Full wwPDB X-ray Structure Validation Report (i)

Jan 3, 2024 – 08:04 am GMT

PDB ID	:	5A2G
Title	:	An esterase from anaerobic Clostridium hathewayi can hydrolyze aliphatic aromatic polyesters
Authors	:	Hromic, A.; Pavkov Keller, T.; Steinkellner, G.; Gruber, K.; Perz, V.; Baumschlager, A.; Bleymaier, K.; Zitzenbacher, S.; Zankel, A.; Mayrhofer, C.; Sinkel, C.; Kueper, U.; Schlegel, K.A.; Ribitsch, D.; Guebitz, G.M.
Deposited on	:	2015-05-19
Resolution	:	1.90 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

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

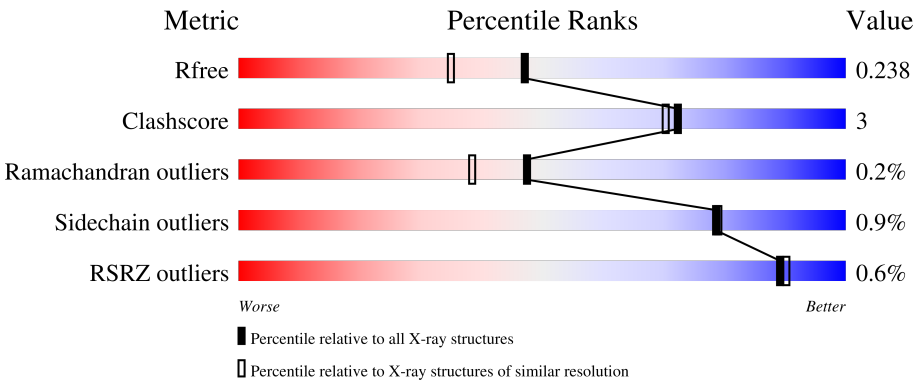
MolProbity	:	4.02b-467
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 1.90 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}	130704	6207 (1.90-1.90)
Clashscore	141614	6847 (1.90-1.90)
Ramachandran outliers	138981	6760 (1.90-1.90)
Sidechain outliers	138945	6760 (1.90-1.90)
RSRZ outliers	127900	6082 (1.90-1.90)

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 of the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5% The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	522	.% 89% 7% .
1	B	522	83% 12% .
1	C	522	.% 89% 7% .
1	D	522	.% 87% 9% .

2 Entry composition (i)

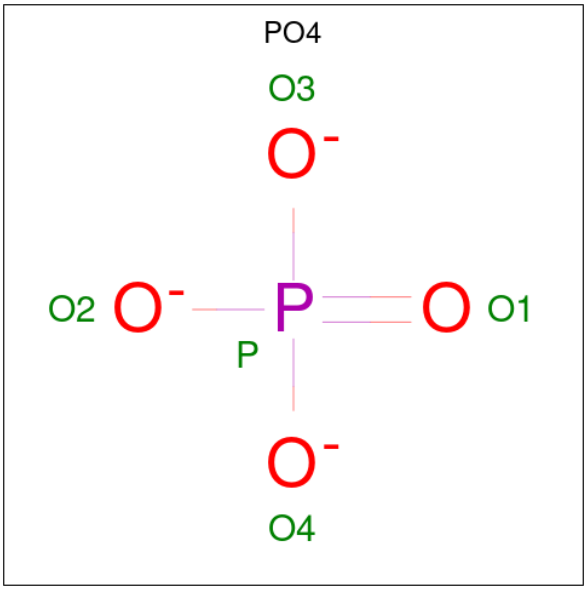
There are 3 unique types of molecules in this entry. The entry contains 17372 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 CARBOXYLIC ESTER HYDROLASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	501	3940	2526	658	737	19	0	0	0
1	B	501	3940	2526	658	737	19	0	0	0
1	C	501	3940	2526	658	737	19	0	0	0
1	D	501	3940	2526	658	737	19	0	0	0

- Molecule 2 is PHOSPHATE ION (three-letter code: PO4) (formula: O_4P).



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

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	O	P		
2	C	1	5	4	1	0	0
			Total	O	P		
2	D	1	5	4	1	0	0

- Molecule 3 is water.

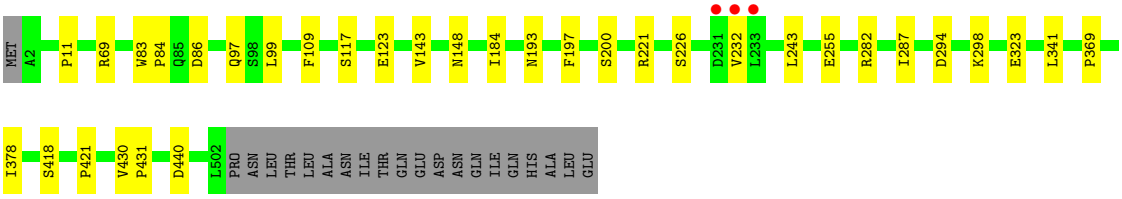
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
3	A	463	463	463	0	0
			Total	O		
3	B	332	332	332	0	0
			Total	O		
3	C	451	451	451	0	0
			Total	O		
3	D	346	346	346	0	0

3 Residue-property plots (i)

These plots are drawn for all protein, RNA, DNA and oligosaccharide 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.

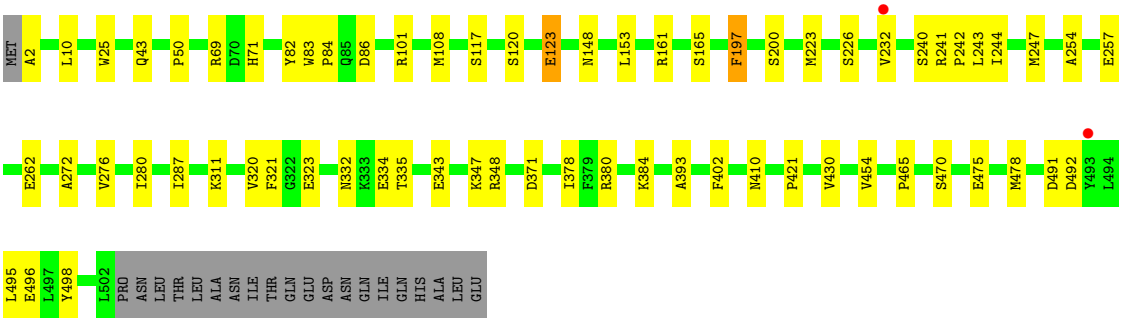
• Molecule 1: CARBOXYLIC ESTER HYDROLASE

Chain A:



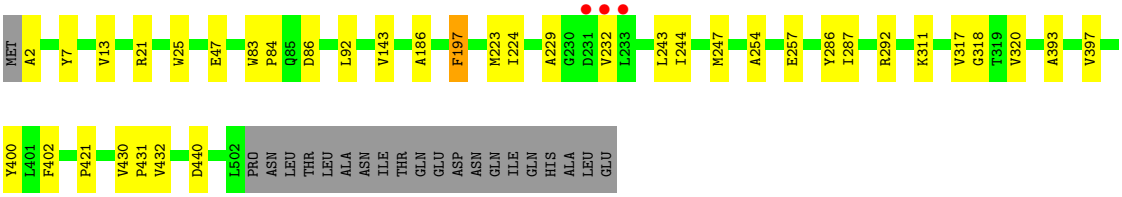
• Molecule 1: CARBOXYLIC ESTER HYDROLASE

Chain B:



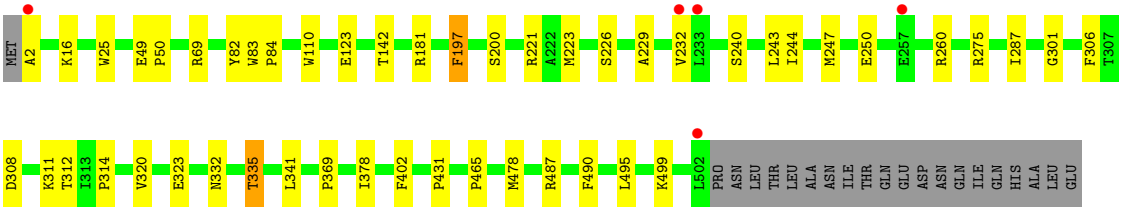
• Molecule 1: CARBOXYLIC ESTER HYDROLASE

Chain C:



• Molecule 1: CARBOXYLIC ESTER HYDROLASE

Chain D:


MET
A2
K16
W25
E49
P50
R69
Y82
W83
P84
W110
E123
T142
R181
F197
S200
R221
A222
M223
S226
A229
V232
L233
S240
L243
I244
M247
E250
E257
R260
R275
I287
G301
F306
T307
D308
K311
T312
I313
P314
V320
E323
N332
T335
L341
P369
I378
F402
P431
P465
M478
R487
F490
L495
K499
L502
PRO
ASN
LEU
THR
LEU
ALA
ASN
ILE
THR
GLN
GLU
ASP
ASN
GLN
ILE
GLN
HIS
ALA
LEU
GLU

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	62.05Å 241.83Å 83.58Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	60.10 – 1.90 60.46 – 1.90	Depositor EDS
% Data completeness (in resolution range)	84.5 (60.10-1.90) 82.3 (60.46-1.90)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.09	Depositor
$< I/\sigma(I) >$ [1]	1.26 (at 1.90Å)	Xtriage
Refinement program	PHENIX (PHENIX.REFINE)	Depositor
R, R_{free}	0.189 , 0.237 0.191 , 0.238	Depositor DCC
R_{free} test set	8047 reflections (4.93%)	wwPDB-VP
Wilson B-factor (Å^2)	18.8	Xtriage
Anisotropy	0.585	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.32 , 24.3	EDS
L-test for twinning[2]	$< \|L\| > = 0.44$, $< L^2 > = 0.26$	Xtriage
Estimated twinning fraction	0.218 for h,-k,-l	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	17372	wwPDB-VP
Average B, all atoms (Å^2)	24.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.98% of the height of the origin peak. No significant pseudotranslation is detected.*

[1]Intensities estimated from amplitudes.

[2]Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 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: PO4

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	0.32	0/4047	0.48	0/5495
1	B	0.29	0/4047	0.46	0/5495
1	C	0.31	0/4047	0.48	0/5495
1	D	0.30	0/4047	0.47	0/5495
All	All	0.31	0/16188	0.47	0/21980

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	3940	0	3821	23	0
1	B	3940	0	3821	37	0
1	C	3940	0	3821	23	0
1	D	3940	0	3821	32	0
2	A	5	0	0	0	0
2	B	5	0	0	0	0
2	C	5	0	0	0	0
2	D	5	0	0	0	0
3	A	463	0	0	5	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	B	332	0	0	4	0
3	C	451	0	0	3	0
3	D	346	0	0	5	0
All	All	17372	0	15284	105	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 3.

All (105) 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)
3:C:2413:HOH:O	1:D:2:ALA:N	2.17	0.77
1:A:86:ASP:OD2	1:B:69:ARG:NH1	2.18	0.76
1:A:69:ARG:NH1	1:B:86:ASP:OD2	2.28	0.67
1:D:221:ARG:NH2	3:D:2213:HOH:O	2.28	0.66
1:B:243:LEU:HA	1:B:280:ILE:HD13	1.78	0.65
1:D:260:ARG:NH2	3:D:2229:HOH:O	2.31	0.64
1:D:332:ASN:HB3	1:D:335:THR:HB	1.81	0.63
1:D:232:VAL:HG11	1:D:378:ILE:HG23	1.80	0.62
1:D:311:LYS:NZ	3:D:2256:HOH:O	2.31	0.62
1:B:101:ARG:NH1	3:B:2016:HOH:O	2.34	0.61
1:B:161:ARG:NH1	1:B:262:GLU:OE1	2.35	0.60
1:B:498:TYR:OH	3:B:2261:HOH:O	2.17	0.59
1:C:311:LYS:HE2	1:C:393:ALA:HB1	1.85	0.59
1:B:465:PRO:HD2	1:B:478:MET:HE1	1.84	0.58
1:B:153:LEU:O	1:B:165:SER:OG	2.19	0.57
1:D:243:LEU:HD22	1:D:287:ILE:HA	1.87	0.56
1:D:244:ILE:HA	1:D:247:MET:HE2	1.87	0.56
1:D:16:LYS:O	3:D:2019:HOH:O	2.18	0.55
1:D:181:ARG:NH2	3:D:2192:HOH:O	2.39	0.55
1:B:243:LEU:HD22	1:B:287:ILE:HA	1.88	0.55
1:B:320:VAL:HG12	1:B:402:PHE:HB3	1.90	0.54
1:C:244:ILE:HD13	1:C:247:MET:HE3	1.88	0.54
1:A:11:PRO:HG2	1:A:99:LEU:HD12	1.88	0.54
1:C:2:ALA:N	3:C:2002:HOH:O	2.39	0.54
1:C:243:LEU:HD22	1:C:287:ILE:HA	1.89	0.53
1:C:421:PRO:HG3	1:C:430:VAL:HG21	1.90	0.51
1:C:92:LEU:HB3	1:C:143:VAL:HG12	1.92	0.51
1:A:421:PRO:HG3	1:A:430:VAL:HG21	1.91	0.50
1:B:421:PRO:HG3	1:B:430:VAL:HG21	1.94	0.50
1:D:320:VAL:HG12	1:D:402:PHE:HB3	1.93	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:83:TRP:CG	1:B:84:PRO:HD2	2.47	0.50
1:B:332:ASN:HB3	1:B:335:THR:HB	1.93	0.50
1:C:440:ASP:OD2	1:D:2:ALA:HB2	2.12	0.49
1:A:83:TRP:CD1	1:A:84:PRO:HD2	2.47	0.49
1:D:301:GLY:HA3	1:D:306:PHE:CE1	2.47	0.49
1:A:97:GLN:NE2	3:A:2154:HOH:O	2.26	0.49
1:B:343:GLU:O	1:B:347:LYS:HG2	2.12	0.49
1:C:86:ASP:OD2	1:D:69:ARG:NH1	2.40	0.48
1:B:348:ARG:NH2	3:B:2260:HOH:O	2.40	0.48
1:D:250:GLU:OE2	1:D:275:ARG:NH1	2.47	0.48
1:D:487:ARG:HB3	1:D:490:PHE:HB3	1.95	0.48
1:A:69:ARG:NE	3:A:2109:HOH:O	2.45	0.47
1:B:232:VAL:HG11	1:B:378:ILE:HG23	1.96	0.47
1:D:465:PRO:HD2	1:D:478:MET:HE1	1.95	0.47
1:B:254:ALA:HB3	1:B:257:GLU:HG3	1.95	0.47
1:A:440:ASP:OD2	1:B:2:ALA:N	2.49	0.46
1:C:25:TRP:CZ3	1:D:431:PRO:HA	2.50	0.46
1:A:83:TRP:CG	1:A:84:PRO:HD2	2.51	0.46
1:A:117:SER:HA	1:A:148:ASN:H	1.80	0.46
1:C:244:ILE:HD13	1:C:247:MET:CE	2.46	0.46
1:A:232:VAL:HG21	1:A:378:ILE:HG23	1.98	0.45
1:A:431:PRO:HA	1:B:25:TRP:CZ3	2.52	0.45
1:D:240:SER:O	1:D:244:ILE:HG12	2.16	0.45
1:B:50:PRO:O	3:B:2065:HOH:O	2.21	0.45
1:B:240:SER:O	1:B:244:ILE:HG12	2.17	0.45
1:B:470:SER:OG	1:B:475:GLU:HA	2.17	0.45
1:D:312:THR:O	1:D:314:PRO:HD3	2.17	0.45
1:B:117:SER:HA	1:B:148:ASN:H	1.82	0.44
1:C:83:TRP:CD1	1:C:84:PRO:HD2	2.53	0.44
1:B:311:LYS:HD3	1:B:393:ALA:HB1	2.00	0.44
1:C:431:PRO:HA	1:D:25:TRP:CZ3	2.52	0.44
1:B:244:ILE:HA	1:B:247:MET:HE2	2.00	0.44
1:B:380:ARG:NE	1:B:384:LYS:HD2	2.33	0.43
1:B:334:GLU:HG3	1:B:410:ASN:HB3	1.99	0.43
1:C:224:ILE:HB	1:C:317:VAL:HG23	1.99	0.43
1:C:286:TYR:CE2	1:C:292:ARG:HD2	2.54	0.43
1:C:7:TYR:CZ	1:C:21:ARG:HD3	2.54	0.43
1:B:491:ASP:O	1:B:495:LEU:HG	2.18	0.43
1:C:318:GLY:HA3	1:C:400:TYR:CZ	2.54	0.43
1:D:341:LEU:HD21	1:D:369:PRO:HB2	2.01	0.43
1:D:308:ASP:HA	1:D:311:LYS:HE2	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:272:ALA:O	1:B:276:VAL:HG22	2.19	0.42
1:D:83:TRP:CG	1:D:84:PRO:HD2	2.53	0.42
1:B:241:ARG:HB2	1:B:242:PRO:HD3	2.00	0.42
1:C:254:ALA:HB3	1:C:257:GLU:HG3	2.02	0.42
1:C:320:VAL:HG12	1:C:402:PHE:HB3	2.00	0.42
1:D:197:PHE:CB	1:D:223:MET:HB3	2.49	0.42
1:D:495:LEU:O	1:D:499:LYS:HG2	2.19	0.42
1:A:193:ASN:OD1	1:A:221:ARG:NH1	2.39	0.42
1:D:110:TRP:HB3	1:D:142:THR:HG22	2.00	0.42
1:D:197:PHE:HB3	1:D:223:MET:HB3	2.01	0.42
1:B:108:MET:SD	1:B:454:VAL:HG11	2.59	0.42
1:C:13:VAL:HG13	1:C:186:ALA:HB1	2.01	0.42
1:C:47:GLU:OE2	3:C:2086:HOH:O	2.22	0.41
1:C:229:ALA:O	1:C:232:VAL:HG12	2.21	0.41
1:D:49:GLU:HA	1:D:50:PRO:HD3	1.91	0.41
1:A:184:ILE:HD12	1:A:184:ILE:HA	1.97	0.41
1:A:109:PHE:CZ	1:A:143:VAL:HG11	2.55	0.41
1:A:243:LEU:HD22	1:A:287:ILE:HA	2.03	0.41
1:C:84:PRO:HD3	1:D:82:TYR:CD2	2.55	0.41
1:A:418:SER:O	1:A:421:PRO:HD2	2.21	0.41
1:B:200:SER:HA	1:B:226:SER:O	2.21	0.41
1:C:197:PHE:HB3	1:C:223:MET:HB3	2.03	0.41
1:D:200:SER:HA	1:D:226:SER:O	2.21	0.40
1:A:84:PRO:HD3	1:B:82:TYR:CD2	2.56	0.40
1:B:197:PHE:CB	1:B:223:MET:HB3	2.52	0.40
1:A:282:ARG:NH1	3:A:2302:HOH:O	2.35	0.40
1:A:294:ASP:HB2	3:A:2305:HOH:O	2.21	0.40
1:B:43:GLN:HG2	1:B:161:ARG:O	2.21	0.40
1:D:229:ALA:HB1	1:D:232:VAL:HG22	2.03	0.40
1:A:298:LYS:NZ	3:A:2311:HOH:O	2.54	0.40
1:B:321:PHE:CZ	1:B:371:ASP:HB3	2.57	0.40
1:A:200:SER:HA	1:A:226:SER:O	2.22	0.40
1:A:341:LEU:HD21	1:A:369:PRO:HB2	2.03	0.40
1:B:120:SER:H	1:B:123:GLU:HB2	1.86	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	499/522 (96%)	479 (96%)	19 (4%)	1 (0%)	47	38
1	B	499/522 (96%)	478 (96%)	20 (4%)	1 (0%)	47	38
1	C	499/522 (96%)	476 (95%)	23 (5%)	0	100	100
1	D	499/522 (96%)	475 (95%)	23 (5%)	1 (0%)	47	38
All	All	1996/2088 (96%)	1908 (96%)	85 (4%)	3 (0%)	47	38

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	323	GLU
1	D	323	GLU
1	A	323	GLU

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	414/433 (96%)	411 (99%)	3 (1%)	84	84
1	B	414/433 (96%)	408 (99%)	6 (1%)	67	65
1	C	414/433 (96%)	411 (99%)	3 (1%)	84	84
1	D	414/433 (96%)	411 (99%)	3 (1%)	84	84
All	All	1656/1732 (96%)	1641 (99%)	15 (1%)	78	79

All (15) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	123	GLU
1	A	197	PHE
1	A	255	GLU
1	B	10	LEU
1	B	71	HIS
1	B	123	GLU
1	B	197	PHE
1	B	492	ASP
1	B	496	GLU
1	C	197	PHE
1	C	397	VAL
1	C	432	VAL
1	D	123	GLU
1	D	197	PHE
1	D	335	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

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 monosaccharides in this entry.

5.6 Ligand geometry (i)

4 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	PO4	B	1503	-	4,4,4	0.81	0	6,6,6	0.50	0
2	PO4	D	1503	-	4,4,4	0.99	0	6,6,6	0.55	0
2	PO4	A	1503	-	4,4,4	0.86	0	6,6,6	0.63	0
2	PO4	C	1503	-	4,4,4	0.77	0	6,6,6	0.33	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 (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, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled 'Q< 0.9' lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
1	A	501/522 (95%)	-0.37	3 (0%)	89	90	13, 20, 33, 58	0
1	B	501/522 (95%)	-0.19	2 (0%)	92	93	13, 25, 46, 62	0
1	C	501/522 (95%)	-0.34	3 (0%)	89	90	13, 21, 33, 67	0
1	D	501/522 (95%)	-0.16	5 (0%)	82	84	14, 25, 49, 60	0
All	All	2004/2088 (95%)	-0.26	13 (0%)	89	90	13, 23, 42, 67	0

All (13) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	232	VAL	7.5
1	D	233	LEU	7.2
1	A	233	LEU	5.5
1	A	232	VAL	4.8
1	C	231	ASP	4.3
1	C	232	VAL	3.6
1	D	502	LEU	3.6
1	D	2	ALA	2.6
1	C	233	LEU	2.5
1	B	232	VAL	2.4
1	B	493	TYR	2.4
1	D	257	GLU	2.3
1	A	231	ASP	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 monosaccharides 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. The B-factors column lists the minimum, median, 95th 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	B-factors(Å^2)	Q<0.9
2	PO4	A	1503	5/5	0.98	0.09	15,15,18,21	0
2	PO4	D	1503	5/5	0.98	0.08	17,17,19,22	0
2	PO4	C	1503	5/5	0.99	0.08	13,14,16,17	0
2	PO4	B	1503	5/5	0.99	0.08	13,15,17,17	0

6.5 Other polymers (i)

There are no such residues in this entry.