.41
1:B:11:VAL:CG1	1:B:181:GLY:HA2	2.50	0.41
1:B:175:MET:O	1:B:179:TYR:HB2	2.21	0.41
1:B:42:ASN:C	1:B:42:ASN:ND2	2.74	0.41
2:D:2:ALA:O	2:D:3:ALA:C	2.59	0.41
1:A:225:ARG:HG2	1:A:225:ARG:HH11	1.86	0.41
1:A:307:LEU:O	1:A:311:VAL:HG23	2.20	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:71:ILE:C	1:A:71:ILE:HD12	2.42	0.40
1:B:246:ILE:O	1:B:251:VAL:HG11	2.21	0.40
1:A:118:LYS:HD3	1:B:276:LYS:HA	2.03	0.40
1:B:29:TRP:HB3	1:B:361:LEU:HD22	2.03	0.40
1:A:175:MET:O	1:A:179:TYR:HB2	2.20	0.40
1:A:99:ILE:HG22	1:A:100:ASP:N	2.35	0.40
1:B:42:ASN:HD22	1:B:43:GLY:N	2.19	0.40
1:A:219:PRO:CG	1:A:293:SER:HB2	2.51	0.40
1:A:2:ILE:N	5:A:524:HOH:O	2.53	0.40
1:B:152:LEU:HD12	1:B:152:LEU:HA	1.78	0.40
1:B:5:MET:SD	1:B:201:LYS:HD3	2.60	0.40
1:B:380:GLN:HB3	1:B:382:GLN:HG2	2.02	0.40
1:A:130:VAL:HG13	1:A:136:ASP:OD2	2.21	0.40
1:A:246:ILE:HD13	1:A:289:SER:HB2	2.03	0.40
1:A:38:SER:HB2	5:A:428:HOH:O	2.21	0.40
1:A:42:ASN:C	1:A:42:ASN:ND2	2.75	0.40
1:B:34:SER:HB3	1:B:156:ILE:HD13	2.03	0.40
1:B:78:PHE:CZ	2:D:6:ALA:HB3	2.55	0.40
1:A:120:ARG:NH2	1:A:166:PHE:O	2.55	0.40
1:B:25:SER:HB3	1:B:350:ASN:HD22	1.86	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles ⓘ

### 5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	412/421 (98%)	379 (92%)	27 (7%)	6 (2%)	12	30
1	B	412/421 (98%)	377 (92%)	29 (7%)	6 (2%)	12	30
2	C	12/17 (71%)	5 (42%)	5 (42%)	2 (17%)	0	0
2	D	15/17 (88%)	7 (47%)	4 (27%)	4 (27%)	0	0
All	All	851/876 (97%)	768 (90%)	65 (8%)	18 (2%)	8	21



All (18) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	39	ALA
2	C	8	ALA
2	D	11	ALA
1	A	39	ALA
1	A	246	ILE
1	A	408	PRO
1	B	31	GLY
2	C	12	ALA
1	A	248	ASP
1	B	306	GLN
1	B	412	ILE
2	D	3	ALA
2	D	13	ALA
1	A	111	PHE
1	B	414	LEU
2	D	6	ALA
1	A	92	ASP
1	B	181	GLY

### 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	365/372 (98%)	348 (95%)	17 (5%)	30	60
1	B	365/372 (98%)	349 (96%)	16 (4%)	33	63
All	All	730/744 (98%)	697 (96%)	33 (4%)	32	62

All (33) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	3	ASN
1	A	35	ARG
1	A	42	ASN
1	A	129	MET
1	A	131	ASP

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Mol	Chain	Res	Type
1	A	163	LEU
1	A	164	ASN
1	A	225	ARG
1	A	275	GLU
1	A	292	ASP
1	A	305	ASP
1	A	308	ASP
1	A	318	THR
1	A	333	ASN
1	A	342	LEU
1	A	351	SER
1	A	404	ASN
1	B	2	ILE
1	B	14	ILE
1	B	34	SER
1	B	42	ASN
1	B	59	ARG
1	B	112	GLN
1	B	129	MET
1	B	152	LEU
1	B	164	ASN
1	B	182	ASP
1	B	191	ASN
1	B	208	LYS
1	B	217	GLU
1	B	269	LEU
1	B	350	ASN
1	B	409	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (27) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	42	ASN
1	A	62	GLN
1	A	94	HIS
1	A	97	GLN
1	A	164	ASN
1	A	224	ASN
1	A	259	ASN
1	A	271	GLN
1	A	304	HIS
1	A	306	GLN

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Mol	Chain	Res	Type
1	A	333	ASN
1	A	377	ASN
1	A	382	GLN
1	A	404	ASN
1	B	42	ASN
1	B	97	GLN
1	B	112	GLN
1	B	164	ASN
1	B	191	ASN
1	B	206	GLN
1	B	215	GLN
1	B	224	ASN
1	B	306	GLN
1	B	315	GLN
1	B	350	ASN
1	B	377	ASN
1	B	413	HIS

### 5.3.3 RNA [i](#)

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](#)

Of 8 ligands modelled in this entry, 2 are monoatomic - leaving 6 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
4	SO4	A	501	-	4,4,4	0.35	0	6,6,6	0.08	0
4	SO4	A	502	-	4,4,4	0.33	0	6,6,6	0.09	0
4	SO4	A	503	-	4,4,4	0.33	0	6,6,6	0.11	0
4	SO4	A	505	-	4,4,4	0.33	0	6,6,6	0.08	0
4	SO4	B	504	-	4,4,4	0.35	0	6,6,6	0.09	0
4	SO4	B	506	-	4,4,4	0.36	0	6,6,6	0.07	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
4	SO4	A	501	-	-	0/0/0/0	0/0/0/0
4	SO4	A	502	-	-	0/0/0/0	0/0/0/0
4	SO4	A	503	-	-	0/0/0/0	0/0/0/0
4	SO4	A	505	-	-	0/0/0/0	0/0/0/0
4	SO4	B	504	-	-	0/0/0/0	0/0/0/0
4	SO4	B	506	-	-	0/0/0/0	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<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	414/421 (98%)	0.05	10 (2%) 59 60	37, 57, 90, 147	0
1	B	414/421 (98%)	0.15	8 (1%) 67 68	38, 61, 84, 146	0
2	C	14/17 (82%)	14.32	14 (100%) 0 0	79, 90, 97, 99	14 (100%)
2	D	17/17 (100%)	12.02	17 (100%) 0 0	78, 93, 99, 101	17 (100%)
All	All	859/876 (98%)	0.57	49 (5%) 24 23	37, 59, 93, 147	31 (3%)

All (49) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	D	6	ALA	24.2
2	C	17	ALA	21.8
2	C	5	ALA	21.5
2	C	4	ALA	20.4
2	D	9	ALA	18.9
2	C	8	ALA	18.1
2	D	17	ALA	17.7
2	D	3	ALA	17.2
2	C	16	ALA	16.5
2	C	6	ALA	14.6
2	D	1	ALA	14.6
2	C	10	ALA	14.4
2	D	16	ALA	14.2
2	D	8	ALA	13.5
2	C	11	ALA	13.4
2	D	7	ALA	12.2
2	C	9	ALA	12.0
2	C	7	ALA	11.9
2	D	12	ALA	11.1
2	D	5	ALA	10.1
2	C	13	ALA	10.1

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Mol	Chain	Res	Type	RSRZ
2	C	12	ALA	9.9
2	C	14	ALA	8.5
2	D	15	ALA	8.5
2	D	10	ALA	8.1
2	D	14	ALA	8.0
2	D	11	ALA	7.8
2	C	15	ALA	7.5
2	D	2	ALA	6.4
2	D	13	ALA	6.0
2	D	4	ALA	5.9
1	B	414	LEU	4.3
1	A	414	LEU	3.7
1	A	412	ILE	3.5
1	B	376	ILE	3.0
1	B	210	THR	2.8
1	A	252	TYR	2.7
1	A	312	TYR	2.5
1	A	405	GLY	2.4
1	A	403	ALA	2.3
1	B	410	ALA	2.3
1	B	331	LEU	2.3
1	A	331	LEU	2.2
1	A	408	PRO	2.2
1	A	407	LEU	2.1
1	B	324	LYS	2.1
1	B	114	GLU	2.1
1	A	415	GLU	2.1
1	B	312	TYR	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<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
4	SO4	B	504	5/5	0.86	0.22	0.66	112,114,115,116	0
3	CO	A	500	1/1	0.99	0.22	-0.55	46,46,46,46	0
3	CO	B	500	1/1	0.99	0.19	-0.55	46,46,46,46	0
4	SO4	A	503	5/5	0.86	0.23	-1.06	137,138,138,139	0
4	SO4	A	502	5/5	0.83	0.19	-	164,165,165,165	0
4	SO4	B	506	5/5	0.90	0.25	-	108,109,109,110	0
4	SO4	A	501	5/5	0.77	0.18	-	149,149,150,150	0
4	SO4	A	505	5/5	0.88	0.20	-	134,135,135,135	0

## 6.5 Other polymers

There are no such residues in this entry.