



# Full wwPDB X-ray Structure Validation Report ⓘ

Jan 31, 2016 – 11:14 PM GMT

PDB ID : 1WNF  
Title : Crystal Structure of PH0066 from *Pyrococcus horikoshii*  
Authors : Ihsanawati; Sekine, S.; Murayama, K.; Sugawara, M.; Shirouzu, M.;  
Yokoyama, S.; RIKEN Structural Genomics/Proteomics Initiative (RSGI)  
Deposited on : 2004-08-02  
Resolution : 2.50 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.

---

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

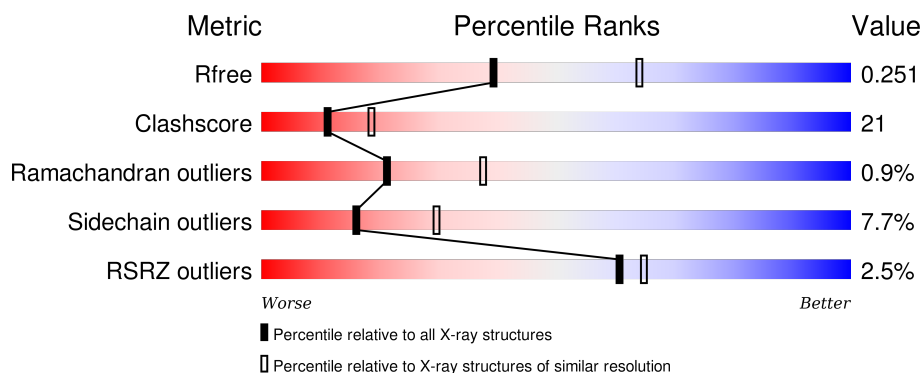
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.50 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	3553 (2.50-2.50)
Clashscore	102246	4242 (2.50-2.50)
Ramachandran outliers	100387	4156 (2.50-2.50)
Sidechain outliers	100360	4158 (2.50-2.50)
RSRZ outliers	91569	3562 (2.50-2.50)

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	328	<div> <div>3%</div> <div> <div></div> <div>61%</div> <div>32%</div> <div>5% •</div> </div> </div>
1	B	328	<div> <div>2%</div> <div> <div></div> <div>62%</div> <div>33%</div> <div>• •</div> </div> </div>

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
2	EDO	A	1001	-	-	-	X
2	EDO	A	1002	-	-	-	X
2	EDO	B	1004	-	-	-	X

## 2 Entry composition [i](#)

There are 3 unique types of molecules in this entry. The entry contains 5437 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 L-asparaginase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	324	Total	C	N	O	S	0	0	0
			2518	1622	420	464	12			
1	B	324	Total	C	N	O	S	0	0	0
			2518	1622	420	464	12			

- Molecule 2 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
2	A	1	Total	C	O	0	0
			4	2	2		
2	A	1	Total	C	O	0	0
			4	2	2		
2	B	1	Total	C	O	0	0
			4	2	2		
2	B	1	Total	C	O	0	0
			4	2	2		

*Continued on next page...*

*Continued from previous page...*

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

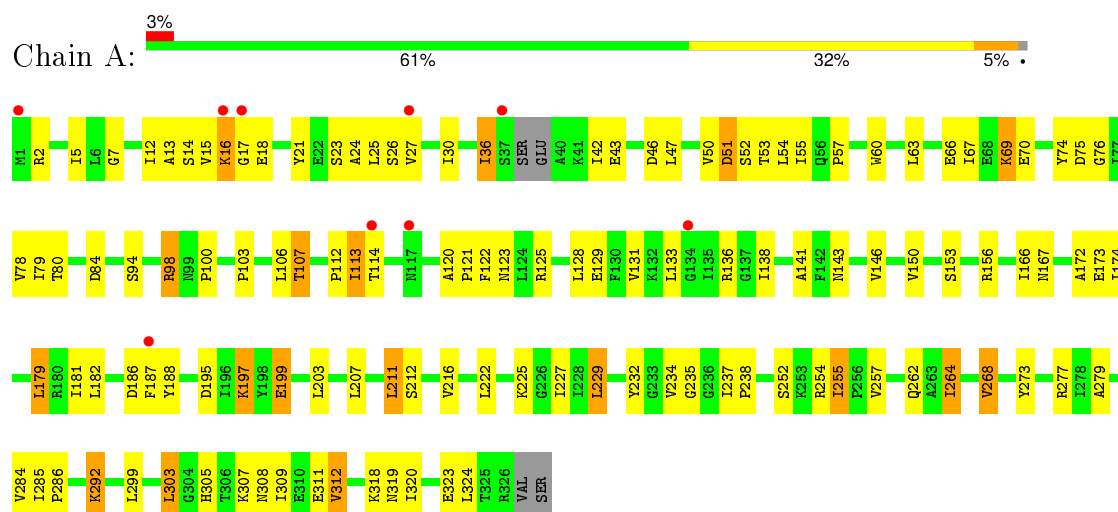
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	180	Total	O	0	0
			180	180		
3	B	201	Total	O	0	0
			201	201		

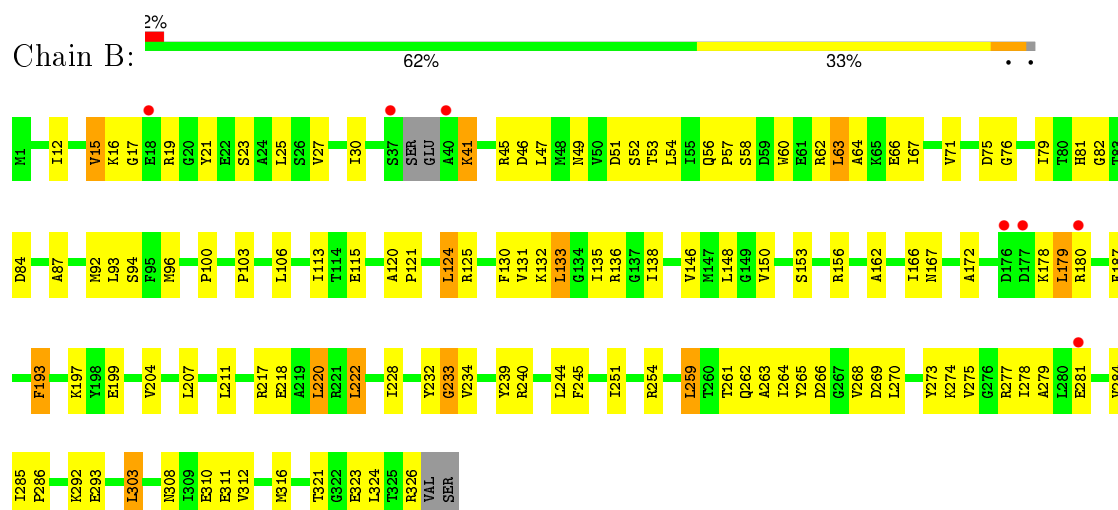
### 3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ( $RSRZ > 2$ ). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

#### • Molecule 1: L-asparaginase



#### • Molecule 1: L-asparaginase



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	125.23 Å 77.14 Å 98.46 Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.23 – 2.50 49.23 – 2.50	Depositor EDS
% Data completeness (in resolution range)	99.7 (49.23-2.50) 99.8 (49.23-2.50)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	4.42 (at 2.51 Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, $R_{free}$	0.199 , 0.251 0.199 , 0.251	Depositor DCC
$R_{free}$ test set	1661 reflections (4.95%)	DCC
Wilson B-factor (Å <sup>2</sup> )	33.5	Xtriage
Anisotropy	0.165	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.31 , 53.3	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.46$ , $\langle L^2 \rangle = 0.29$	Xtriage
Outliers	0 of 33574 reflections	Xtriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	5437	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	37.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.84% 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

### 5.1 Standard geometry

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	0.33	0/2560	0.59	0/3453
1	B	0.36	0/2560	0.61	0/3453
All	All	0.35	0/5120	0.60	0/6906

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

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	2518	0	2624	132	0
1	B	2518	0	2624	93	0
2	A	8	0	12	3	0
2	B	12	0	18	1	0
3	A	180	0	0	5	0
3	B	201	0	0	12	0
All	All	5437	0	5278	214	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 21.

All (214) 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:A:98:ARG:HB3	1:A:98:ARG:HH21	1.13	1.14
1:A:98:ARG:NH2	1:A:98:ARG:HB3	1.74	1.02
1:A:55:ILE:HG12	2:A:1002:EDO:H22	1.50	0.92
1:A:69:LYS:HD2	1:A:70:GLU:HG2	1.52	0.91
1:B:261:THR:HG22	1:B:263:ALA:H	1.45	0.82
1:B:41:LYS:HA	1:B:41:LYS:HE2	1.61	0.82
1:A:98:ARG:CB	1:A:98:ARG:HH21	1.94	0.81
1:B:270:LEU:HD12	1:B:286:PRO:HG3	1.65	0.78
1:A:308:ASN:HD22	1:A:311:GLU:H	1.33	0.75
1:B:261:THR:O	1:B:292:LYS:HE2	1.88	0.73
1:A:264:ILE:CD1	1:B:264:ILE:HG13	2.19	0.72
1:A:42:ILE:HG22	1:A:43:GLU:H	1.54	0.71
1:B:30:ILE:HG23	1:B:113:ILE:HD11	1.71	0.71
1:A:30:ILE:HG12	1:A:113:ILE:HD11	1.73	0.71
1:B:27:VAL:HG23	1:B:46:ASP:OD1	1.91	0.70
1:A:42:ILE:HG22	1:A:43:GLU:N	2.06	0.70
1:A:30:ILE:HG23	1:A:113:ILE:HD13	1.74	0.68
1:A:14:SER:HA	1:A:23:SER:HA	1.76	0.68
1:A:197:LYS:NZ	1:A:305:HIS:HD2	1.90	0.67
1:A:13:ALA:HB2	1:A:30:ILE:HD11	1.77	0.67
1:A:308:ASN:O	1:A:312:VAL:HG12	1.95	0.67
1:A:232:TYR:HB3	1:B:84:ASP:HB3	1.76	0.67
1:A:47:LEU:HD21	1:A:66:GLU:HG2	1.78	0.65
1:A:264:ILE:HD13	1:B:264:ILE:HG13	1.78	0.64
1:A:53:THR:HA	2:A:1002:EDO:H11	1.80	0.63
1:A:225:LYS:HD3	1:A:307:LYS:NZ	2.13	0.63
1:A:172:ALA:HB1	1:A:179:LEU:HD22	1.80	0.62
1:A:27:VAL:HG23	1:A:46:ASP:OD2	2.00	0.62
1:A:133:LEU:HD23	1:A:181:ILE:HD11	1.82	0.62
1:A:234:VAL:HG11	1:A:273:TYR:CD1	2.35	0.62
1:A:186:ASP:O	1:A:188:TYR:N	2.33	0.62
1:A:121:PRO:O	1:A:125:ARG:HG3	2.00	0.61
1:A:237:ILE:CD1	1:A:284:VAL:HG11	2.31	0.61
1:B:51:ASP:HB2	1:B:54:LEU:HD22	1.82	0.61
1:B:47:LEU:HD21	1:B:66:GLU:HG2	1.83	0.61
1:B:45:ARG:HD3	3:B:1138:HOH:O	2.00	0.61
1:B:277:ARG:O	1:B:281:GLU:HG2	2.01	0.61
1:A:128:LEU:O	1:A:131:VAL:HG12	2.02	0.60
1:A:199:GLU:HG3	1:A:225:LYS:HD2	1.82	0.60
1:A:53:THR:HG22	1:A:84:ASP:OD1	2.03	0.59
1:B:172:ALA:HB1	1:B:179:LEU:HD22	1.85	0.58

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:1139:HOH:O	1:B:156:ARG:HD3	2.03	0.58
1:A:197:LYS:HZ1	1:A:305:HIS:HD2	1.51	0.58
1:A:308:ASN:ND2	1:A:311:GLU:H	2.01	0.58
1:B:274:LYS:NZ	1:B:278:ILE:HD11	2.19	0.58
1:A:54:LEU:HB3	1:B:240:ARG:HD3	1.85	0.58
1:A:76:GLY:HA3	1:A:131:VAL:CG2	2.35	0.57
1:B:125:ARG:HD3	3:B:1258:HOH:O	2.03	0.57
1:B:259:LEU:HD13	1:B:270:LEU:HD21	1.86	0.57
1:B:41:LYS:CE	1:B:41:LYS:HA	2.35	0.57
1:A:186:ASP:C	1:A:188:TYR:H	2.08	0.57
1:A:254:ARG:HG2	1:A:254:ARG:HH21	1.70	0.57
1:A:36:ILE:O	1:A:36:ILE:HG23	2.04	0.57
1:B:156:ARG:HB2	1:B:162:ALA:HA	1.85	0.57
1:B:16:LYS:HB3	3:B:1375:HOH:O	2.05	0.56
1:A:203:LEU:CD2	1:A:227:ILE:HG12	2.35	0.56
1:A:94:SER:HA	1:A:138:ILE:HD12	1.87	0.56
1:B:218:GLU:O	1:B:222:LEU:HD22	2.05	0.56
1:B:12:ILE:HD11	1:B:124:LEU:HD21	1.86	0.56
1:B:17:GLY:C	1:B:19:ARG:H	2.08	0.56
1:B:233:GLY:O	1:B:261:THR:HG23	2.06	0.56
1:B:81:HIS:HD2	1:B:82:GLY:O	1.89	0.56
1:B:133:LEU:HB3	1:B:135:ILE:HD13	1.87	0.56
1:A:16:LYS:CG	1:A:21:TYR:HE2	2.18	0.55
1:B:239:TYR:HE1	1:B:275:VAL:HG12	1.72	0.55
1:B:120:ALA:HB3	1:B:121:PRO:HD3	1.88	0.55
1:A:133:LEU:CD2	1:A:181:ILE:HD11	2.37	0.54
1:B:308:ASN:HD21	1:B:310:GLU:HB2	1.72	0.54
1:A:216:VAL:HG13	1:A:227:ILE:CD1	2.37	0.54
1:B:12:ILE:HD11	1:B:124:LEU:CD2	2.38	0.54
1:A:107:THR:CG2	1:A:123:ASN:HB3	2.37	0.54
1:A:150:VAL:HG21	1:A:323:GLU:HB3	1.90	0.54
1:A:16:LYS:HG2	1:A:21:TYR:HE2	1.73	0.53
1:B:23:SER:HB2	1:B:49:ASN:OD1	2.08	0.53
1:B:274:LYS:HZ3	1:B:278:ILE:HD11	1.74	0.53
1:B:167:ASN:HD21	1:B:266:ASP:H	1.56	0.53
1:A:305:HIS:HE1	1:A:311:GLU:OE2	1.92	0.52
1:A:237:ILE:HD11	1:A:284:VAL:HG11	1.91	0.52
1:A:42:ILE:CG2	1:A:43:GLU:H	2.21	0.52
1:A:234:VAL:HG11	1:A:273:TYR:CE1	2.43	0.52
1:A:107:THR:HG23	1:A:141:ALA:O	2.09	0.52
1:A:156:ARG:HG3	1:B:265:TYR:HB2	1.91	0.52

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:76:GLY:HA3	1:B:131:VAL:HG13	1.92	0.52
1:A:146:VAL:HB	1:A:172:ALA:HB3	1.92	0.52
1:B:308:ASN:HD22	1:B:311:GLU:H	1.57	0.51
1:A:15:VAL:O	1:A:17:GLY:N	2.44	0.51
1:A:7:GLY:HA3	1:A:27:VAL:HG22	1.91	0.51
1:B:197:LYS:HG3	3:B:1074:HOH:O	2.10	0.51
1:A:309:ILE:O	1:A:312:VAL:HG13	2.11	0.51
1:A:225:LYS:HD3	1:A:307:LYS:HZ3	1.73	0.51
1:B:153:SER:HB2	1:B:166:ILE:HD12	1.93	0.51
1:A:42:ILE:CG2	1:A:43:GLU:N	2.74	0.50
1:B:92:MET:HG3	1:B:96:MET:HE2	1.93	0.50
1:B:130:PHE:CE2	1:B:146:VAL:HG11	2.46	0.50
1:B:15:VAL:HG22	3:B:1067:HOH:O	2.10	0.50
1:A:113:ILE:HG23	1:A:120:ALA:CB	2.42	0.50
1:A:75:ASP:O	1:A:103:PRO:HD2	2.11	0.50
1:B:57:PRO:HA	1:B:60:TRP:CE3	2.47	0.50
1:A:2:ARG:HG2	1:A:74:TYR:CD1	2.46	0.49
1:A:203:LEU:HD21	1:A:227:ILE:HG12	1.92	0.49
1:A:166:ILE:HG22	1:A:167:ASN:ND2	2.27	0.49
1:B:262:GLN:HB3	3:B:1385:HOH:O	2.11	0.49
1:B:312:VAL:O	1:B:316:MET:HB2	2.12	0.49
1:A:36:ILE:HD12	3:A:1290:HOH:O	2.12	0.48
1:B:234:VAL:O	1:B:268:VAL:HG13	2.13	0.48
1:A:207:LEU:HD21	1:A:229:LEU:HG	1.93	0.48
1:B:19:ARG:NH1	3:B:1178:HOH:O	2.46	0.48
1:B:133:LEU:O	1:B:135:ILE:HD12	2.12	0.48
1:A:7:GLY:HA2	1:A:80:THR:OG1	2.13	0.48
1:B:133:LEU:HB3	1:B:135:ILE:CD1	2.43	0.48
1:A:112:PRO:HB2	1:A:114:THR:HG22	1.94	0.48
1:A:7:GLY:HA3	1:A:27:VAL:CG2	2.42	0.48
1:A:234:VAL:O	1:A:268:VAL:HG22	2.13	0.48
1:A:237:ILE:HD12	1:A:284:VAL:HG11	1.95	0.48
1:B:193:PHE:HB2	3:B:1050:HOH:O	2.13	0.48
1:A:131:VAL:HG22	1:A:131:VAL:O	2.14	0.47
1:A:279:ALA:O	1:A:284:VAL:HG22	2.14	0.47
1:A:26:SER:O	1:A:30:ILE:HG13	2.14	0.47
1:A:273:TYR:CD2	1:B:21:TYR:HB2	2.50	0.47
1:A:173:GLU:HG3	1:A:182:LEU:HD11	1.97	0.47
1:A:324:LEU:HD12	1:A:324:LEU:C	2.35	0.47
1:B:135:ILE:HD12	1:B:135:ILE:N	2.30	0.47
1:B:239:TYR:CE1	1:B:275:VAL:HG12	2.49	0.47

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:273:TYR:CE2	1:B:21:TYR:HD2	2.32	0.47
1:A:16:LYS:HA	1:A:21:TYR:CD2	2.50	0.47
1:A:107:THR:HG21	1:A:123:ASN:HB3	1.97	0.46
1:B:130:PHE:CD2	1:B:146:VAL:HG11	2.49	0.46
1:A:211:LEU:HD22	1:A:212:SER:N	2.29	0.46
1:B:279:ALA:O	1:B:284:VAL:HG22	2.14	0.46
1:B:87:ALA:HB3	1:B:293:GLU:HG2	1.97	0.46
1:A:308:ASN:HD22	1:A:311:GLU:N	2.09	0.46
1:B:308:ASN:ND2	1:B:311:GLU:H	2.14	0.46
1:B:41:LYS:CA	1:B:41:LYS:HE2	2.40	0.46
1:A:120:ALA:HB3	1:A:121:PRO:HD3	1.97	0.46
1:A:128:LEU:HA	1:A:131:VAL:HG12	1.97	0.46
1:A:227:ILE:HG22	1:A:229:LEU:HD13	1.99	0.45
1:A:5:ILE:HD11	1:A:128:LEU:HD21	1.97	0.45
1:A:103:PRO:HB2	1:A:131:VAL:HG23	1.98	0.45
1:B:245:PHE:CE2	1:B:278:ILE:HG22	2.52	0.45
1:A:255:ILE:HD11	3:A:1298:HOH:O	2.16	0.45
1:B:56:GLN:HG3	1:B:58:SER:HB3	1.98	0.45
1:A:234:VAL:HA	3:B:1370:HOH:O	2.15	0.45
1:A:16:LYS:HA	1:A:21:TYR:HD2	1.81	0.45
1:B:217:ARG:NH1	3:B:1273:HOH:O	2.50	0.45
1:B:220:LEU:HD12	1:B:251:ILE:HD12	1.97	0.45
1:A:25:LEU:HD23	1:A:113:ILE:HD11	1.98	0.45
1:A:150:VAL:CG2	1:A:323:GLU:HB3	2.46	0.45
1:B:148:LEU:HD21	1:B:187:PHE:HZ	1.81	0.45
1:A:50:VAL:CG1	1:A:54:LEU:HB2	2.46	0.44
1:A:238:PRO:HG3	1:B:53:THR:O	2.16	0.44
1:A:98:ARG:NH2	1:A:98:ARG:CB	2.63	0.44
1:B:150:VAL:HG21	1:B:323:GLU:HB3	1.99	0.44
1:B:199:GLU:HB3	1:B:303:LEU:HB3	1.98	0.44
1:B:67:ILE:HD11	1:B:79:ILE:HD11	1.99	0.44
1:B:150:VAL:HB	2:B:1004:EDO:H22	1.99	0.44
1:A:252:SER:HA	1:A:257:VAL:HG13	2.00	0.44
1:A:234:VAL:HG13	1:A:235:GLY:N	2.33	0.44
1:A:21:TYR:HB2	1:B:273:TYR:CD1	2.53	0.44
1:A:123:ASN:HD21	1:A:143:ASN:H	1.66	0.44
1:A:225:LYS:HD3	1:A:307:LYS:HZ1	1.82	0.44
1:B:30:ILE:HG23	1:B:113:ILE:CD1	2.45	0.44
1:A:129:GLU:O	1:A:133:LEU:HD13	2.18	0.44
1:A:195:ASP:OD1	1:A:197:LYS:HE3	2.18	0.43
1:A:53:THR:HB	1:B:232:TYR:CD1	2.53	0.43

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:197:LYS:O	1:A:197:LYS:HD2	2.18	0.43
1:B:178:LYS:HD2	1:B:178:LYS:HA	1.88	0.43
1:B:64:ALA:HB2	1:B:96:MET:HE3	2.00	0.43
1:A:47:LEU:CD2	1:A:66:GLU:HG2	2.47	0.43
1:A:16:LYS:HG2	1:A:21:TYR:CE2	2.53	0.43
1:A:57:PRO:HA	1:A:60:TRP:CE3	2.53	0.43
1:A:292:LYS:HD3	3:A:1372:HOH:O	2.17	0.43
1:A:318:LYS:HE2	1:A:318:LYS:HB3	1.82	0.43
1:B:232:TYR:O	1:B:233:GLY:C	2.57	0.43
1:A:307:LYS:HD3	1:A:307:LYS:HA	1.83	0.43
1:A:186:ASP:C	1:A:188:TYR:N	2.71	0.43
1:A:63:LEU:O	1:A:67:ILE:HG13	2.18	0.43
1:A:100:PRO:O	1:A:136:ARG:HD2	2.18	0.43
1:B:52:SER:HA	3:B:1120:HOH:O	2.19	0.43
1:B:220:LEU:HD12	1:B:251:ILE:CD1	2.49	0.43
1:B:148:LEU:HD21	1:B:187:PHE:CZ	2.54	0.43
1:B:106:LEU:N	1:B:106:LEU:HD12	2.34	0.43
1:A:254:ARG:HG2	1:A:254:ARG:NH2	2.32	0.42
1:A:5:ILE:HG12	1:A:78:VAL:HB	2.01	0.42
1:B:324:LEU:HD11	1:B:326:ARG:HG3	2.02	0.42
1:A:106:LEU:N	1:A:106:LEU:HD12	2.35	0.42
1:A:12:ILE:O	1:A:113:ILE:HG12	2.19	0.42
1:A:285:ILE:HA	1:A:286:PRO:HD3	1.82	0.42
1:A:51:ASP:HB3	1:A:52:SER:H	1.73	0.42
1:B:62:ARG:HG2	1:B:62:ARG:HH11	1.85	0.42
1:B:204:VAL:HG22	1:B:228:ILE:HB	2.02	0.42
1:B:268:VAL:CG1	1:B:269:ASP:N	2.83	0.41
1:B:324:LEU:CD1	1:B:326:ARG:HG3	2.50	0.41
1:B:75:ASP:O	1:B:103:PRO:HD2	2.20	0.41
1:A:122:PHE:CZ	1:A:174:ILE:HD12	2.55	0.41
1:A:264:ILE:HD11	1:B:264:ILE:HG13	2.00	0.41
1:A:234:VAL:CG1	3:A:1101:HOH:O	2.68	0.41
1:B:63:LEU:HD22	1:B:67:ILE:CD1	2.50	0.41
1:B:93:LEU:HD23	1:B:96:MET:CE	2.50	0.41
1:A:2:ARG:HG3	1:A:2:ARG:HH11	1.85	0.41
1:A:264:ILE:HG13	1:A:264:ILE:H	1.61	0.41
1:A:107:THR:HG22	1:A:123:ASN:HB3	2.02	0.41
1:A:52:SER:OG	2:A:1001:EDO:H12	2.21	0.41
1:A:216:VAL:HG13	1:A:227:ILE:HD12	2.01	0.41
1:B:100:PRO:O	1:B:136:ARG:HD2	2.21	0.41
1:A:199:GLU:CG	1:A:225:LYS:HD2	2.49	0.41

*Continued on next page...*

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:67:ILE:HD11	1:A:79:ILE:HD11	2.02	0.41
1:A:98:ARG:HE	1:A:320:ILE:CG2	2.34	0.40
1:A:122:PHE:HZ	1:A:174:ILE:HD12	1.86	0.40
1:B:285:ILE:HA	1:B:286:PRO:HD3	1.95	0.40
1:A:299:LEU:HG	1:A:303:LEU:HD22	2.03	0.40
1:B:94:SER:HA	1:B:138:ILE:HD12	2.03	0.40
1:B:292:LYS:HG2	3:B:1018:HOH:O	2.20	0.40
1:A:47:LEU:HD11	1:A:66:GLU:HG2	2.04	0.40
1:A:123:ASN:ND2	1:A:143:ASN:H	2.20	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	320/328 (98%)	290 (91%)	25 (8%)	5 (2%)	12	21
1	B	320/328 (98%)	305 (95%)	14 (4%)	1 (0%)	46	68
All	All	640/656 (98%)	595 (93%)	39 (6%)	6 (1%)	21	37

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	51	ASP
1	A	187	PHE
1	A	16	LYS
1	A	36	ILE
1	B	233	GLY
1	A	24	ALA

### 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	273 / 277 (99%)	252 (92%)	21 (8%)	16	30
1	B	273 / 277 (99%)	252 (92%)	21 (8%)	16	30
All	All	546 / 554 (99%)	504 (92%)	42 (8%)	16	30

All (42) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	18	GLU
1	A	69	LYS
1	A	98	ARG
1	A	107	THR
1	A	113	ILE
1	A	153	SER
1	A	179	LEU
1	A	197	LYS
1	A	199	GLU
1	A	211	LEU
1	A	222	LEU
1	A	229	LEU
1	A	255	ILE
1	A	262	GLN
1	A	264	ILE
1	A	268	VAL
1	A	277	ARG
1	A	292	LYS
1	A	303	LEU
1	A	312	VAL
1	A	319	ASN
1	B	15	VAL
1	B	25	LEU
1	B	41	LYS
1	B	63	LEU
1	B	71	VAL
1	B	115	GLU

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	B	124	LEU
1	B	132	LYS
1	B	133	LEU
1	B	179	LEU
1	B	180	ARG
1	B	193	PHE
1	B	207	LEU
1	B	211	LEU
1	B	220	LEU
1	B	222	LEU
1	B	244	LEU
1	B	254	ARG
1	B	259	LEU
1	B	303	LEU
1	B	321	THR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (12) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	56	GLN
1	A	123	ASN
1	A	143	ASN
1	A	271	GLN
1	A	305	HIS
1	A	308	ASN
1	A	319	ASN
1	B	81	HIS
1	B	117	ASN
1	B	167	ASN
1	B	170	ASN
1	B	308	ASN

### 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

5 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	$\# Z  > 2$
2	EDO	A	1001	-	3,3,3	0.59	0	2,2,2	0.31	0
2	EDO	A	1002	-	3,3,3	0.62	0	2,2,2	0.27	0
2	EDO	B	1003	-	3,3,3	0.65	0	2,2,2	0.27	0
2	EDO	B	1004	-	3,3,3	0.92	0	2,2,2	0.14	0
2	EDO	B	1005	-	3,3,3	0.63	0	2,2,2	0.33	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
2	EDO	A	1001	-	-	0/1/1/1	0/0/0/0
2	EDO	A	1002	-	-	0/1/1/1	0/0/0/0
2	EDO	B	1003	-	-	0/1/1/1	0/0/0/0
2	EDO	B	1004	-	-	0/1/1/1	0/0/0/0
2	EDO	B	1005	-	-	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.

3 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	1001	EDO	1	0
2	A	1002	EDO	2	0
2	B	1004	EDO	1	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 [i](#)

### 6.1 Protein, DNA and RNA chains [i](#)

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	324/328 (98%)	-0.11	9 (2%) 56 61	16, 36, 74, 99	0
1	B	324/328 (98%)	-0.32	7 (2%) 65 69	14, 29, 57, 72	0
All	All	648/656 (98%)	-0.22	16 (2%) 61 65	14, 32, 66, 99	0

All (16) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	37	SER	4.2
1	B	40	ALA	3.7
1	A	1	MET	3.7
1	A	114	THR	3.3
1	A	17	GLY	3.3
1	B	177	ASP	3.1
1	B	37	SER	2.8
1	B	176	ASP	2.8
1	B	180	ARG	2.7
1	A	187	PHE	2.4
1	A	27	VAL	2.3
1	B	281	GLU	2.2
1	A	16	LYS	2.1
1	A	117	ASN	2.1
1	A	134	GLY	2.1
1	B	18	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](#)

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( $\text{\AA}^2$ )	Q<0.9
2	EDO	B	1004	4/4	0.83	0.26	6.07	21,29,29,31	0
2	EDO	A	1001	4/4	0.81	0.28	3.34	60,61,63,64	0
2	EDO	A	1002	4/4	0.89	0.22	2.73	48,48,48,50	0
2	EDO	B	1005	4/4	0.92	0.17	-	63,63,63,63	0
2	EDO	B	1003	4/4	0.91	0.14	-	55,56,57,57	0

### 6.5 Other polymers [i](#)

There are no such residues in this entry.