



# Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 08:52 PM UTC

PDB ID : 2FPP / pdb\_00002fpp  
Title : Crystal structure of pig GTP-specific succinyl-CoA synthetase from polyethylene glycol with chloride ions  
Authors : Fraser, M.E.; Hayakawa, K.; Hume, M.S.; Ryan, D.G.; Brownie, E.R.  
Deposited on : 2006-01-16  
Resolution : 2.35 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

<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>.

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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

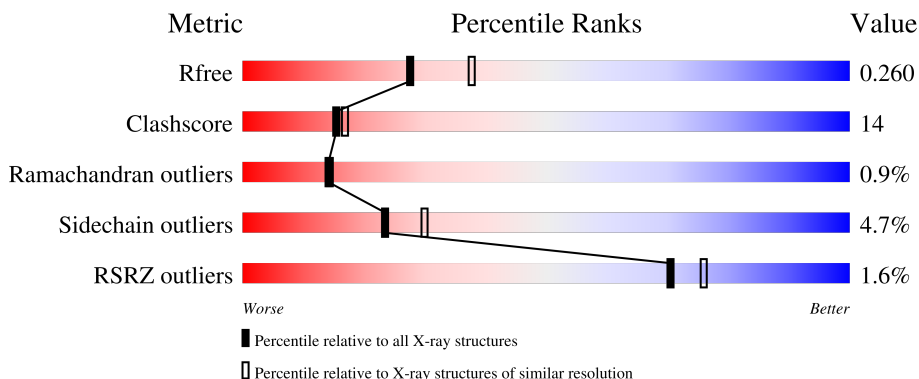
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*


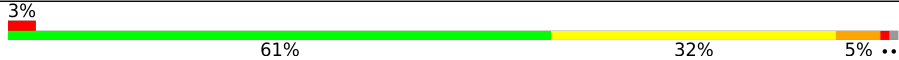
The reported resolution of this entry is 2.35 Å.

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	1596 (2.36-2.36)
Clashscore	190562	1663 (2.36-2.36)
Ramachandran outliers	187476	1646 (2.36-2.36)
Sidechain outliers	187428	1646 (2.36-2.36)
RSRZ outliers	180081	1598 (2.36-2.36)

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  $\geq 3$ , 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	305	 74% 24% .
2	B	395	 3% 61% 32% 5% ..

## 2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 5367 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 Succinyl-CoA ligase [GDP-forming] alpha-chain, mitochondrial.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace	
			Total	C	N	O	P				S
1	A	305	2255	1418	400	425	1	11	0	0	0

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	2	SER	-	cloning artifact	UNP O19069-2
A	259	NEP	HIS	modified residue	UNP O19069-2

- Molecule 2 is a protein called Succinyl-CoA ligase [GDP-forming] beta-chain, mitochondrial.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	B	393	2970	1876	502	578	14	0	0	0

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	1	MET	-	initiating methionine	UNP P53590

- Molecule 3 is SULFATE ION (CCD ID: SO4) (formula: O<sub>4</sub>S).



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

- Molecule 4 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total Cl 1 1	0	0

- Molecule 5 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	77	Total O 77 77	0	0
5	B	49	Total O 49 49	0	0



## 4 Data and refinement statistics i

Property	Value	Source
Space group	P 65	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	123.41Å 123.41Å 84.86Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	100.00 – 2.35 100.00 – 2.35	Depositor EDS
% Data completeness (in resolution range)	87.8 (100.00-2.35) 87.8 (100.00-2.35)	Depositor EDS
$R_{merge}$	0.11	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	4.50 (at 2.33Å)	Xtrriage
Refinement program	CNS	Depositor
R, $R_{free}$	0.192 , 0.259 0.191 , 0.260	Depositor DCC
$R_{free}$ test set	1074 reflections (3.97%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	29.9	Xtrriage
Anisotropy	0.037	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.35 , 39.1	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtrriage
Estimated twinning fraction	0.049 for h,-h-k,-l	Xtrriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	5367	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	31.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.69% 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, 0.333 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: CL, NEP, SO4

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	1.03	1/2281 (0.0%)	1.33	26/3081 (0.8%)
2	B	0.91	1/3007 (0.0%)	1.26	26/4059 (0.6%)
All	All	0.96	2/5288 (0.0%)	1.29	52/7140 (0.7%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	104	MET	SD-CE	-5.15	1.66	1.79
1	A	101	VAL	CA-CB	-5.09	1.47	1.53

All (52) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	201	THR	N-CA-C	-10.56	100.13	113.23
2	B	161	GLY	N-CA-C	-9.79	102.06	112.04
2	B	373	LEU	N-CA-C	-8.20	97.55	110.10
1	A	18	VAL	N-CA-C	8.09	120.13	108.48
2	B	366	ASN	N-CA-C	-7.81	101.17	111.24
2	B	293	PHE	N-CA-C	-7.57	97.06	109.40
1	A	82	PRO	N-CA-C	7.37	119.69	110.70
1	A	97	VAL	N-CA-C	-7.26	101.84	108.95
2	B	246	GLU	CA-C-N	7.09	128.70	119.84
2	B	246	GLU	C-N-CA	7.09	128.70	119.84
2	B	280	CYS	N-CA-C	-7.08	103.56	111.28
1	A	157	GLY	N-CA-C	-7.07	99.11	111.62
2	B	197	LYS	N-CA-C	6.98	118.89	111.28
1	A	231	LYS	N-CA-C	-6.80	103.80	111.07
1	A	22	GLY	N-CA-C	-6.80	103.94	115.08
2	B	219	PHE	N-CA-C	6.57	118.44	111.28
2	B	262	LEU	N-CA-C	-6.55	100.26	109.69

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	78	ILE	N-CA-C	6.36	117.02	107.80
1	A	145	ILE	N-CA-C	6.33	117.55	111.91
1	A	155	ARG	N-CA-C	6.29	121.73	113.30
2	B	202	GLN	N-CA-C	6.28	117.94	108.46
1	A	58	LEU	CA-C-N	6.24	126.00	119.76
1	A	58	LEU	C-N-CA	6.24	126.00	119.76
1	A	187	GLY	N-CA-C	6.16	121.93	112.81
1	A	233	HIS	N-CA-C	6.12	121.68	113.72
2	B	305	VAL	N-CA-C	-6.07	103.50	111.09
1	A	160	SER	N-CA-C	5.92	118.29	108.99
1	A	51	GLY	N-CA-C	-5.92	104.44	111.36
1	A	89	ILE	N-CA-C	-5.88	105.00	110.53
2	B	194	LEU	N-CA-C	-5.74	105.11	111.36
1	A	145	ILE	CB-CA-C	-5.68	105.65	112.19
2	B	332	CYS	N-CA-C	5.65	122.83	110.80
1	A	179	GLY	N-CA-C	5.61	119.95	112.65
2	B	391	SER	N-CA-C	5.59	118.91	111.75
1	A	227	ALA	N-CA-C	-5.59	105.09	111.07
2	B	140	ILE	N-CA-C	5.59	115.78	110.42
1	A	117	HIS	N-CA-C	-5.58	104.22	111.02
2	B	269	PHE	N-CA-CB	-5.54	102.28	110.37
1	A	170	VAL	CB-CA-C	-5.46	104.99	111.97
2	B	368	LEU	N-CA-C	-5.44	105.00	111.03
2	B	344	ARG	N-CA-C	-5.34	105.10	111.03
1	A	33	GLN	N-CA-C	-5.25	105.46	111.14
1	A	68	LYS	N-CA-C	-5.22	105.48	111.07
1	A	244	SER	N-CA-C	5.21	117.31	109.23
2	B	121	MET	N-CA-C	-5.20	100.25	108.73
2	B	121	MET	CA-C-N	-5.20	114.86	122.19
2	B	121	MET	C-N-CA	-5.20	114.86	122.19
2	B	315	ASP	CA-C-N	5.15	125.19	119.32
2	B	315	ASP	C-N-CA	5.15	125.19	119.32
1	A	125	THR	N-CA-C	5.08	117.89	109.46
2	B	260	ILE	CB-CA-C	-5.07	104.70	110.73
1	A	134	GLY	N-CA-C	5.04	120.80	112.84

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	2255	0	2295	36	0
2	B	2970	0	3023	110	0
3	A	5	0	0	0	0
3	B	10	0	0	1	0
4	A	1	0	0	0	0
5	A	77	0	0	2	0
5	B	49	0	0	1	0
All	All	5367	0	5318	143	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 14.

All (143) 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:360:ASN:OD1	2:B:363:GLU:HB3	1.59	1.02
1:A:154:GLY:HA3	1:A:179:GLY:HA3	1.47	0.93
2:B:350:VAL:HG12	2:B:351:PRO:HD2	1.52	0.91
2:B:352:LEU:HD23	2:B:375:ILE:HG12	1.58	0.85
2:B:336:ALA:O	2:B:340:THR:HG23	1.76	0.84
2:B:241:ASP:HB3	5:B:440:HOH:O	1.77	0.82
2:B:383:ASP:OD1	2:B:387:LYS:HE3	1.82	0.80
2:B:340:THR:O	2:B:344:ARG:HG3	1.81	0.79
2:B:329:ILE:HG13	2:B:330:VAL:H	1.50	0.76
2:B:117:LEU:HD21	2:B:188:ILE:HG12	1.69	0.73
2:B:333:ALA:HB1	2:B:367:ILE:HD12	1.71	0.72
2:B:122:ASP:HB3	2:B:125:CYS:SG	2.30	0.72
1:A:168:GLU:OE2	2:B:355:ARG:NH2	2.20	0.72
2:B:365:GLN:O	2:B:369:THR:HB	1.91	0.71
2:B:44:VAL:HG13	2:B:69:LEU:HD23	1.72	0.70
2:B:21:ARG:HB2	2:B:107:GLU:HG2	1.76	0.67
2:B:44:VAL:HG22	2:B:108:ALA:HB2	1.76	0.66
2:B:44:VAL:HG13	2:B:69:LEU:CD2	2.26	0.66
2:B:236:ILE:HA	2:B:239:MET:HE2	1.79	0.65
2:B:355:ARG:HD3	2:B:355:ARG:C	2.23	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:303:ARG:HB2	1:A:305:MET:HG3	1.79	0.63
2:B:307:GLN:O	2:B:311:LEU:HG	1.99	0.62
2:B:383:ASP:O	2:B:387:LYS:HG3	1.99	0.62
2:B:385:ALA:O	2:B:389:VAL:HG23	2.00	0.61
2:B:333:ALA:HB1	2:B:367:ILE:CD1	2.30	0.61
1:A:154:GLY:HA3	1:A:179:GLY:CA	2.27	0.61
2:B:341:LYS:O	2:B:345:GLU:HG3	2.01	0.60
2:B:1:MET:HE1	2:B:3:LEU:CD2	2.31	0.60
2:B:282:ILE:HA	2:B:285:LEU:HD12	1.86	0.58
2:B:71:LYS:O	2:B:73:PRO:HD3	2.04	0.58
2:B:363:GLU:O	2:B:366:ASN:HB3	2.05	0.57
1:A:49:GLY:N	1:A:62:ASN:OD1	2.38	0.56
2:B:164:ASP:OD1	2:B:189:LYS:NZ	2.36	0.56
2:B:241:ASP:OD2	2:B:243:SER:HB3	2.06	0.56
2:B:119:ILE:HD13	2:B:192:TYR:HA	1.88	0.56
1:A:65:LYS:O	1:A:69:GLU:HG3	2.06	0.56
2:B:80:ALA:O	2:B:84:ILE:HG12	2.05	0.56
2:B:119:ILE:HG12	2:B:130:LEU:HD12	1.88	0.55
2:B:1:MET:HE2	2:B:240:ASP:HB2	1.88	0.55
2:B:210:GLU:HA	2:B:215:GLN:O	2.07	0.55
2:B:184:ALA:O	2:B:188:ILE:HG13	2.08	0.54
2:B:5:GLU:HG2	2:B:104:MET:HE1	1.89	0.54
1:A:61:PHE:CD1	1:A:67:ALA:HB2	2.43	0.54
2:B:1:MET:HE1	2:B:3:LEU:HD21	1.89	0.54
1:A:156:ILE:HD11	1:A:300:PHE:CE2	2.43	0.54
1:A:3:TYR:CZ	1:A:119:LEU:HD21	2.44	0.53
2:B:135:GLN:OE1	2:B:143:VAL:HG22	2.07	0.53
2:B:306:TYR:CE1	2:B:346:LEU:HD21	2.43	0.53
1:A:40:THR:HG22	1:A:41:ASN:N	2.23	0.53
2:B:241:ASP:O	2:B:242:LYS:HB2	2.08	0.53
2:B:249:GLU:HG2	2:B:259:TYR:HD1	1.75	0.52
2:B:348:LEU:HD11	2:B:350:VAL:O	2.09	0.52
2:B:98:VAL:HG11	2:B:244:GLU:CD	2.35	0.52
2:B:343:CYS:SG	2:B:348:LEU:HD22	2.49	0.52
2:B:18:LYS:HE3	2:B:216:VAL:O	2.10	0.52
2:B:355:ARG:C	2:B:355:ARG:CD	2.83	0.52
2:B:255:TYR:O	2:B:304:GLN:NE2	2.33	0.51
2:B:373:LEU:O	2:B:375:ILE:N	2.38	0.51
2:B:350:VAL:CG1	2:B:351:PRO:HD2	2.35	0.51
1:A:19:ILE:HG23	1:A:73:ALA:HB2	1.91	0.51
2:B:361:VAL:HG23	2:B:362:HIS:N	2.25	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:29:THR:OG1	1:A:55:HIS:NE2	2.39	0.50
2:B:192:TYR:O	2:B:195:PHE:HB3	2.11	0.50
2:B:96:GLU:H	2:B:96:GLU:CD	2.19	0.50
2:B:128:PRO:HB2	2:B:156:ILE:HB	1.92	0.50
1:A:161:ARG:HD3	5:A:309:HOH:O	2.12	0.50
2:B:21:ARG:NH1	2:B:107:GLU:OE1	2.43	0.49
1:A:12:VAL:HG11	1:A:143:ILE:HD12	1.94	0.49
1:A:201:GLU:OE2	1:A:205:ASN:ND2	2.46	0.49
2:B:21:ARG:HB2	2:B:107:GLU:CG	2.42	0.49
2:B:112:SER:OG	2:B:212:PRO:HG3	2.12	0.49
2:B:51:ALA:CB	2:B:93:THR:HG22	2.43	0.49
2:B:333:ALA:CB	2:B:367:ILE:HD12	2.42	0.49
2:B:363:GLU:OE1	2:B:366:ASN:HB3	2.13	0.48
1:A:63:THR:HG23	1:A:66:GLU:OE2	2.13	0.48
2:B:156:ILE:HD12	2:B:162:ILE:HG13	1.97	0.47
1:A:161:ARG:CD	5:A:309:HOH:O	2.63	0.47
1:A:156:ILE:N	1:A:156:ILE:HD13	2.30	0.47
2:B:246:GLU:OE2	2:B:248:ILE:HB	2.15	0.46
2:B:116:TYR:CE2	2:B:140:ILE:HB	2.50	0.46
2:B:270:VAL:HA	2:B:324:ASN:O	2.15	0.46
1:A:218:ILE:HG23	1:A:248:GLY:HA3	1.97	0.46
2:B:1:MET:HG3	2:B:237:PHE:CE2	2.51	0.46
2:B:164:ASP:CG	2:B:189:LYS:HZ3	2.23	0.46
1:A:156:ILE:HD11	1:A:300:PHE:HE2	1.79	0.46
2:B:347:GLU:O	2:B:348:LEU:C	2.59	0.45
2:B:302:GLU:OE1	2:B:341:LYS:HD3	2.16	0.45
2:B:74:GLU:O	2:B:78:GLN:NE2	2.49	0.45
2:B:206:ASN:HA	2:B:207:PRO:HA	1.72	0.45
2:B:306:TYR:CE1	2:B:346:LEU:CD2	3.00	0.45
1:A:3:TYR:OH	1:A:119:LEU:HD21	2.17	0.45
2:B:331:ASN:HB2	2:B:359:THR:HG22	1.98	0.45
1:A:106:GLY:O	2:B:228:ASN:HB3	2.16	0.45
2:B:146:SER:HB3	2:B:147:ASN:OD1	2.17	0.44
2:B:164:ASP:CG	2:B:189:LYS:NZ	2.75	0.44
2:B:155:GLN:OE1	2:B:155:GLN:CA	2.65	0.44
2:B:251:GLU:O	2:B:254:LYS:HB2	2.17	0.44
2:B:342:ALA:O	2:B:346:LEU:HG	2.18	0.44
1:A:40:THR:CG2	1:A:41:ASN:N	2.80	0.44
2:B:352:LEU:HD11	2:B:354:VAL:HG22	2.00	0.44
2:B:365:GLN:O	2:B:369:THR:CB	2.63	0.44
2:B:99:LYS:HE2	2:B:99:LYS:HB2	1.83	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:24:THR:HG21	1:A:50:LYS:HD3	1.98	0.43
2:B:368:LEU:O	2:B:371:SER:HB3	2.17	0.43
2:B:111:ILE:HG12	2:B:219:PHE:CZ	2.53	0.43
2:B:129:VAL:HG13	2:B:155:GLN:OE1	2.18	0.43
2:B:72:ASP:OD1	2:B:74:GLU:HB2	2.19	0.43
2:B:115:THR:HB	2:B:174:LEU:HD22	2.00	0.43
1:A:245:PHE:HB2	1:A:292:LEU:HD21	1.99	0.43
2:B:300:VAL:O	2:B:300:VAL:HG13	2.18	0.43
1:A:162:SER:OG	1:A:165:LEU:HB3	2.18	0.43
2:B:125:CYS:O	2:B:126:ASN:HB2	2.19	0.43
2:B:44:VAL:HG22	2:B:108:ALA:CB	2.47	0.43
2:B:361:VAL:O	2:B:365:GLN:HG3	2.18	0.43
1:A:109:GLN:HE21	1:A:191:PHE:HE2	1.67	0.43
2:B:359:THR:O	2:B:360:ASN:HB3	2.19	0.43
2:B:117:LEU:CD2	2:B:188:ILE:HG12	2.45	0.42
2:B:269:PHE:HE1	2:B:325:ILE:HD11	1.83	0.42
1:A:245:PHE:CE1	1:A:289:PRO:HD3	2.54	0.42
1:A:191:PHE:CE1	2:B:123:ARG:HA	2.54	0.42
2:B:116:TYR:O	2:B:132:GLY:HA2	2.19	0.42
1:A:164:THR:HA	1:A:167:TYR:CD2	2.54	0.42
2:B:18:LYS:NZ	2:B:215:GLN:OE1	2.53	0.42
2:B:301:LYS:HG2	2:B:303:SER:H	1.85	0.42
2:B:178:GLY:HA3	2:B:179:PRO:HD2	1.90	0.42
1:A:92:ALA:O	1:A:97:VAL:HG23	2.20	0.42
1:A:300:PHE:O	1:A:301:GLU:C	2.63	0.42
1:A:4:THR:HG22	1:A:7:ARG:CZ	2.50	0.41
2:B:163:LYS:HD2	3:B:397:SO4:O3	2.20	0.41
1:A:80:VAL:O	1:A:85:ALA:HB2	2.19	0.41
2:B:1:MET:CE	2:B:240:ASP:HB2	2.49	0.41
2:B:120:LEU:N	2:B:120:LEU:HD23	2.35	0.41
2:B:51:ALA:HB3	2:B:93:THR:HG22	2.03	0.41
2:B:371:SER:OG	2:B:373:LEU:HG	2.20	0.41
2:B:293:PHE:CD1	2:B:293:PHE:C	2.99	0.41
2:B:363:GLU:OE1	2:B:363:GLU:CA	2.69	0.40
2:B:6:TYR:CD2	2:B:24:VAL:HG21	2.56	0.40
1:A:178:LEU:HD12	1:A:178:LEU:HA	1.80	0.40
2:B:241:ASP:O	2:B:242:LYS:CB	2.69	0.40
2:B:393:THR:O	2:B:393:THR:HG22	2.21	0.40
2:B:388:ALA:O	2:B:391:SER:HB2	2.21	0.40
1:A:25:GLY:O	1:A:29:THR:HB	2.22	0.40
2:B:155:GLN:OE1	2:B:155:GLN:HA	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	302/305 (99%)	291 (96%)	9 (3%)	2 (1%)	18	20
2	B	391/395 (99%)	365 (93%)	22 (6%)	4 (1%)	12	12
All	All	693/700 (99%)	656 (95%)	31 (4%)	6 (1%)	14	14

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	300	VAL
2	B	329	ILE
1	A	177	GLY
2	B	146	SER
2	B	328	GLY
1	A	138	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	237/237 (100%)	230 (97%)	7 (3%)	36	48
2	B	317/319 (99%)	298 (94%)	19 (6%)	17	21
All	All	554/556 (100%)	528 (95%)	26 (5%)	23	30

All (26) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	4	THR
1	A	29	THR
1	A	41	ASN
1	A	53	LYS
1	A	168	GLU
1	A	178	LEU
1	A	272	LYS
2	B	44	VAL
2	B	46	LYS
2	B	96	GLU
2	B	107	GLU
2	B	125	CYS
2	B	130	LEU
2	B	140	ILE
2	B	146	SER
2	B	149	GLU
2	B	155	GLN
2	B	246	GLU
2	B	258	LYS
2	B	293	PHE
2	B	310	LYS
2	B	348	LEU
2	B	350	VAL
2	B	355	ARG
2	B	369	THR
2	B	371	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (11) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	33	GLN
1	A	131	ASN
1	A	205	ASN
1	A	225	ASN
1	A	233	HIS
2	B	78	GLN
2	B	101	ASN
2	B	126	ASN
2	B	173	ASN
2	B	337	ASN
2	B	366	ASN

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

1 non-standard protein/DNA/RNA residue is 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
1	NEP	A	259	1	11,14,15	1.53	1 (9%)	8,20,22	1.17	1 (12%)

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
1	NEP	A	259	1	-	2/5/12/14	0/1/1/1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	259	NEP	P-O1P	-4.58	1.44	1.56

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	259	NEP	CE1-ND1-CG	2.29	109.47	105.80

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	A	259	NEP	CA-CB-CG-CD2

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Mol	Chain	Res	Type	Atoms
1	A	259	NEP	CA-CB-CG-ND1

There are no ring outliers.

No monomer is involved in short contacts.

## 5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

Of 4 ligands modelled in this entry, 1 is monoatomic - leaving 3 for Mogul analysis.

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	SO4	B	396	-	4,4,4	0.43	0	6,6,6	0.34	0
3	SO4	B	397	-	4,4,4	0.47	0	6,6,6	0.16	0
3	SO4	A	307	-	4,4,4	0.29	0	6,6,6	0.55	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.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	397	SO4	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	304/305 (99%)	-0.39	0 <b>100</b> <b>100</b>	13, 25, 41, 53	0
2	B	393/395 (99%)	-0.03	11 (2%) 55 61	14, 33, 57, 71	0
All	All	697/700 (99%)	-0.19	11 (1%) 70 76	13, 29, 52, 71	0

All (11) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	329	ILE	4.3
2	B	369	THR	2.9
2	B	366	ASN	2.7
2	B	370	ASN	2.6
2	B	314	ALA	2.4
2	B	364	ALA	2.3
2	B	371	SER	2.3
2	B	300	VAL	2.3
2	B	313	THR	2.2
2	B	330	VAL	2.1
2	B	346	LEU	2.0

### 6.2 Non-standard residues in protein, DNA, RNA chains [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<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	B-factors(Å <sup>2</sup> )	Q<0.9
1	NEP	A	259	14/15	0.98	0.05	11,15,21,23	0

### 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, 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	B-factors(Å <sup>2</sup> )	Q<0.9
3	SO4	B	397	5/5	0.82	0.14	73,73,74,75	0
3	SO4	B	396	5/5	0.90	0.11	56,57,58,60	0
3	SO4	A	307	5/5	0.97	0.09	45,46,48,49	0
4	CL	A	308	1/1	0.99	0.03	22,22,22,22	0

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

There are no such residues in this entry.