



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 17, 2018 – 05:46 pm GMT

PDB ID : 1OR0  
Title : Crystal Structures of Glutaryl 7-Aminocephalosporanic Acid Acylase: Insight into Autoproteolytic Activation  
Authors : Kim, J.K.; Yang, I.S.; Rhee, S.; Dauter, Z.; Lee, Y.S.; Park, S.S.; Kim, K.H.  
Deposited on : 2003-03-11  
Resolution : 2.00 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

<https://www.wwpdb.org/validation/2017/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 : 1.7.3 (157068), CSD as539be (2018)  
Xtriage (Phenix) : **NOT EXECUTED**  
EDS : **NOT EXECUTED**  
Percentile statistics : 20171227.v01 (using entries in the PDB archive December 27th 2017)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : trunk30686

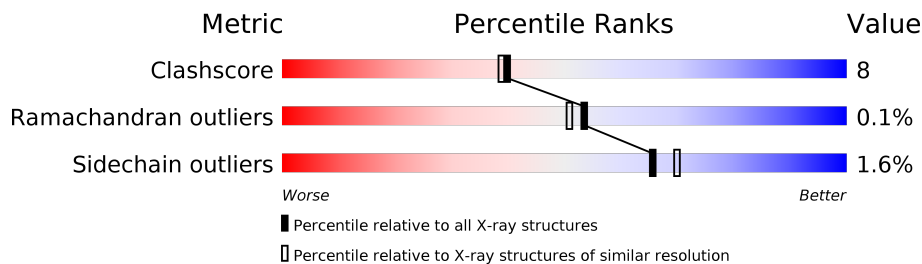
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.00 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	122078	8264 (2.00-2.00)
Ramachandran outliers	120005	8163 (2.00-2.00)
Sidechain outliers	119972	8162 (2.00-2.00)

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.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	160	
1	C	160	
2	B	528	
2	D	528	

## 2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 12046 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 Glutaryl 7-Aminocephalosporanic Acid Acylase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	153	Total	C	N	O	Se	0	0	0
			1197	761	211	224	1			
1	C	152	Total	C	N	O	Se	0	0	0
			1192	758	210	223	1			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	125	ASP	GLU	SEE REMARK 999	UNP Q84I62
A	145	MSE	MET	MODIFIED RESIDUE	UNP Q84I62
C	125	ASP	GLU	SEE REMARK 999	UNP Q84I62
C	145	MSE	MET	MODIFIED RESIDUE	UNP Q84I62

- Molecule 2 is a protein called glutaryl acylase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	521	Total	C	N	O	Se	0	0	0
			4110	2600	723	776	11			
2	D	521	Total	C	N	O	Se	0	0	0
			4110	2600	723	776	11			

There are 34 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	64	MSE	MET	MODIFIED RESIDUE	UNP Q84I62
B	73	MSE	MET	MODIFIED RESIDUE	UNP Q84I62
B	149	MSE	MET	MODIFIED RESIDUE	UNP Q84I62
B	156	MSE	MET	MODIFIED RESIDUE	UNP Q84I62
B	172	MSE	MET	MODIFIED RESIDUE	UNP Q84I62
B	282	MSE	MET	MODIFIED RESIDUE	UNP Q84I62
B	294	MSE	MET	MODIFIED RESIDUE	UNP Q84I62
B	304	MSE	MET	MODIFIED RESIDUE	UNP Q84I62

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Chain	Residue	Modelled	Actual	Comment	Reference
B	416	MSE	MET	MODIFIED RESIDUE	UNP Q84I62
B	460	MSE	MET	MODIFIED RESIDUE	UNP Q84I62
B	473	MSE	MET	MODIFIED RESIDUE	UNP Q84I62
B	523	HIS	-	EXPRESSION TAG	UNP Q84I62
B	524	HIS	-	EXPRESSION TAG	UNP Q84I62
B	525	HIS	-	EXPRESSION TAG	UNP Q84I62
B	526	HIS	-	EXPRESSION TAG	UNP Q84I62
B	527	HIS	-	EXPRESSION TAG	UNP Q84I62
B	528	HIS	-	EXPRESSION TAG	UNP Q84I62
D	64	MSE	MET	MODIFIED RESIDUE	UNP Q84I62
D	73	MSE	MET	MODIFIED RESIDUE	UNP Q84I62
D	149	MSE	MET	MODIFIED RESIDUE	UNP Q84I62
D	156	MSE	MET	MODIFIED RESIDUE	UNP Q84I62
D	172	MSE	MET	MODIFIED RESIDUE	UNP Q84I62
D	282	MSE	MET	MODIFIED RESIDUE	UNP Q84I62
D	294	MSE	MET	MODIFIED RESIDUE	UNP Q84I62
D	304	MSE	MET	MODIFIED RESIDUE	UNP Q84I62
D	416	MSE	MET	MODIFIED RESIDUE	UNP Q84I62
D	460	MSE	MET	MODIFIED RESIDUE	UNP Q84I62
D	473	MSE	MET	MODIFIED RESIDUE	UNP Q84I62
D	523	HIS	-	EXPRESSION TAG	UNP Q84I62
D	524	HIS	-	EXPRESSION TAG	UNP Q84I62
D	525	HIS	-	EXPRESSION TAG	UNP Q84I62
D	526	HIS	-	EXPRESSION TAG	UNP Q84I62
D	527	HIS	-	EXPRESSION TAG	UNP Q84I62
D	528	HIS	-	EXPRESSION TAG	UNP Q84I62

- Molecule 3 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: C<sub>2</sub>H<sub>6</sub>O<sub>2</sub>).



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

- Molecule 4 is water.


Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	158	Total	O	0	0
			158	158		
4	B	577	Total	O	0	0
			577	577		
4	C	158	Total	O	0	0
			158	158		
4	D	536	Total	O	0	0
			536	536		

### 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 the various outlier classes 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.

Note EDS was not executed.

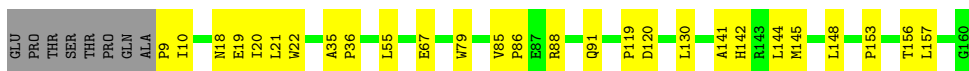
- Molecule 1: Glutaryl 7-Aminocephalosporanic Acid Acylase

Chain A: 




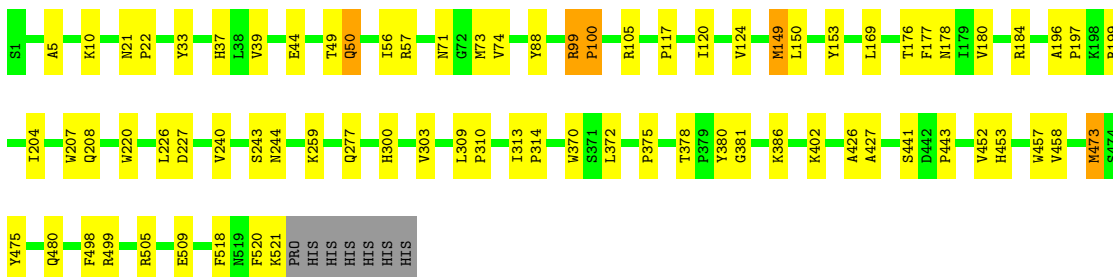
- Molecule 1: Glutaryl 7-Aminocephalosporanic Acid Acylase

Chain C: 




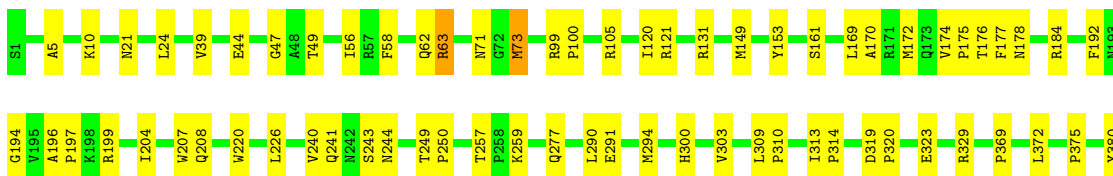
- Molecule 2: glutaryl acylase

Chain B: 



- Molecule 2: glutaryl acylase

Chain D: 



G381	K400	A426	A427	W440	S441	R449	Y452	H453	Y475	E506	Q507	E514	R515	T516	P517	R518	H519	F520	K521	PRO	HIS	HIS	HIS	HIS	HIS	HIS
------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	-----	-----	-----	-----	-----	-----	-----

## 4 Data and refinement statistics

Xtriage (Phenix) and EDS were not executed - this section is therefore incomplete.

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	229.67Å 69.91Å 113.73Å 90.00° 97.63° 90.00°	Depositor
Resolution (Å)	19.95 – 2.00	Depositor
% Data completeness (in resolution range)	91.8 (19.95-2.00)	Depositor
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
Refinement program	CNS 1.1	Depositor
R, $R_{free}$	0.171 , 0.184	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	12046	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	14.0	wwPDB-VP



## 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: 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	0.31	0/1235	0.53	0/1687
1	C	0.31	0/1230	0.55	0/1679
2	B	0.31	0/4214	0.60	0/5736
2	D	0.31	0/4214	0.60	0/5736
All	All	0.31	0/10893	0.59	0/14838

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	1197	0	1113	15	0
1	C	1192	0	1109	35	0
2	B	4110	0	3943	66	0
2	D	4110	0	3943	77	0
3	B	4	0	6	2	0
3	D	4	0	6	2	0
4	A	158	0	0	3	0
4	B	577	0	0	7	0
4	C	158	0	0	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	D	536	0	0	8	0
All	All	12046	0	10120	164	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 8.

All (164) 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:D:290:LEU:HG	2:D:294:MSE:HE2	1.40	1.03
2:D:169:LEU:O	2:D:172:MSE:HE2	1.76	0.85
2:D:291:GLU:HA	2:D:294:MSE:HE3	1.58	0.84
2:B:33:TYR:HB3	2:B:473:MSE:HE1	1.59	0.83
2:D:100:PRO:HD2	2:D:120:ILE:O	1.79	0.82
1:C:145:MSE:HE3	2:D:175:PRO:HD2	1.62	0.81
2:D:73:MSE:HE3	2:D:192:PHE:CE2	2.17	0.78
2:D:170:ALA:HA	2:D:172:MSE:CE	2.15	0.77
2:D:172:MSE:HE3	2:D:226:LEU:HB2	1.67	0.77
2:D:172:MSE:CE	2:D:226:LEU:HB2	2.17	0.75
1:C:9:PRO:HG2	2:D:184:ARG:NH2	2.02	0.75
2:D:170:ALA:HA	2:D:172:MSE:HE3	1.68	0.74
1:C:145:MSE:HG3	2:D:149:MSE:HE2	1.69	0.74
1:C:141:ALA:HB1	2:D:149:MSE:HE1	1.71	0.72
1:C:141:ALA:HB1	2:D:149:MSE:CE	2.19	0.72
2:D:73:MSE:HE3	2:D:192:PHE:HE2	1.54	0.72
2:B:33:TYR:CB	2:B:473:MSE:HE1	2.19	0.71
1:C:88:ARG:HH11	1:C:142:HIS:HE2	1.38	0.69
2:D:58:PHE:HZ	3:D:2002:EDO:H12	1.58	0.68
2:D:372:LEU:O	2:D:375:PRO:HG3	1.93	0.67
2:D:73:MSE:HA	2:D:73:MSE:HE2	1.75	0.66
2:B:117:PRO:HG3	1:C:120:ASP:HA	1.79	0.65
2:D:24:LEU:HG	4:D:2458:HOH:O	1.97	0.65
1:A:52:ASP:H	2:B:480:GLN:HE22	1.44	0.64
2:B:39:VAL:HG22	2:B:44:GLU:HG3	1.80	0.63
1:A:117:GLN:HG2	4:A:245:HOH:O	1.98	0.63
2:B:259:LYS:HG3	4:B:2276:HOH:O	1.97	0.63
1:A:35:ALA:HB3	1:A:36:PRO:HD3	1.81	0.62
1:C:35:ALA:HB3	1:C:36:PRO:HD3	1.81	0.61
1:C:157:LEU:C	2:D:131:ARG:HD2	2.21	0.61
1:C:91:GLN:HG3	4:C:178:HOH:O	2.01	0.61
2:B:100:PRO:HD3	4:B:2175:HOH:O	2.00	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:199:ARG:HG2	2:D:207:TRP:CZ2	2.37	0.59
2:B:50:GLN:HE22	2:B:57:ARG:HH11	1.48	0.59
2:D:290:LEU:O	2:D:294:MSE:HG3	2.02	0.59
2:B:313:ILE:HB	2:B:314:PRO:HD3	1.83	0.58
2:D:199:ARG:HG2	2:D:207:TRP:CE2	2.39	0.57
1:C:145:MSE:CG	2:D:149:MSE:HE2	2.34	0.57
2:B:457:TRP:HE3	2:B:473:MSE:HG2	1.70	0.56
1:C:10:ILE:O	1:C:10:ILE:HG13	2.06	0.56
1:C:22:TRP:HB2	2:D:514:GLU:HB2	1.88	0.55
2:D:39:VAL:HG22	2:D:44:GLU:HG3	1.88	0.55
2:B:169:LEU:HD23	2:B:169:LEU:O	2.07	0.55
2:B:199:ARG:HG2	2:B:207:TRP:CZ2	2.41	0.55
1:C:67:GLU:HG3	2:D:105:ARG:HB2	1.88	0.55
2:B:50:GLN:HE22	2:B:57:ARG:HD3	1.72	0.55
2:B:50:GLN:HE21	2:B:50:GLN:H	1.55	0.54
2:D:49:THR:HB	2:D:56:ILE:HA	1.87	0.54
1:C:145:MSE:HE1	2:D:174:VAL:HG13	1.89	0.54
2:B:5:ALA:HB3	2:B:240:VAL:HG22	1.90	0.54
2:D:290:LEU:HG	2:D:294:MSE:CE	2.27	0.54
1:C:157:LEU:O	2:D:131:ARG:HD2	2.09	0.53
2:D:313:ILE:HB	2:D:314:PRO:HD3	1.90	0.53
2:B:73:MSE:CE	4:B:2196:HOH:O	2.57	0.53
2:D:99:ARG:HG2	2:D:121:ARG:HG2	1.91	0.51
4:C:205:HOH:O	2:D:149:MSE:HE3	2.10	0.51
2:B:100:PRO:CD	2:B:120:ILE:O	2.59	0.51
2:D:100:PRO:CD	2:D:120:ILE:O	2.55	0.51
1:C:79:TRP:CD1	1:C:153:PRO:HG3	2.46	0.51
1:A:52:ASP:H	2:B:480:GLN:NE2	2.08	0.51
1:A:117:GLN:HG3	4:A:242:HOH:O	2.10	0.51
3:D:2002:EDO:H11	4:D:2458:HOH:O	2.11	0.51
2:D:369:PRO:HG3	4:D:2417:HOH:O	2.11	0.51
2:B:73:MSE:HE1	4:B:2196:HOH:O	2.12	0.50
2:D:99:ARG:HD3	4:D:2484:HOH:O	2.10	0.50
2:B:88:TYR:OH	2:B:124:VAL:HG13	2.11	0.50
1:C:20:ILE:HB	2:D:516:THR:HB	1.93	0.49
2:B:426:ALA:O	2:B:427:ALA:HB3	2.13	0.49
2:B:149:MSE:HG3	2:B:150:LEU:N	2.27	0.49
2:B:402:LYS:HB3	2:B:443:PRO:HG3	1.94	0.49
2:B:99:ARG:N	2:B:99:ARG:HD3	2.27	0.49
2:D:73:MSE:SE	2:D:196:ALA:HB2	2.62	0.49
2:D:5:ALA:HB3	2:D:240:VAL:HG22	1.93	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:73:MSE:HE3	2:B:74:VAL:N	2.28	0.48
2:D:176:THR:O	2:D:177:PHE:HB2	2.14	0.48
1:C:145:MSE:CE	2:D:174:VAL:HG13	2.42	0.48
1:C:19:GLU:HG3	1:C:21:LEU:CD1	2.43	0.48
2:B:386:LYS:O	2:B:386:LYS:HD3	2.14	0.48
2:B:441:SER:HB3	2:B:452:VAL:CG1	2.44	0.47
1:C:144:LEU:HA	1:C:148:LEU:HD12	1.95	0.47
2:B:100:PRO:HD2	2:B:120:ILE:O	2.14	0.47
2:B:176:THR:O	2:B:177:PHE:HB2	2.14	0.47
1:C:18:ASN:HB3	2:D:518:PHE:CE1	2.50	0.47
1:C:145:MSE:HE3	2:D:175:PRO:CD	2.40	0.47
2:D:441:SER:HB3	2:D:452:VAL:HG13	1.97	0.47
2:B:441:SER:HB3	2:B:452:VAL:HG13	1.97	0.47
2:B:204:ILE:O	2:B:208:GLN:HG3	2.15	0.47
2:D:426:ALA:O	2:D:427:ALA:HB3	2.15	0.46
2:B:5:ALA:HB3	2:B:240:VAL:CG2	2.45	0.46
1:A:18:ASN:HB3	2:B:518:PHE:CE1	2.51	0.46
1:C:9:PRO:HG2	2:D:184:ARG:HH22	1.77	0.46
2:D:519:ASN:HA	4:D:2385:HOH:O	2.15	0.46
2:B:99:ARG:HA	2:B:100:PRO:HD3	1.66	0.46
2:B:243:SER:O	2:B:244:ASN:HB2	2.15	0.46
2:B:49:THR:HB	2:B:56:ILE:HA	1.97	0.46
1:C:156:THR:O	2:D:131:ARG:HD3	2.15	0.46
1:A:85:VAL:HB	1:A:86:PRO:HD3	1.97	0.46
2:B:386:LYS:HD3	2:B:386:LYS:C	2.36	0.46
2:B:458:VAL:O	2:B:458:VAL:HG23	2.15	0.46
2:D:323:GLU:OE1	2:D:400:LYS:CE	2.64	0.45
1:C:85:VAL:HB	1:C:86:PRO:HD3	1.98	0.45
1:A:80:LEU:HD11	1:A:143:ARG:HD2	1.99	0.45
1:C:9:PRO:HD2	2:D:184:ARG:CZ	2.47	0.45
2:B:372:LEU:O	2:B:375:PRO:HD3	2.17	0.45
2:B:99:ARG:HD3	4:B:2489:HOH:O	2.17	0.45
2:D:174:VAL:HA	2:D:175:PRO:HD3	1.78	0.45
2:D:277:GLN:HG2	2:D:303:VAL:HG21	1.98	0.45
2:D:243:SER:O	2:D:244:ASN:HB2	2.17	0.45
2:D:73:MSE:HG3	2:D:194:GLY:HA3	1.97	0.45
2:D:197:PRO:HB3	2:D:220:TRP:CD2	2.52	0.44
1:C:55:LEU:HD13	1:C:130:LEU:HD21	1.99	0.44
1:A:67:GLU:HG3	2:B:105:ARG:HB2	2.00	0.44
2:D:257:THR:OG1	2:D:259:LYS:HG2	2.18	0.44
4:A:318:HOH:O	3:B:2001:EDO:H12	2.16	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:319:ASP:HA	2:D:320:PRO:HD3	1.85	0.44
1:A:97:SER:HB3	4:B:2374:HOH:O	2.18	0.44
2:B:71:ASN:HB3	2:B:178:ASN:ND2	2.33	0.44
2:D:441:SER:HB3	2:D:452:VAL:CG1	2.48	0.44
2:B:277:GLN:HG2	2:B:303:VAL:HG21	2.00	0.43
2:B:380:TYR:CG	2:B:381:GLY:N	2.86	0.43
2:B:199:ARG:HG2	2:B:207:TRP:CE2	2.53	0.43
2:D:5:ALA:HB3	2:D:240:VAL:CG2	2.48	0.43
2:B:57:ARG:HH22	3:B:2001:EDO:C2	2.30	0.43
1:C:10:ILE:HD11	2:D:62:GLN:HG3	2.00	0.43
2:B:149:MSE:HE1	2:B:153:TYR:CE1	2.54	0.43
1:C:21:LEU:N	1:C:21:LEU:HD12	2.34	0.42
2:D:172:MSE:HE1	2:D:226:LEU:HD13	2.01	0.42
1:C:9:PRO:CD	2:D:184:ARG:CZ	2.97	0.42
2:B:10:LYS:HG3	4:B:2172:HOH:O	2.19	0.42
2:D:249:THR:O	2:D:249:THR:HG22	2.19	0.42
2:B:370:TRP:HD1	2:B:378:THR:O	2.02	0.42
2:B:505:ARG:O	2:B:509:GLU:HG3	2.19	0.42
2:D:10:LYS:HG3	4:D:2140:HOH:O	2.20	0.42
2:D:71:ASN:HB3	2:D:178:ASN:CG	2.40	0.42
1:A:144:LEU:HA	1:A:148:LEU:HD12	2.01	0.42
2:D:506:GLU:HG2	2:D:507:GLN:N	2.34	0.42
2:B:197:PRO:HB3	2:B:220:TRP:CD2	2.55	0.42
2:B:169:LEU:HD22	2:B:226:LEU:HD22	2.01	0.42
2:B:99:ARG:HH11	2:B:99:ARG:HG3	1.85	0.41
1:C:19:GLU:HG3	1:C:21:LEU:HD11	2.02	0.41
2:D:73:MSE:CE	4:D:2184:HOH:O	2.69	0.41
2:B:169:LEU:HD22	2:B:226:LEU:HD13	2.02	0.41
2:B:458:VAL:CG2	2:B:498:PHE:HE2	2.34	0.41
2:D:380:TYR:CG	2:D:381:GLY:N	2.87	0.41
1:A:154:GLY:HA3	1:A:160:GLY:O	2.21	0.41
2:B:22:PRO:HD2	2:B:457:TRP:O	2.20	0.41
2:B:309:LEU:N	2:B:310:PRO:CD	2.84	0.41
2:B:520:PHE:O	2:B:521:LYS:HG2	2.21	0.41
2:B:73:MSE:HE3	2:B:74:VAL:H	1.86	0.41
2:B:117:PRO:CD	1:C:119:PRO:HB2	2.51	0.41
2:D:440:TRP:HB3	2:D:449:ARG:HD2	2.03	0.41
2:B:73:MSE:SE	2:B:196:ALA:HB2	2.70	0.41
1:C:18:ASN:HB3	2:D:518:PHE:CZ	2.56	0.41
2:D:47:GLY:HA3	2:D:58:PHE:O	2.21	0.41
1:A:25:TYR:CE1	2:B:499:ARG:HD3	2.56	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:5:ALA:HB2	2:B:180:VAL:CG1	2.51	0.40
2:D:204:ILE:O	2:D:208:GLN:HG3	2.21	0.40
2:D:249:THR:N	2:D:250:PRO:CD	2.84	0.40
2:D:63:ARG:NH2	2:D:161:SER:HA	2.36	0.40
2:B:117:PRO:HD3	1:C:119:PRO:HB2	2.04	0.40
1:A:9:PRO:HG3	2:B:184:ARG:HD3	2.03	0.40
2:D:329:ARG:NH2	4:D:2378:HOH:O	2.54	0.40
1:A:29:HIS:HA	2:B:37:HIS:HB3	2.04	0.40
2:D:309:LEU:N	2:D:310:PRO:CD	2.85	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	151/160 (94%)	147 (97%)	4 (3%)	0	100	100
1	C	150/160 (94%)	147 (98%)	3 (2%)	0	100	100
2	B	519/528 (98%)	505 (97%)	13 (2%)	1 (0%)	49	46
2	D	519/528 (98%)	506 (98%)	13 (2%)	0	100	100
All	All	1339/1376 (97%)	1305 (98%)	33 (2%)	1 (0%)	53	51

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	100	PRO

### 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	116/122 (95%)	115 (99%)	1 (1%)	81	85
1	C	116/122 (95%)	116 (100%)	0	100	100
2	B	430/426 (101%)	421 (98%)	9 (2%)	56	60
2	D	430/426 (101%)	422 (98%)	8 (2%)	60	64
All	All	1092/1096 (100%)	1074 (98%)	18 (2%)	65	70

All (18) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	116	GLN
2	B	21	ASN
2	B	50	GLN
2	B	99	ARG
2	B	149	MSE
2	B	227	ASP
2	B	300	HIS
2	B	453	HIS
2	B	473	MSE
2	B	475	TYR
2	D	21	ASN
2	D	63	ARG
2	D	73	MSE
2	D	153	TYR
2	D	241	GLN
2	D	300	HIS
2	D	453	HIS
2	D	475	TYR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (18) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	53	ASN
1	A	83	ASN
2	B	15	ASN
2	B	50	GLN
2	B	78	ASN

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Mol	Chain	Res	Type
2	B	268	GLN
2	B	300	HIS
2	B	480	GLN
2	B	485	HIS
1	C	53	ASN
1	C	95	GLN
1	C	146	ASN
2	D	13	ASN
2	D	178	ASN
2	D	241	GLN
2	D	268	GLN
2	D	446	ASN
2	D	513	GLN

### 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](#)

2 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	EDO	B	2001	-	3,3,3	0.36	0	2,2,2	1.08	0



Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z  > 2$	Counts	RMSZ	$\# Z  > 2$
3	EDO	D	2002	-	3,3,3	0.24	0	2,2,2	1.17	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	EDO	B	2001	-	-	0/1/1/1	0/0/0/0
3	EDO	D	2002	-	-	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.

2 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	2001	EDO	2	0
3	D	2002	EDO	2	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 ⓘ

EDS was not executed - this section is therefore empty.

### 6.2 Non-standard residues in protein, DNA, RNA chains ⓘ

EDS was not executed - this section is therefore empty.

### 6.3 Carbohydrates ⓘ

EDS was not executed - this section is therefore empty.

### 6.4 Ligands ⓘ

EDS was not executed - this section is therefore empty.

### 6.5 Other polymers ⓘ

EDS was not executed - this section is therefore empty.