



wwPDB X-ray Structure Validation Summary Report ⓘ

Feb 28, 2026 – 05:41 PM UTC

PDB ID : 2OAQ / pdb_00002oaq
Title : Crystal structure of the archaeal secretion ATPase GspE in complex with phosphate
Authors : Yamagata, A.; Tainer, J.A.
Deposited on : 2006-12-17
Resolution : 3.15 Å(reported)

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

We welcome your comments at validation@mail.wwpdb.org

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<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ 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 ⓘ](#)) were used in the production of this report:

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

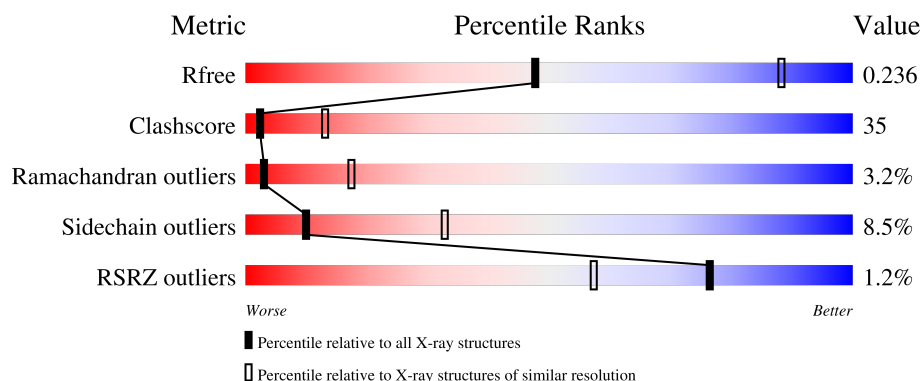
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.15 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}	180053	2361 (3.20-3.12)
Clashscore	190562	2486 (3.20-3.12)
Ramachandran outliers	187476	2405 (3.20-3.12)
Sidechain outliers	187428	2404 (3.20-3.12)
RSRZ outliers	180081	2361 (3.20-3.12)

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 $\leq 5\%$. 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	1	511	2% 42% 45% 9% ..
1	2	511	% 42% 47% 9% .

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	PO4	2	512	-	-	X	-
2	PO4	2	513	-	-	X	-
2	PO4	2	514	-	-	X	-

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 7997 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 Type II secretion system protein.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	1	498	Total	C	N	O	S	Se	0	0	0
			3916	2501	669	728	1	17			
1	2	503	Total	C	N	O	S	Se	0	0	0
			4061	2593	681	770	1	16			

There are 36 discrepancies between the modelled and reference sequences:

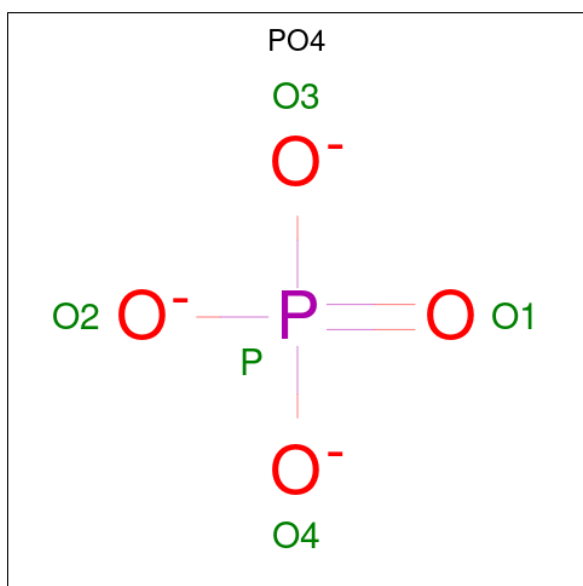
Chain	Residue	Modelled	Actual	Comment	Reference
1	1	MSE	MET	modified residue	UNP O29598
1	121	MSE	MET	modified residue	UNP O29598
1	139	MSE	MET	modified residue	UNP O29598
1	180	MSE	MET	modified residue	UNP O29598
1	281	MSE	MET	modified residue	UNP O29598
1	282	MSE	MET	modified residue	UNP O29598
1	315	MSE	MET	modified residue	UNP O29598
1	322	MSE	MET	modified residue	UNP O29598
1	354	MSE	MET	modified residue	UNP O29598
1	372	MSE	MET	modified residue	UNP O29598
1	387	MSE	MET	modified residue	UNP O29598
1	399	MSE	MET	modified residue	UNP O29598
1	446	MSE	MET	modified residue	UNP O29598
1	453	MSE	MET	modified residue	UNP O29598
1	468	MSE	MET	modified residue	UNP O29598
1	478	MSE	MET	modified residue	UNP O29598
1	504	MSE	MET	modified residue	UNP O29598
1	507	MSE	MET	modified residue	UNP O29598
2	1	MSE	MET	modified residue	UNP O29598
2	121	MSE	MET	modified residue	UNP O29598
2	139	MSE	MET	modified residue	UNP O29598
2	180	MSE	MET	modified residue	UNP O29598
2	281	MSE	MET	modified residue	UNP O29598
2	282	MSE	MET	modified residue	UNP O29598
2	315	MSE	MET	modified residue	UNP O29598

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Chain	Residue	Modelled	Actual	Comment	Reference
2	322	MSE	MET	modified residue	UNP O29598
2	354	MSE	MET	modified residue	UNP O29598
2	372	MSE	MET	modified residue	UNP O29598
2	387	MSE	MET	modified residue	UNP O29598
2	399	MSE	MET	modified residue	UNP O29598
2	446	MSE	MET	modified residue	UNP O29598
2	453	MSE	MET	modified residue	UNP O29598
2	468	MSE	MET	modified residue	UNP O29598
2	478	MSE	MET	modified residue	UNP O29598
2	504	MSE	MET	modified residue	UNP O29598
2	507	MSE	MET	modified residue	UNP O29598

- Molecule 2 is PHOSPHATE ION (CCD ID: PO4) (formula: O_4P).

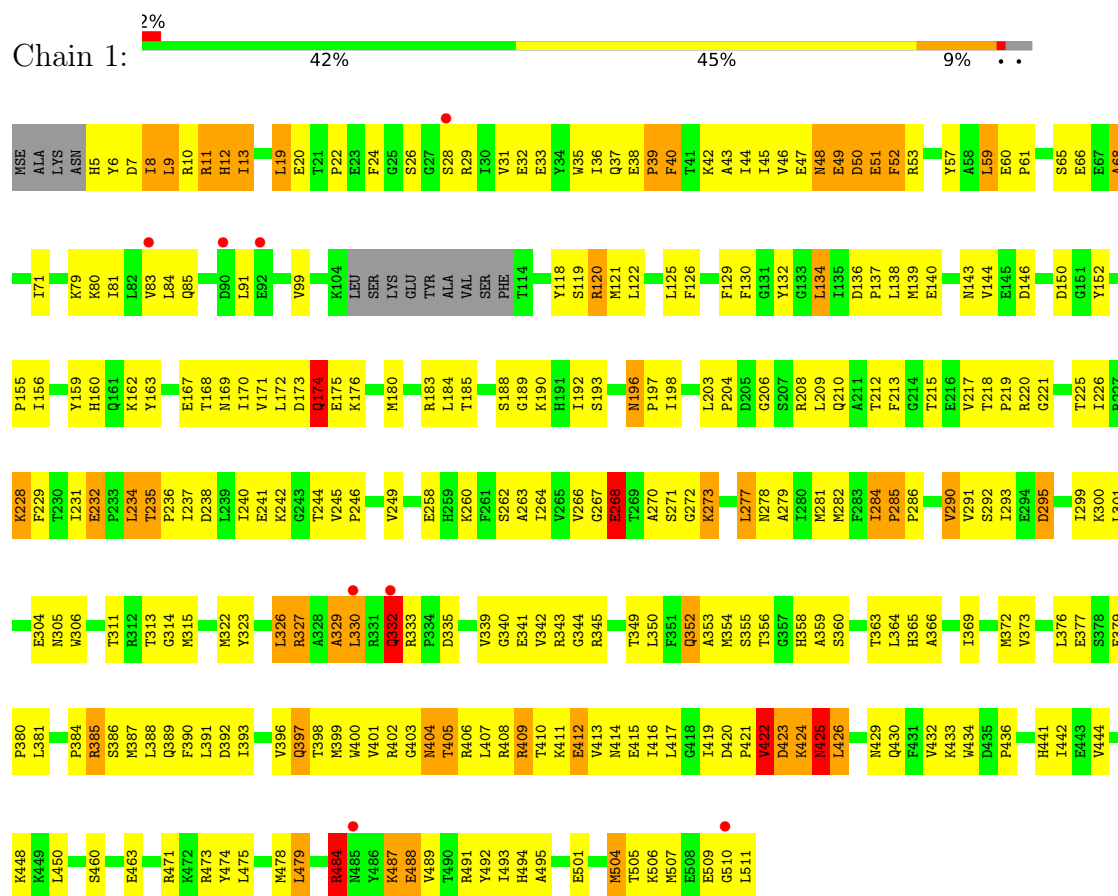


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	1	1	Total	O	P	0	0
			5	4	1		
2	2	1	Total	O	P	0	0
			5	4	1		
2	2	1	Total	O	P	0	0
			5	4	1		
2	2	1	Total	O	P	0	0
			5	4	1		

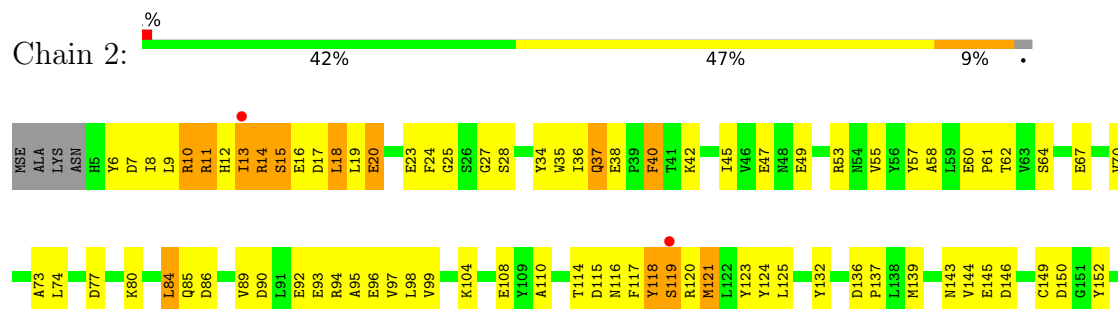
3 Residue-property plots

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: Type II secretion system protein



• Molecule 1: Type II secretion system protein



M446	P155	I226	T296	D369	M446
P447	I156	R227	R297	I369	P447
K449	F157	K228	E298	I370	K449
L450	I158	E232	I299	Q371	L450
E451	Y159	P233	K300	E379	E451
L457	H160	L234	I301	P380	L457
V461	Q161	L235	Y302	L381	V461
Y465	Y163	P236	H303	P384	Y465
D466	G164	I237	E304	M387	D466
E467	E167	D238	W306	I387	E467
M468	T168	L239	A308	D392	M468
L469	M169	I240	E309	I393	L469
S470	I170	E241	V310	A394	S470
R471	V171	T244	T311	L395	R471
K472	L172	V245	R312	T398	K472
R473	D173	L280	T313	M399	R473
L477	Q174	A251	G314	W400	L477
M478	E176	Y252	NSE	V401	M478
R484	K176	L253	GLY	T405	R484
M485	L177	W254	GLU	R406	M485
K486	M180	L255	E319	L407	K486
E488	R183	A256	I320	R408	E488
V489	L184	I257	D321	R409	V489
T490	T185	E258	M322	T410	T490
R491	Q186	K259	D324	K411	R491
Y492	R187	P261	L325	E412	Y492
I493	S188	S262	R326	E415	I493
H494	G189	A263	R327	L416	H494
A495	K190	I264	R331	L417	A495
Y496	H191	V265	Q332	Q418	Y496
Y497	I192	E268	R333	T419	Y497
R498	I194	T269	P334	D420	R498
E501	A195	A270	I338	P421	E501
L502	M196	S271	V339	V422	L502
M503	P197	G272	G340	D423	M503
M504	D200	K273	E341	K424	M504
T505	A201	T274	V342	N425	T505
K506	T202	T275	R345	L426	K506
M507	L203	T276	T349	L427	M507
E508	P204	L277	L350	V428	E508
E509	L209	N278	F351	N429	E509
G510	Q210	M281	Q352	Q430	G510
L511	A211	P283	A353	F431	L511
	T212	I284	M354	V432	
	T215	P285	Y361	K433	
	E216	P286	S362	W434	
	V217	D287	T363	K437	
	T218	A288	L364	E438	
	P219	K289	H365	D439	
	R220	V290	A366	K440	
	S223	D295	G367	V444	
				S445	

4 Data and refinement statistics

Property	Value	Source
Space group	H 3 2	Depositor
Cell constants a, b, c, α , β , γ	132.61Å 132.61Å 445.28Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	20.00 – 3.15 20.00 – 3.16	Depositor EDS
% Data completeness (in resolution range)	93.2 (20.00-3.15) 93.2 (20.00-3.16)	Depositor EDS
R_{merge}	0.12	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.67 (at 3.19Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.221 , 0.236 0.218 , 0.236	Depositor DCC
R_{free} test set	1248 reflections (4.81%)	wwPDB-VP
Wilson B-factor (Å ²)	64.6	Xtriage
Anisotropy	0.577	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 43.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	7997	wwPDB-VP
Average B, all atoms (Å ²)	60.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.64% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical 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

5.1 Standard geometry

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	1	0.59	2/3977 (0.1%)	1.08	26/5365 (0.5%)
1	2	0.55	0/4125	1.07	26/5560 (0.5%)
All	All	0.57	2/8102 (0.0%)	1.08	52/10925 (0.5%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	1	327	ARG	N-CA	6.93	1.55	1.46
1	1	270	ALA	CA-CB	6.38	1.63	1.53

The worst 5 of 52 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	1	330	LEU	N-CA-C	-10.55	99.58	111.82
1	1	404	ASN	N-CA-C	-10.42	100.52	113.02
1	1	335	ASP	N-CA-C	-8.91	100.72	111.69
1	2	36	ILE	N-CA-C	-8.37	102.71	111.58
1	1	424	LYS	N-CA-C	-8.03	93.70	110.80

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	1	3916	0	3816	287	0
1	2	4061	0	4040	285	0
2	1	5	0	0	1	0
2	2	15	0	0	9	0
All	All	7997	0	7856	561	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 35.

The worst 5 of 561 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)
1:1:180:MSE:HE2	1:1:184:LEU:HG	1.43	0.99
1:2:446:MSE:HG2	1:2:447:PRO:HD2	1.42	0.98
1:1:215:THR:HG22	1:1:221:GLY:HA2	1.47	0.95
1:2:180:MSE:HE2	1:2:184:LEU:HG	1.50	0.94
1:1:391:LEU:HD22	1:1:416:ILE:HD12	1.52	0.90

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	1	494/511 (97%)	417 (84%)	54 (11%)	23 (5%)	2	11
1	2	499/511 (98%)	441 (88%)	49 (10%)	9 (2%)	6	29
All	All	993/1022 (97%)	858 (86%)	103 (10%)	32 (3%)	3	17

5 of 32 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	1	11	ARG

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Mol	Chain	Res	Type
1	1	52	PHE
1	1	68	ALA
1	2	13	ILE
1	1	120	ARG

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	1	406/439 (92%)	372 (92%)	34 (8%)	10	33
1	2	444/439 (101%)	406 (91%)	38 (9%)	10	32
All	All	850/878 (97%)	778 (92%)	72 (8%)	10	33

5 of 72 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	2	311	THR
1	2	504	MSE
1	2	326	LEU
1	2	433	LYS
1	1	424	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 29 such sidechains are listed below:

Mol	Chain	Res	Type
1	2	174	GLN
1	2	441	HIS
1	2	278	ASN
1	2	414	ASN
1	2	259	HIS

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides 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	1	512	-	4,4,4	1.64	1 (25%)	6,6,6	0.81	0
2	PO4	2	512	-	4,4,4	1.78	1 (25%)	6,6,6	1.01	0
2	PO4	2	514	-	4,4,4	1.69	1 (25%)	6,6,6	1.04	0
2	PO4	2	513	-	4,4,4	1.42	1 (25%)	6,6,6	1.32	2 (33%)

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	2	512	PO4	P-O1	3.07	1.57	1.50
2	1	512	PO4	P-O1	2.76	1.57	1.50
2	2	514	PO4	P-O1	2.74	1.57	1.50
2	2	513	PO4	P-O1	2.23	1.55	1.50

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	2	513	PO4	O3-P-O2	2.17	114.65	107.91
2	2	513	PO4	O3-P-O1	-2.06	103.67	110.95

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

4 monomers are involved in 10 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	1	512	PO4	1	0
2	2	512	PO4	3	0
2	2	514	PO4	4	0
2	2	513	PO4	4	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, 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	1	481/511 (94%)	-0.11	8 (1%) 69 48	24, 58, 118, 127	0
1	2	487/511 (95%)	-0.22	4 (0%) 82 66	32, 56, 89, 104	0
All	All	968/1022 (94%)	-0.16	12 (1%) 76 57	24, 57, 110, 127	0

The worst 5 of 12 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	2	296	THR	3.1
1	1	28	SER	2.9
1	2	119	SER	2.7
1	1	90	ASP	2.4
1	1	330	LEU	2.4

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 oligosaccharides 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($\text{\AA}^2$)	Q<0.9
2	PO4	2	513	5/5	0.68	0.25	53,53,55,57	5
2	PO4	1	512	5/5	0.75	0.18	51,52,53,54	5
2	PO4	2	512	5/5	0.83	0.20	55,57,57,57	5
2	PO4	2	514	5/5	0.89	0.10	61,61,62,62	0

6.5 Other polymers [i](#)

There are no such residues in this entry.