



Full wwPDB X-ray Structure Validation Report ⓘ

May 7, 2026 – 07:55 AM EDT

PDB ID : 6SXL / pdb_00006sxl
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 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

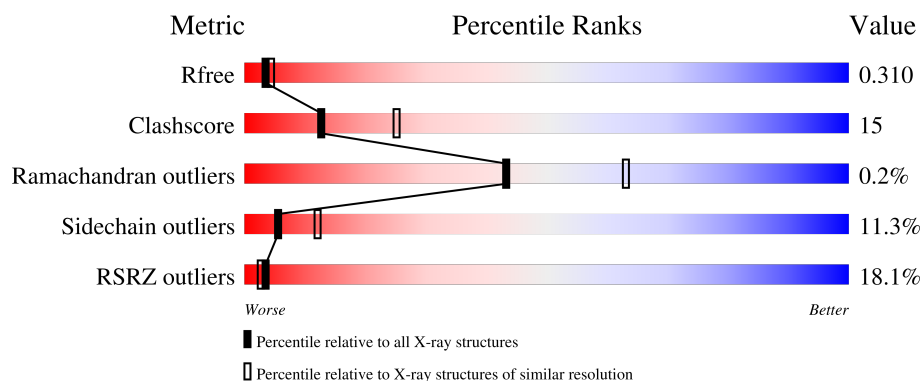
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 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}	180053	5829 (2.50-2.50)
Clashscore	190562	6492 (2.50-2.50)
Ramachandran outliers	187476	6378 (2.50-2.50)
Sidechain outliers	187428	6380 (2.50-2.50)
RSRZ outliers	180081	5833 (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 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	A	277	8% 75% 22% .
2	B	258	29% 67% 29% .

2 Entry composition [i](#)

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:

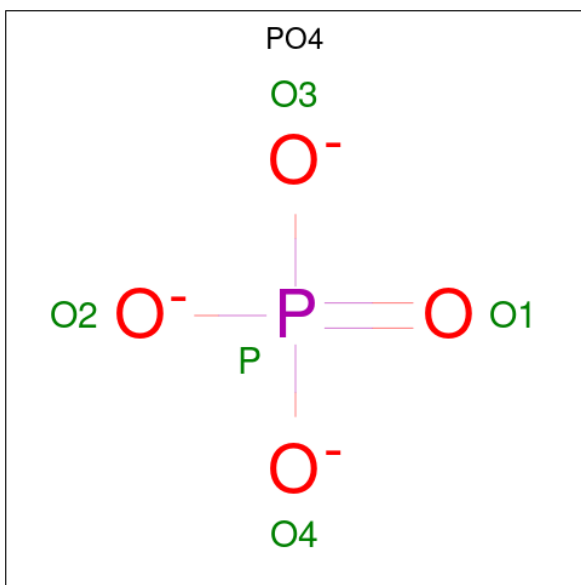
Chain	Residue	Modelled	Actual	Comment	Reference
B	19	ALA	GLU	conflict	UNP B1XJV9

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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 (CCD ID: PO4) (formula: O₄P).



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

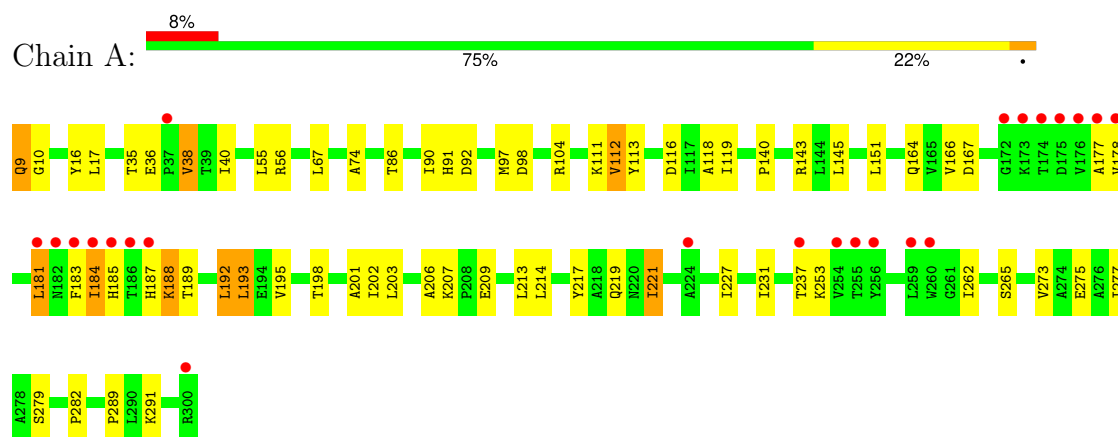
- Molecule 4 is water.

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

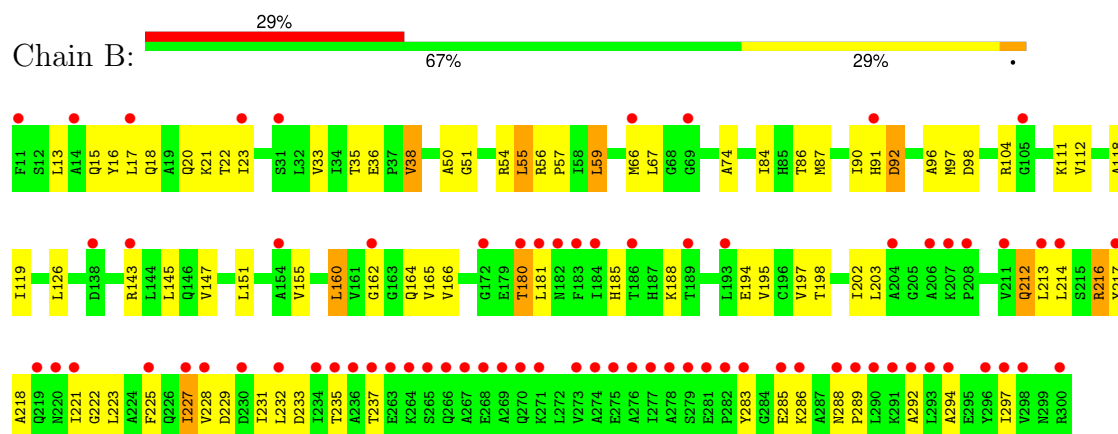
3 Residue-property plots

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: Geranylgeranyl pyrophosphate synthase



- Molecule 2: Geranylgeranyl pyrophosphate synthase



4 Data and refinement statistics

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) 99.9 (68.72-2.50)	Depositor EDS
R_{merge}	0.03	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ 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 (4.86%)	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)	0.33 , 55.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.34$	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.*

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	A	0.60	0/2060	1.21	0/2799
2	B	0.56	0/1910	1.21	1/2596 (0.0%)
All	All	0.58	0/3970	1.21	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(°)	Ideal(°)
2	B	180	THR	CA-CB-OG1	-5.04	102.04	109.60

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	62	0
2	B	1888	0	1871	59	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	119	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 (119) 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:66:MET:HE2	2:B:67:LEU:HD21	1.61	0.82
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
1:A:209:GLU:H	1:A:209:GLU:CD	2.07	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:56:ARG:CD	1:A:192:LEU:HD11	2.33	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:104:ARG:HD2	4:A:511:HOH:O	2.02	0.58
2:B:13:LEU:HB2	2:B:292:ALA:HB3	1.85	0.58
2:B:283:TYR:CB	2:B:286:LYS:HB2	2.33	0.58
2:B:151:LEU:O	2:B:155:VAL:HG23	2.04	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:HD12	2:B:160:LEU:O	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:56:ARG:NE	1:A:192:LEU:CD1	2.71	0.53
1:A:188:LYS:O	1:A:189:THR:CG2	2.56	0.53
2:B:160:LEU:HD12	2:B:160:LEU:C	2.34	0.52
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
1:A:118:ALA:O	1:A:119:ILE:C	2.56	0.47
2:B:111:LYS:HA	2:B:111:LYS:HD2	1.67	0.47
2:B:185:HIS:CD2	2:B:185:HIS:C	2.93	0.47
1:A:35:THR:CG2	1:A:36:GLU:N	2.77	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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
2:B:118:ALA:O	2:B:119:ILE:C	2.58	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:86:THR:O	2:B:90:ILE:HG13	2.17	0.45
2:B:143:ARG:O	2:B:147:VAL:HG23	2.16	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:209:GLU:CD	1:A:209:GLU:N	2.75	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:35:THR:CG2	1:A:36:GLU:H	2.31	0.43
1:A:112:VAL:HG22	1:A:113:TYR:CD2	2.53	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:HA	1:A:111:LYS:HD2	1.63	0.43
1:A:188:LYS:C	1:A:189:THR:HB	2.43	0.43
2:B:56:ARG:N	2:B:57:PRO:HD2	2.34	0.43
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
1:A:116:ASP:HB3	2:B:96:ALA:O	2.21	0.41
2:B:87:MET:HG2	2:B:126:LEU:HB2	2.03	0.41
2:B:104:ARG:HG2	2:B:104:ARG:HH11	1.85	0.41
1:A:192:LEU:O	1:A:195:VAL:HG12	2.20	0.41
2:B:13:LEU:HD22	2:B:292:ALA:C	2.45	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
2:B:221:ILE:O	2:B:222:GLY:C	2.64	0.40
1:A:188:LYS:O	1:A:189:THR:HB	2.21	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%)	30	49
2	B	250/258 (97%)	230 (92%)	20 (8%)	0	100	100
All	All	521/535 (97%)	487 (94%)	33 (6%)	1 (0%)	43	63

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%)	186 (92%)	17 (8%)	10	22
2	B	188/203 (93%)	161 (86%)	27 (14%)	3	6
All	All	391/423 (92%)	347 (89%)	44 (11%)	5	12

All (44) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	9	GLN
1	A	38	VAL

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Mol	Chain	Res	Type
1	A	55	LEU
1	A	112	VAL
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	193	LEU
1	A	207	LYS
1	A	219	GLN
1	A	221	ILE
1	A	237	THR
1	A	262	ILE
1	A	275	GLU
2	B	15	GLN
2	B	17	LEU
2	B	18	GLN
2	B	21	LYS
2	B	22	THR
2	B	23	ILE
2	B	33	VAL
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	145	LEU
2	B	160	LEU
2	B	180	THR
2	B	181	LEU
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	231	ILE
2	B	233	ASP
2	B	235	THR
2	B	237	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	146	GLN
1	A	270	GLN
2	B	109	ASN
2	B	185	HIS
2	B	187	HIS

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 oligosaccharides 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	PO4	A	401	-	4,4,4	0.79	0	6,6,6	0.51	0
3	PO4	B	401	-	4,4,4	0.66	0	6,6,6	0.65	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](#)

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, 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	277/277 (100%)	0.27	23 (8%)	17 15	36, 58, 116, 160	0
2	B	258/258 (100%)	1.41	74 (28%)	1 1	38, 82, 161, 211	1 (0%)
All	All	535/535 (100%)	0.82	97 (18%)	3 3	36, 69, 143, 211	1 (0%)

All (97) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	297	ILE	5.7
2	B	267	ALA	5.4
2	B	276	ALA	5.2
2	B	279	SER	5.2
2	B	208	PRO	4.9
2	B	66	MET	4.8
2	B	290	LEU	4.8
2	B	17	LEU	4.8
2	B	214	LEU	4.7
2	B	232	LEU	4.5
2	B	221	ILE	4.4
1	A	182	ASN	4.4
2	B	11	PHE	4.3
2	B	189	THR	4.3
2	B	282	PRO	4.3
1	A	260	TRP	4.1
2	B	275	GLU	4.0
2	B	138	ASP	3.9
2	B	213	LEU	3.9
2	B	265	SER	3.9
2	B	288	ASN	3.8
2	B	283	TYR	3.7
2	B	220	ASN	3.7
2	B	292	ALA	3.6

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Mol	Chain	Res	Type	RSRZ
1	A	184	ILE	3.6
1	A	177	ALA	3.6
2	B	186	THR	3.5
2	B	217	TYR	3.5
2	B	294	ALA	3.5
2	B	14	ALA	3.4
2	B	236	ALA	3.4
1	A	175	ASP	3.4
1	A	178	VAL	3.3
2	B	291	LYS	3.3
2	B	273	VAL	3.3
2	B	235	THR	3.3
2	B	269	ALA	3.3
2	B	225	PHE	3.2
2	B	293	LEU	3.2
2	B	184	ILE	3.2
2	B	296	TYR	3.1
2	B	278	ALA	3.1
2	B	274	ALA	3.0
1	A	173	LYS	2.9
2	B	230	ASP	2.9
1	A	187	HIS	2.9
1	A	254	VAL	2.9
1	A	259	LEU	2.9
2	B	211	VAL	2.9
2	B	237	THR	2.9
2	B	289	PRO	2.8
2	B	234	ILE	2.8
2	B	298	VAL	2.8
1	A	185	HIS	2.8
1	A	255	THR	2.8
2	B	105	GLY	2.8
1	A	176	VAL	2.8
2	B	193	LEU	2.7
1	A	186	THR	2.7
1	A	237	THR	2.7
2	B	263	GLU	2.7
2	B	206	ALA	2.7
2	B	204	ALA	2.7
2	B	219	GLN	2.7
2	B	266	GLN	2.6
2	B	69	GLY	2.5

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Mol	Chain	Res	Type	RSRZ
2	B	277	ILE	2.5
2	B	228	VAL	2.5
2	B	227	ILE	2.5
1	A	181	LEU	2.5
2	B	143	ARG	2.5
2	B	264	LYS	2.5
1	A	300	ARG	2.5
2	B	183	PHE	2.4
1	A	224	ALA	2.4
2	B	31	SER	2.4
2	B	172	GLY	2.4
1	A	37	PRO	2.4
1	A	174	THR	2.3
2	B	281	GLU	2.3
2	B	268	GLU	2.3
2	B	162	GLY	2.3
2	B	286	LYS	2.2
2	B	91	HIS	2.2
2	B	182	ASN	2.2
2	B	154	ALA	2.2
2	B	207	LYS	2.2
2	B	180	THR	2.1
2	B	181	LEU	2.1
2	B	285	GLU	2.1
2	B	300	ARG	2.1
2	B	271	LYS	2.1
1	A	183	PHE	2.1
2	B	270	GLN	2.1
2	B	23	ILE	2.0
1	A	256	TYR	2.0
1	A	172	GLY	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 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(Å ²)	Q<0.9
3	PO4	A	401	5/5	0.61	0.13	99,115,125,135	0
3	PO4	B	401	5/5	0.76	0.11	102,103,115,120	0

6.5 Other polymers [i](#)

There are no such residues in this entry.