Full wwPDB X-ray Structure Validation Report ⓘ

Aug 6, 2020 – 07:13 PM BST

PDB ID	:	6SXL
Title	:	Crystal structure of CrtE
Authors	:	Feng, Y.; Morgan, R.M.L.; Nixon, P.J.
Deposited on	:	2019-09-26
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*
A user guide is available at
https://www.wwpdb.org/validation/2017/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:

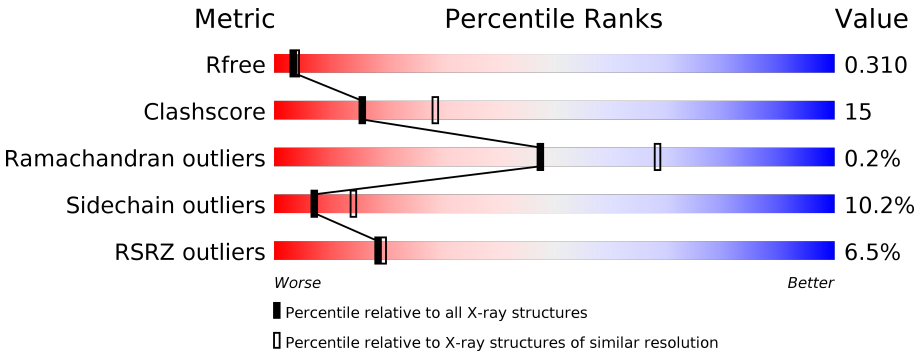
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.13.1
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.13.1

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 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}	130704	4661 (2.50-2.50)
Clashscore	141614	5346 (2.50-2.50)
Ramachandran outliers	138981	5231 (2.50-2.50)
Sidechain outliers	138945	5233 (2.50-2.50)
RSRZ outliers	127900	4559 (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 >=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	277	3% 75% 22% .
2	B	258	10% 69% 28% .

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 3963 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 Geranylgeranyl pyrophosphate synthase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	277	Total	C	N	O	S	0	0	0
			2036	1285	344	396	11			

There are 15 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	?	-	ALA	deletion	UNP B1XJV9
A	?	-	GLU	deletion	UNP B1XJV9
A	?	-	GLU	deletion	UNP B1XJV9
A	?	-	LEU	deletion	UNP B1XJV9
A	?	-	GLY	deletion	UNP B1XJV9
A	?	-	LYS	deletion	UNP B1XJV9
A	?	-	THR	deletion	UNP B1XJV9
A	?	-	ALA	deletion	UNP B1XJV9
A	?	-	GLY	deletion	UNP B1XJV9
A	?	-	LYS	deletion	UNP B1XJV9
A	?	-	ASP	deletion	UNP B1XJV9
A	?	-	LEU	deletion	UNP B1XJV9
A	?	-	GLU	deletion	UNP B1XJV9
A	?	-	ALA	deletion	UNP B1XJV9
A	?	-	GLN	deletion	UNP B1XJV9

- Molecule 2 is a protein called Geranylgeranyl pyrophosphate synthase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	258	Total	C	N	O	S	0	0	0
			1888	1191	322	364	11			

There are 33 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	19	ALA	GLU	conflict	UNP B1XJV9

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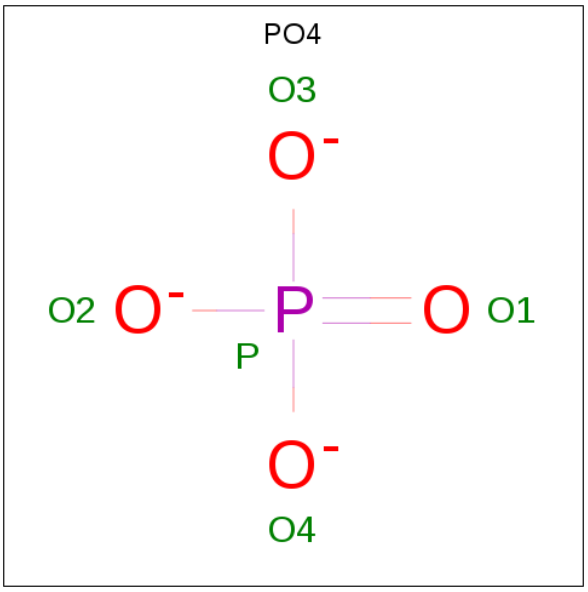
Chain	Residue	Modelled	Actual	Comment	Reference
B	?	-	LYS	deletion	UNP B1XJV9
B	?	-	THR	deletion	UNP B1XJV9
B	?	-	ASP	deletion	UNP B1XJV9
B	?	-	VAL	deletion	UNP B1XJV9
B	?	-	ALA	deletion	UNP B1XJV9
B	?	-	VAL	deletion	UNP B1XJV9
B	?	-	ALA	deletion	UNP B1XJV9
B	?	-	GLU	deletion	UNP B1XJV9
B	?	-	GLU	deletion	UNP B1XJV9
B	?	-	LEU	deletion	UNP B1XJV9
B	?	-	GLY	deletion	UNP B1XJV9
B	?	-	LYS	deletion	UNP B1XJV9
B	?	-	THR	deletion	UNP B1XJV9
B	?	-	ALA	deletion	UNP B1XJV9
B	?	-	GLY	deletion	UNP B1XJV9
B	?	-	LYS	deletion	UNP B1XJV9
B	?	-	ASP	deletion	UNP B1XJV9
B	?	-	LEU	deletion	UNP B1XJV9
B	?	-	GLU	deletion	UNP B1XJV9
B	?	-	ALA	deletion	UNP B1XJV9
B	?	-	GLN	deletion	UNP B1XJV9
B	?	-	LYS	deletion	UNP B1XJV9
B	?	-	VAL	deletion	UNP B1XJV9
B	?	-	THR	deletion	UNP B1XJV9
B	?	-	TYR	deletion	UNP B1XJV9
B	?	-	PRO	deletion	UNP B1XJV9
B	?	-	SER	deletion	UNP B1XJV9
B	?	-	LEU	deletion	UNP B1XJV9
B	?	-	TRP	deletion	UNP B1XJV9
B	?	-	GLY	deletion	UNP B1XJV9
B	?	-	ILE	deletion	UNP B1XJV9
B	?	-	LEU	deletion	UNP B1XJV9

- Molecule 3 is PHOSPHATE ION (three-letter code: PO4) (formula: O_4P).



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

- Molecule 4 is water.

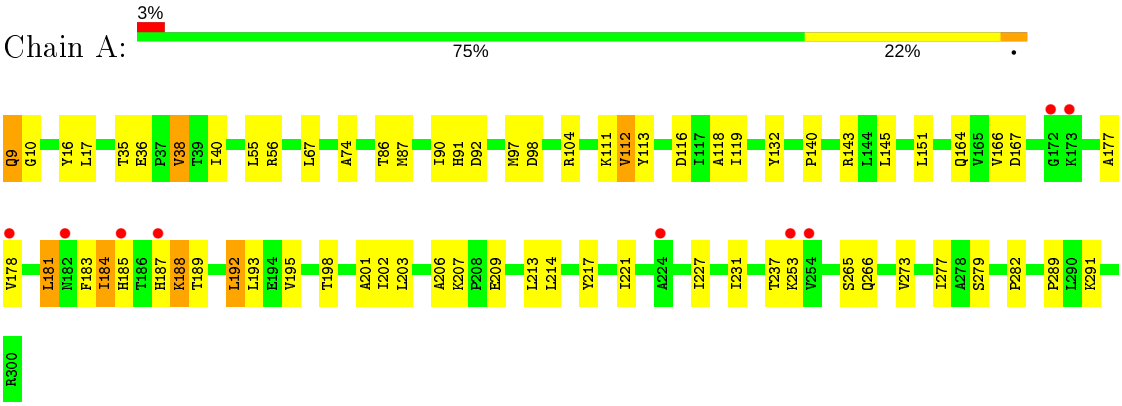
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	19	Total O 19 19	0	0
4	B	10	Total O 10 10	0	0

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.

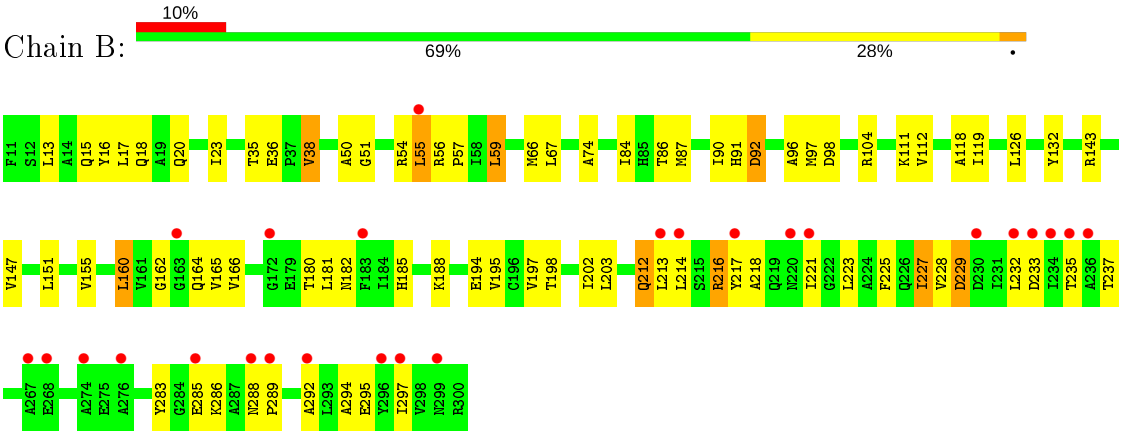
- Molecule 1: Geranylgeranyl pyrophosphate synthase

Chain A:



- Molecule 2: Geranylgeranyl pyrophosphate synthase

Chain B:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	70.20Å 89.47Å 107.32Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	68.82 – 2.50 68.72 – 2.50	Depositor EDS
% Data completeness (in resolution range)	99.9 (68.82-2.50) 100.0 (68.72-2.50)	Depositor EDS
R_{merge}	0.03	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.27 (at 2.51Å)	Xtriage
Refinement program	REFMAC 5.8.0258	Depositor
R, R_{free}	0.243 , 0.306 0.245 , 0.310	Depositor DCC
R_{free} test set	1205 reflections (5.02%)	wwPDB-VP
Wilson B-factor (Å^2)	55.3	Xtriage
Anisotropy	0.568	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.32 , 56.3	EDS
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	3963	wwPDB-VP
Average B, all atoms (Å^2)	77.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.36% 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

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	A	0.41	0/2060	0.77	0/2799
2	B	0.38	0/1910	0.79	1/2596 (0.0%)
All	All	0.39	0/3970	0.78	1/5395 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	229	ASP	CB-CA-C	5.18	120.76	110.40

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	2036	0	2015	61	0
2	B	1888	0	1871	56	0
3	A	5	0	0	0	0
3	B	5	0	0	0	0
4	A	19	0	0	4	0
4	B	10	0	0	1	0
All	All	3963	0	3886	115	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 15.

All (115) 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:B:13:LEU:HD13	2:B:292:ALA:HB3	1.44	0.98
1:A:167:ASP:HA	1:A:185:HIS:NE2	1.91	0.86
1:A:213:LEU:HD11	1:A:279:SER:HB2	1.60	0.83
1:A:56:ARG:HG2	1:A:192:LEU:HD11	1.61	0.83
2:B:198:THR:O	2:B:202:ILE:HG13	1.85	0.76
1:A:198:THR:O	1:A:202:ILE:HG13	1.90	0.72
2:B:51:GLY:HA3	2:B:104:ARG:NH2	2.04	0.72
2:B:197:VAL:CG1	2:B:214:LEU:HB3	2.19	0.71
2:B:228:VAL:O	2:B:232:LEU:HB2	1.91	0.70
2:B:228:VAL:HG12	2:B:229:ASP:OD1	1.93	0.69
2:B:213:LEU:O	2:B:216:ARG:HG3	1.93	0.69
2:B:217:TYR:HE1	2:B:294:ALA:HB2	1.58	0.68
2:B:35:THR:HG22	2:B:36:GLU:N	2.08	0.68
1:A:56:ARG:CG	1:A:192:LEU:HD11	2.24	0.67
2:B:194:GLU:HA	2:B:218:ALA:CB	2.24	0.67
2:B:13:LEU:HD22	2:B:292:ALA:HB1	1.76	0.66
2:B:197:VAL:HG11	2:B:214:LEU:HB3	1.77	0.66
2:B:13:LEU:HB2	2:B:292:ALA:CB	2.27	0.65
2:B:13:LEU:CD1	2:B:292:ALA:HB3	2.24	0.65
1:A:167:ASP:HB2	1:A:185:HIS:HD2	1.63	0.64
2:B:38:VAL:HG13	4:B:502:HOH:O	1.95	0.64
2:B:35:THR:HG22	2:B:36:GLU:H	1.62	0.63
1:A:201:ALA:HB2	1:A:214:LEU:HD12	1.80	0.62
2:B:51:GLY:HA3	2:B:104:ARG:HH21	1.63	0.61
1:A:67:LEU:HD12	1:A:201:ALA:HA	1.80	0.61
2:B:194:GLU:HA	2:B:218:ALA:HB1	1.82	0.61
1:A:167:ASP:HB2	1:A:185:HIS:CD2	2.34	0.61
2:B:212:GLN:OE1	2:B:216:ARG:NH2	2.33	0.61
1:A:56:ARG:HE	1:A:192:LEU:HD13	1.66	0.60
1:A:167:ASP:CA	1:A:185:HIS:NE2	2.65	0.59
1:A:188:LYS:O	1:A:189:THR:HG21	2.03	0.59
1:A:192:LEU:HG	1:A:193:LEU:N	2.18	0.59
2:B:217:TYR:CE1	2:B:294:ALA:HB2	2.37	0.58
2:B:221:ILE:HG23	2:B:297:ILE:HG21	1.85	0.58
1:A:104:ARG:HD2	4:A:511:HOH:O	2.02	0.58
1:A:56:ARG:CD	1:A:192:LEU:HD11	2.33	0.58
2:B:283:TYR:CB	2:B:286:LYS:HB2	2.33	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:13:LEU:HB2	2:B:292:ALA:HB3	1.85	0.58
2:B:151:LEU:O	2:B:155:VAL:HG23	2.04	0.57
1:A:209:GLU:H	1:A:209:GLU:CD	2.07	0.57
1:A:140:PRO:HG2	1:A:143:ARG:HD2	1.86	0.57
1:A:74:ALA:HA	1:A:203:LEU:HD13	1.87	0.57
2:B:285:GLU:O	2:B:288:ASN:HB2	2.05	0.56
1:A:56:ARG:CD	1:A:192:LEU:CD1	2.83	0.56
2:B:84:ILE:HD13	2:B:155:VAL:HG21	1.87	0.56
2:B:16:TYR:CE2	2:B:289:PRO:HB3	2.41	0.55
2:B:221:ILE:HD13	2:B:297:ILE:CD1	2.37	0.55
1:A:67:LEU:HD13	1:A:206:ALA:HB2	1.88	0.55
1:A:178:VAL:HB	1:A:181:LEU:HB2	1.89	0.55
2:B:160:LEU:O	2:B:160:LEU:HD12	2.07	0.55
1:A:183:PHE:O	1:A:187:HIS:HB2	2.06	0.54
2:B:221:ILE:HD13	2:B:297:ILE:HD13	1.88	0.54
2:B:74:ALA:HA	2:B:203:LEU:HD13	1.89	0.54
1:A:184:ILE:HG23	4:A:513:HOH:O	2.07	0.53
1:A:178:VAL:HG11	1:A:181:LEU:HD12	1.90	0.53
2:B:50:ALA:O	2:B:54:ARG:NH2	2.42	0.53
1:A:188:LYS:O	1:A:189:THR:CG2	2.56	0.53
1:A:56:ARG:NE	1:A:192:LEU:CD1	2.71	0.53
2:B:197:VAL:HG12	2:B:214:LEU:HB3	1.91	0.52
1:A:184:ILE:CG2	4:A:513:HOH:O	2.58	0.51
2:B:13:LEU:HD22	2:B:292:ALA:CB	2.40	0.51
2:B:223:LEU:O	2:B:227:ILE:HD13	2.11	0.50
2:B:55:LEU:O	2:B:59:LEU:HD12	2.12	0.49
1:A:273:VAL:HG12	1:A:277:ILE:HD12	1.93	0.49
1:A:92:ASP:O	1:A:97:MET:HB2	2.12	0.49
2:B:66:MET:HG2	2:B:67:LEU:HD23	1.94	0.49
1:A:56:ARG:NE	1:A:192:LEU:HD13	2.27	0.49
1:A:35:THR:HG22	1:A:36:GLU:N	2.28	0.49
2:B:35:THR:CG2	2:B:36:GLU:N	2.75	0.48
2:B:214:LEU:O	2:B:217:TYR:HB3	2.13	0.48
2:B:92:ASP:OD1	2:B:164:GLN:NE2	2.46	0.48
1:A:16:TYR:CE2	1:A:289:PRO:HB3	2.49	0.47
2:B:160:LEU:HD12	2:B:160:LEU:C	2.34	0.47
2:B:111:LYS:HA	2:B:111:LYS:HD2	1.67	0.47
1:A:35:THR:CG2	1:A:36:GLU:N	2.77	0.47
1:A:56:ARG:HE	1:A:192:LEU:CD1	2.27	0.46
1:A:92:ASP:OD2	1:A:164:GLN:NE2	2.48	0.46
1:A:231:ILE:HD11	1:A:265:SER:HB3	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:20:GLN:HA	2:B:20:GLN:OE1	2.15	0.46
2:B:35:THR:CG2	2:B:36:GLU:H	2.26	0.46
1:A:214:LEU:O	1:A:217:TYR:HB3	2.16	0.45
1:A:227:ILE:O	1:A:231:ILE:HG13	2.15	0.45
1:A:277:ILE:HG23	1:A:291:LYS:HG2	1.98	0.45
1:A:166:VAL:CG1	1:A:181:LEU:HD23	2.47	0.45
2:B:143:ARG:O	2:B:147:VAL:HG23	2.16	0.45
2:B:86:THR:O	2:B:90:ILE:HG13	2.17	0.45
1:A:56:ARG:NE	1:A:192:LEU:HD11	2.32	0.45
1:A:86:THR:O	1:A:90:ILE:HG13	2.16	0.45
1:A:112:VAL:HG22	1:A:113:TYR:CE2	2.53	0.44
2:B:16:TYR:CE1	2:B:289:PRO:HG3	2.52	0.44
1:A:36:GLU:OE1	1:A:38:VAL:HG12	2.17	0.44
1:A:97:MET:HB2	1:A:98:ASP:H	1.62	0.44
1:A:217:TYR:O	1:A:221:ILE:HD12	2.17	0.44
1:A:112:VAL:HG22	1:A:113:TYR:CD2	2.53	0.43
1:A:35:THR:CG2	1:A:36:GLU:H	2.31	0.43
2:B:91:HIS:O	2:B:97:MET:HG3	2.18	0.43
1:A:214:LEU:HA	1:A:214:LEU:HD23	1.78	0.43
1:A:111:LYS:HD2	1:A:111:LYS:HA	1.63	0.43
2:B:56:ARG:N	2:B:57:PRO:HD2	2.34	0.43
1:A:118:ALA:O	1:A:119:ILE:C	2.56	0.42
2:B:185:HIS:C	2:B:185:HIS:CD2	2.93	0.42
1:A:177:ALA:H	1:A:253:LYS:HA	1.84	0.42
1:A:91:HIS:O	1:A:97:MET:HG3	2.19	0.42
2:B:162:GLY:O	2:B:166:VAL:HG23	2.21	0.41
1:A:9:GLN:HG2	1:A:10:GLY:H	1.85	0.41
1:A:40:ILE:HB	2:B:165:VAL:HG21	2.02	0.41
2:B:87:MET:HG2	2:B:126:LEU:HB2	2.03	0.41
1:A:116:ASP:HB3	2:B:96:ALA:O	2.21	0.41
2:B:104:ARG:HH11	2:B:104:ARG:HG2	1.85	0.41
1:A:192:LEU:O	1:A:195:VAL:HG12	2.20	0.41
2:B:118:ALA:O	2:B:119:ILE:C	2.58	0.41
1:A:17:LEU:HB3	4:A:514:HOH:O	2.20	0.40
1:A:56:ARG:HD3	1:A:192:LEU:CD1	2.51	0.40
1:A:188:LYS:O	1:A:189:THR:HB	2.21	0.40
1:A:209:GLU:N	1:A:209:GLU:CD	2.75	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	271/277 (98%)	257 (95%)	13 (5%)	1 (0%)	34 54
2	B	250/258 (97%)	230 (92%)	20 (8%)	0	100 100
All	All	521/535 (97%)	487 (94%)	33 (6%)	1 (0%)	47 68

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	282	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	203/220 (92%)	188 (93%)	15 (7%)	13 27
2	B	188/203 (93%)	163 (87%)	25 (13%)	4 7
All	All	391/423 (92%)	351 (90%)	40 (10%)	7 14

All (40) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	9	GLN
1	A	38	VAL
1	A	55	LEU
1	A	87	MET
1	A	112	VAL

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Mol	Chain	Res	Type
1	A	132	TYR
1	A	145	LEU
1	A	151	LEU
1	A	181	LEU
1	A	184	ILE
1	A	188	LYS
1	A	192	LEU
1	A	207	LYS
1	A	237	THR
1	A	266	GLN
2	B	15	GLN
2	B	17	LEU
2	B	18	GLN
2	B	23	ILE
2	B	38	VAL
2	B	55	LEU
2	B	59	LEU
2	B	92	ASP
2	B	98	ASP
2	B	112	VAL
2	B	132	TYR
2	B	160	LEU
2	B	180	THR
2	B	181	LEU
2	B	182	ASN
2	B	188	LYS
2	B	195	VAL
2	B	212	GLN
2	B	216	ARG
2	B	225	PHE
2	B	227	ILE
2	B	233	ASP
2	B	235	THR
2	B	237	THR
2	B	295	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	15	GLN
2	B	185	HIS

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 monosaccharides in this entry.

5.6 Ligand geometry

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	PO4	B	401	-	4,4,4	0.61	0	6,6,6	0.62	0
3	PO4	A	401	-	4,4,4	0.74	0	6,6,6	0.47	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

There are no such residues in this entry.

5.8 Polymer linkage issues

The following chains have linkage breaks:

Mol	Chain	Number of breaks
2	B	3
1	A	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	B	237:THR	C	263:GLU	N	19.74
1	A	237:THR	C	253:LYS	N	15.62
1	B	172:GLY	C	179:GLU	N	12.91
1	B	279:SER	C	281:GLU	N	7.31

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^{th} 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	277/277 (100%)	0.19	9 (3%) 47 51	36, 58, 116, 160	0
2	B	258/258 (100%)	0.70	26 (10%) 7 6	38, 82, 161, 211	1 (0%)
All	All	535/535 (100%)	0.44	35 (6%) 18 19	36, 69, 143, 211	1 (0%)

All (35) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	236	ALA	8.9
2	B	172	GLY	7.8
2	B	230	ASP	7.0
2	B	235	THR	5.2
2	B	288	ASN	5.0
2	B	292	ALA	4.9
2	B	267	ALA	4.8
1	A	182	ASN	4.3
2	B	297	ILE	4.3
2	B	234	ILE	3.8
2	B	221	ILE	3.6
2	B	214	LEU	3.6
2	B	276	ALA	3.5
1	A	254	VAL	3.4
2	B	299	ASN	3.3
2	B	268	GLU	3.2
1	A	187	HIS	3.2
2	B	285	GLU	3.1
1	A	172	GLY	3.1
2	B	217	TYR	3.1
1	A	253	LYS	2.9
2	B	213	LEU	2.8
1	A	224	ALA	2.7
2	B	274	ALA	2.7

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Mol	Chain	Res	Type	RSRZ
2	B	220	ASN	2.6
2	B	232	LEU	2.6
1	A	178	VAL	2.4
2	B	296	TYR	2.2
1	A	185	HIS	2.2
2	B	55	LEU	2.2
2	B	289	PRO	2.1
2	B	233	ASP	2.0
2	B	183	PHE	2.0
2	B	163	GLY	2.0
1	A	173	LYS	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, 95^{th} 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
3	PO4	A	401	5/5	0.85	0.14	99,115,125,135	0
3	PO4	B	401	5/5	0.86	0.17	102,103,115,120	0

6.5 Other polymers (i)

There are no such residues in this entry.