



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 10, 2026 – 05:40 AM UTC

PDB ID : 2FPI / pdb_00002fpi
Title : Crystal structure of pig GTP-specific succinyl-CoA synthetase from polyethylene glycol
Authors : Fraser, M.E.
Deposited on : 2006-01-16
Resolution : 2.70 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)
Xtrriage (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

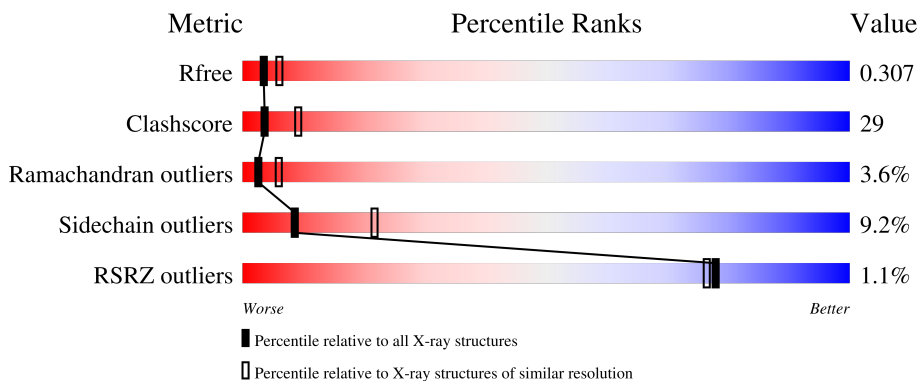
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.70 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	3538 (2.70-2.70)
Clashscore	190562	3843 (2.70-2.70)
Ramachandran outliers	187476	3778 (2.70-2.70)
Sidechain outliers	187428	3778 (2.70-2.70)
RSRZ outliers	180081	3538 (2.70-2.70)

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	305	 59% 32% 9%
2	B	395	 38% 49% 12% ..

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 5299 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: O₄S).



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

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	39	Total	O	0	0
			39	39		
4	B	25	Total	O	0	0
			25	25		



4 Data and refinement statistics

Property	Value	Source
Space group	P 65	Depositor
Cell constants a, b, c, α , β , γ	135.79Å 135.79Å 77.15Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	100.00 – 2.70 100.00 – 2.70	Depositor EDS
% Data completeness (in resolution range)	99.8 (100.00-2.70) 99.8 (100.00-2.70)	Depositor EDS
R_{merge}	0.05	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	5.88 (at 2.68Å)	Xtrriage
Refinement program	CNS	Depositor
R, R_{free}	0.215 , 0.310 0.213 , 0.307	Depositor DCC
R_{free} test set	1143 reflections (5.03%)	wwPDB-VP
Wilson B-factor (Å ²)	50.0	Xtrriage
Anisotropy	0.021	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.29 , 41.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtrriage
Estimated twinning fraction	0.034 for h,-h-k,-l	Xtrriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	5299	wwPDB-VP
Average B, all atoms (Å ²)	44.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.83% 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 [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: 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	0.97	1/2281 (0.0%)	1.38	29/3081 (0.9%)
2	B	0.93	5/3007 (0.2%)	1.32	31/4059 (0.8%)
All	All	0.95	6/5288 (0.1%)	1.35	60/7140 (0.8%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
2	B	0	1

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	329	ILE	CA-CB	6.89	1.63	1.54
2	B	44	VAL	CA-CB	6.50	1.62	1.54
1	A	101	VAL	CA-CB	6.10	1.61	1.53
2	B	335	ILE	CA-CB	6.05	1.62	1.54
2	B	277	MET	SD-CE	-5.35	1.66	1.79
2	B	1	MET	SD-CE	-5.31	1.66	1.79

All (60) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	143	VAL	N-CA-C	-9.01	101.56	110.30
1	A	82	PRO	N-CA-C	8.97	121.64	110.70
1	A	23	PHE	N-CA-C	8.84	120.52	111.07
1	A	236	GLY	CA-C-N	8.73	130.76	119.84
1	A	236	GLY	C-N-CA	8.73	130.76	119.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	201	GLU	N-CA-C	-8.65	101.54	110.97
2	B	344	ARG	N-CA-C	-8.61	101.84	111.14
2	B	161	GLY	N-CA-C	-8.51	103.48	112.08
2	B	201	THR	N-CA-C	-8.37	102.51	112.89
1	A	155	ARG	N-CA-C	7.90	123.10	113.38
2	B	61	SER	N-CA-C	-7.90	103.22	113.17
2	B	317	LYS	N-CA-C	-7.81	103.57	113.72
1	A	104	THR	N-CA-C	7.69	121.64	110.42
2	B	209	GLY	N-CA-C	7.40	125.80	111.66
1	A	176	VAL	N-CA-C	-7.28	105.45	112.29
1	A	87	ALA	N-CA-C	-7.27	103.29	111.07
1	A	81	PRO	CA-C-N	7.20	127.80	120.38
1	A	81	PRO	C-N-CA	7.20	127.80	120.38
1	A	187	GLY	N-CA-C	7.11	120.25	112.29
1	A	134	GLY	N-CA-C	7.07	118.70	111.56
1	A	58	LEU	CA-C-N	7.02	127.01	119.78
1	A	58	LEU	C-N-CA	7.02	127.01	119.78
1	A	178	LEU	N-CA-C	6.93	120.97	112.23
1	A	18	VAL	N-CA-C	6.70	118.25	108.53
2	B	300	VAL	N-CA-C	-6.66	100.15	109.21
2	B	198	ILE	N-CA-C	6.52	120.30	112.80
2	B	121	MET	CA-C-N	-6.34	113.25	122.19
2	B	121	MET	C-N-CA	-6.34	113.25	122.19
2	B	217	VAL	N-CA-C	6.33	117.60	108.48
2	B	208	PHE	N-CA-C	-6.28	98.96	109.07
2	B	241	ASP	N-CA-C	6.21	118.56	111.11
1	A	291	GLN	N-CA-C	6.07	120.27	112.26
2	B	134	PRO	N-CA-C	-6.05	106.59	114.03
2	B	21	ARG	N-CA-C	-6.03	102.00	110.50
1	A	271	ALA	N-CA-C	5.88	117.69	111.28
1	A	244	SER	N-CA-C	5.87	118.20	108.99
1	A	30	PHE	N-CA-C	5.82	118.37	111.33
1	A	132	CYS	CA-C-N	5.75	125.37	119.56
1	A	132	CYS	C-N-CA	5.75	125.37	119.56
1	A	156	ILE	N-CA-C	5.75	116.58	108.36
2	B	298	GLY	N-CA-C	-5.63	106.01	115.80
2	B	211	THR	CA-C-N	-5.62	113.23	119.19
2	B	211	THR	C-N-CA	-5.62	113.23	119.19
2	B	305	VAL	N-CA-C	-5.60	103.44	111.17
1	A	141	CYS	N-CA-C	5.53	118.44	108.48
2	B	332	CYS	N-CA-C	5.46	119.42	112.87
2	B	16	GLY	N-CA-C	5.39	123.20	114.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	9	LYS	N-CA-C	-5.38	105.07	111.69
2	B	343	CYS	N-CA-C	5.32	117.89	111.40
2	B	194	LEU	N-CA-C	-5.31	105.38	111.07
2	B	72	ASP	N-CA-C	5.23	118.11	108.69
2	B	348	LEU	N-CA-C	5.21	117.84	110.50
2	B	36	LYS	N-CA-C	-5.16	105.10	111.40
1	A	78	ILE	N-CA-C	5.16	115.39	108.17
1	A	114	ARG	N-CA-C	-5.14	105.76	111.36
2	B	263	ASP	N-CA-C	5.13	118.41	112.97
2	B	214	GLY	N-CA-C	5.09	122.86	115.32
1	A	82	PRO	CA-C-N	5.07	124.85	119.28
1	A	82	PRO	C-N-CA	5.07	124.85	119.28
2	B	318	VAL	N-CA-C	5.01	115.56	109.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	B	86	TYR	Sidechain

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	2255	0	2295	96	0
2	B	2970	0	3023	220	0
3	A	5	0	0	0	0
3	B	5	0	0	0	0
4	A	39	0	0	0	0
4	B	25	0	0	2	0
All	All	5299	0	5318	309	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 29.

All (309) 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:70:THR:HG21	2:B:75:VAL:HB	1.47	0.97
1:A:89:ILE:HG22	1:A:93:ILE:HD11	1.53	0.89
2:B:113:ARG:HG3	2:B:113:ARG:HH11	1.37	0.88
2:B:180:LEU:HD13	2:B:210:GLU:OE1	1.72	0.88
1:A:90:ASN:HA	1:A:93:ILE:HD12	1.55	0.87
2:B:360:ASN:HD21	2:B:363:GLU:HG2	1.39	0.87
2:B:329:ILE:O	2:B:330:VAL:HB	1.75	0.87
2:B:352:LEU:HD12	2:B:353:VAL:N	1.91	0.86
2:B:360:ASN:ND2	2:B:363:GLU:HG2	1.91	0.86
2:B:330:VAL:HG11	2:B:335:ILE:HD11	1.58	0.83
2:B:335:ILE:O	2:B:339:ILE:HG13	1.79	0.82
2:B:352:LEU:HD12	2:B:353:VAL:H	1.45	0.81
1:A:256:ARG:HH12	2:B:258:LYS:NZ	1.81	0.79
2:B:392:VAL:HG23	2:B:392:VAL:O	1.83	0.79
2:B:329:ILE:O	2:B:329:ILE:HG13	1.82	0.77
2:B:310:LYS:O	2:B:313:THR:HB	1.83	0.77
2:B:35:ALA:HB1	2:B:43:ILE:HD13	1.66	0.76
2:B:212:PRO:HD2	2:B:213:GLU:OE2	1.85	0.76
2:B:122:ASP:HB3	2:B:125:CYS:SG	2.26	0.75
2:B:269:PHE:CE1	2:B:296:LEU:HD11	2.21	0.75
2:B:348:LEU:HD21	2:B:373:LEU:CD2	2.16	0.75
1:A:23:PHE:CE2	1:A:55:HIS:HB3	2.24	0.73
2:B:21:ARG:HD3	2:B:107:GLU:OE2	1.89	0.73
2:B:270:VAL:HG22	2:B:324:ASN:HB3	1.69	0.72
2:B:269:PHE:HE1	2:B:296:LEU:HD11	1.52	0.72
2:B:122:ASP:OD2	2:B:125:CYS:SG	2.46	0.72
2:B:135:GLN:O	2:B:135:GLN:HG2	1.88	0.72
1:A:171:HIS:O	1:A:175:GLN:HG2	1.91	0.71
2:B:179:PRO:HG2	2:B:180:LEU:H	1.56	0.70
2:B:1:MET:HE3	2:B:2:ASN:C	2.16	0.70
2:B:38:LEU:O	2:B:39:ASN:HB3	1.92	0.70
2:B:120:LEU:HD23	2:B:120:LEU:N	2.07	0.69
2:B:1:MET:HE1	2:B:3:LEU:HG	1.75	0.69
2:B:348:LEU:HD21	2:B:373:LEU:HD23	1.75	0.69
1:A:90:ASN:HA	1:A:93:ILE:CD1	2.23	0.68
1:A:6:SER:OG	1:A:126:ARG:HB2	1.94	0.68
2:B:144:ALA:HA	2:B:151:ILE:CD1	2.24	0.67
1:A:241:PRO:HB3	1:A:303:ARG:CZ	2.25	0.67
2:B:111:ILE:HD12	2:B:111:ILE:H	1.59	0.67
2:B:350:VAL:HG12	2:B:351:PRO:HD2	1.78	0.66
1:A:10:LEU:HD23	1:A:128:ILE:HD11	1.78	0.66
1:A:256:ARG:HH12	2:B:258:LYS:HZ3	1.41	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:221:ASN:H	1:A:221:ASN:HD22	1.44	0.66
1:A:61:PHE:CD1	1:A:61:PHE:N	2.66	0.64
2:B:88:LEU:HD12	2:B:89:ALA:N	2.12	0.64
2:B:176:PHE:O	2:B:181:GLN:HG3	1.98	0.64
2:B:90:THR:C	2:B:92:GLN:H	2.04	0.64
2:B:251:GLU:OE2	2:B:254:LYS:HD2	1.98	0.63
2:B:330:VAL:CG1	2:B:335:ILE:HD11	2.27	0.63
2:B:342:ALA:O	2:B:346:LEU:HB2	1.99	0.63
2:B:41:LYS:O	2:B:71:LYS:HB3	1.98	0.63
1:A:82:PRO:HB2	1:A:83:PRO:HD3	1.80	0.63
2:B:387:LYS:O	2:B:388:ALA:C	2.42	0.63
1:A:17:LYS:HA	1:A:41:ASN:HB3	1.81	0.62
1:A:221:ASN:H	1:A:221:ASN:ND2	1.97	0.61
2:B:111:ILE:HD12	2:B:111:ILE:N	2.15	0.61
2:B:138:VAL:HG12	2:B:139:ASP:N	2.15	0.61
2:B:267:ALA:HA	2:B:291:ALA:HB3	1.83	0.61
1:A:168:GLU:OE2	2:B:355:ARG:NH1	2.34	0.60
2:B:59:PHE:CZ	2:B:83:MET:HG2	2.36	0.60
1:A:94:ASP:OD1	1:A:118:ARG:NH2	2.20	0.60
1:A:127:LEU:HD23	1:A:193:GLY:HA3	1.82	0.60
1:A:90:ASN:CA	1:A:93:ILE:HD12	2.29	0.60
2:B:38:LEU:O	2:B:39:ASN:CB	2.50	0.59
1:A:122:GLN:NE2	1:A:125:THR:HB	2.17	0.59
2:B:107:GLU:O	2:B:107:GLU:HG3	2.02	0.59
2:B:144:ALA:HA	2:B:151:ILE:HD11	1.85	0.59
2:B:269:PHE:HB2	2:B:294:LEU:HD23	1.85	0.59
2:B:189:LYS:O	2:B:193:ASN:ND2	2.36	0.58
2:B:113:ARG:HH11	2:B:113:ARG:CG	2.12	0.58
1:A:17:LYS:HE2	1:A:41:ASN:OD1	2.03	0.58
2:B:90:THR:C	2:B:92:GLN:N	2.61	0.57
2:B:107:GLU:C	2:B:108:ALA:O	2.47	0.57
2:B:257:LEU:HD12	2:B:311:LEU:HD11	1.87	0.56
2:B:369:THR:HG22	2:B:370:ASN:ND2	2.20	0.56
1:A:245:PHE:HB2	1:A:292:LEU:HD21	1.86	0.56
2:B:140:ILE:HG23	2:B:141:GLU:N	2.20	0.56
2:B:129:VAL:HG22	2:B:155:GLN:HE21	1.69	0.56
1:A:36:LEU:HD11	1:A:58:LEU:HD11	1.88	0.56
2:B:178:GLY:O	2:B:181:GLN:HB2	2.06	0.56
1:A:156:ILE:HD12	1:A:296:ILE:HD13	1.87	0.55
2:B:303:SER:O	2:B:306:TYR:HB3	2.06	0.55
2:B:245:ASN:HB2	2:B:250:ASN:HD21	1.72	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:61:PHE:CG	1:A:67:ALA:HB2	2.42	0.55
2:B:144:ALA:HA	2:B:151:ILE:HD12	1.89	0.55
1:A:94:ASP:C	1:A:96:GLU:H	2.14	0.54
2:B:120:LEU:HD23	2:B:120:LEU:H	1.70	0.54
2:B:319:GLU:O	2:B:350:VAL:HG12	2.07	0.54
1:A:173:THR:O	1:A:176:VAL:HG22	2.08	0.54
2:B:90:THR:OG1	2:B:93:THR:HG23	2.07	0.54
2:B:288:GLY:O	2:B:289:LYS:HD3	2.07	0.54
1:A:19:ILE:HG13	1:A:19:ILE:O	2.06	0.54
1:A:36:LEU:HD21	1:A:42:LEU:HB3	1.90	0.54
2:B:164:ASP:HB2	4:B:403:HOH:O	2.07	0.54
2:B:186:ASP:O	2:B:190:LYS:HG3	2.08	0.54
2:B:198:ILE:HD12	2:B:225:PHE:CE1	2.43	0.53
2:B:113:ARG:HG3	2:B:113:ARG:NH1	2.15	0.53
2:B:192:TYR:OH	2:B:196:LEU:HD11	2.09	0.53
1:A:14:LYS:H	1:A:140:GLU:HB3	1.74	0.53
1:A:155:ARG:NH2	1:A:305:MET:O	2.29	0.53
2:B:144:ALA:CA	2:B:151:ILE:HD11	2.38	0.53
2:B:170:MET:O	2:B:171:ALA:C	2.50	0.53
1:A:119:LEU:HD21	1:A:127:LEU:HB3	1.89	0.53
2:B:365:GLN:HG2	2:B:377:SER:OG	2.08	0.53
2:B:163:LYS:N	2:B:166:GLN:OE1	2.32	0.53
2:B:122:ASP:CB	2:B:125:CYS:SG	2.97	0.53
2:B:304:GLN:O	2:B:305:VAL:C	2.50	0.53
2:B:194:LEU:O	2:B:198:ILE:HG12	2.09	0.53
1:A:36:LEU:HD11	1:A:58:LEU:CD1	2.39	0.52
2:B:135:GLN:HE21	2:B:150:LEU:HD13	1.75	0.52
1:A:174:THR:O	1:A:177:GLY:N	2.36	0.52
2:B:32:LEU:HD13	2:B:73:PRO:O	2.09	0.52
2:B:157:ASP:HB3	2:B:160:GLU:HB3	1.92	0.52
2:B:188:ILE:HA	2:B:191:LEU:HD12	1.92	0.52
1:A:60:VAL:C	1:A:61:PHE:CD1	2.88	0.51
2:B:217:VAL:HB	2:B:219:PHE:CZ	2.46	0.51
2:B:109:LEU:HD22	2:B:211:THR:HG22	1.93	0.51
1:A:290:ALA:HB3	2:B:382:GLU:OE1	2.10	0.51
2:B:182:ASN:HD22	2:B:182:ASN:H	1.57	0.51
2:B:231:PHE:CD1	2:B:231:PHE:C	2.88	0.51
2:B:246:GLU:HG2	2:B:247:PRO:HD2	1.93	0.51
1:A:57:GLY:O	1:A:58:LEU:HG	2.10	0.51
2:B:98:VAL:CG1	2:B:244:GLU:HG2	2.41	0.51
2:B:343:CYS:HB3	2:B:373:LEU:HD22	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:113:VAL:HG11	2:B:127:GLY:HA2	1.93	0.51
1:A:24:THR:OG1	1:A:47:THR:HG21	2.11	0.51
2:B:379:VAL:HG12	2:B:383:ASP:HB2	1.93	0.51
2:B:379:VAL:HG12	2:B:383:ASP:CB	2.41	0.50
1:A:223:GLU:HB2	1:A:274:LYS:HE3	1.93	0.50
1:A:122:GLN:HE22	1:A:125:THR:CA	2.24	0.50
1:A:14:LYS:N	1:A:140:GLU:HB3	2.27	0.50
1:A:43:VAL:O	1:A:58:LEU:HD22	2.11	0.50
2:B:308:ALA:O	2:B:312:LEU:HG	2.12	0.50
2:B:113:ARG:CG	2:B:113:ARG:NH1	2.74	0.50
2:B:340:THR:HG22	2:B:373:LEU:HD13	1.94	0.50
1:A:4:THR:O	1:A:7:ARG:HG3	2.12	0.49
1:A:162:SER:HB2	1:A:259:NEP:O1P	2.11	0.49
1:A:299:GLU:OE2	1:A:302:LYS:NZ	2.36	0.49
2:B:116:TYR:CD2	2:B:140:ILE:HD13	2.47	0.49
2:B:270:VAL:HA	2:B:324:ASN:O	2.12	0.49
1:A:164:THR:HA	1:A:167:TYR:CD2	2.47	0.49
2:B:388:ALA:O	2:B:391:SER:HB3	2.12	0.49
2:B:138:VAL:CG1	2:B:139:ASP:N	2.75	0.49
1:A:51:GLY:HA3	1:A:62:ASN:CG	2.38	0.49
2:B:128:PRO:C	2:B:129:VAL:HG23	2.37	0.49
1:A:89:ILE:C	1:A:93:ILE:HD12	2.38	0.49
2:B:147:ASN:HB3	2:B:150:LEU:CD1	2.43	0.49
2:B:80:ALA:O	2:B:81:LYS:C	2.54	0.49
2:B:120:LEU:N	2:B:120:LEU:CD2	2.76	0.49
2:B:125:CYS:O	2:B:126:ASN:O	2.31	0.49
2:B:152:PHE:CD1	2:B:152:PHE:N	2.80	0.49
1:A:36:LEU:CD2	1:A:42:LEU:HB3	2.42	0.48
2:B:304:GLN:C	2:B:306:TYR:N	2.68	0.48
2:B:348:LEU:O	2:B:348:LEU:HG	2.13	0.48
2:B:192:TYR:O	2:B:195:PHE:HB3	2.13	0.48
1:A:66:GLU:O	1:A:68:LYS:N	2.47	0.48
2:B:1:MET:C	2:B:1:MET:HE2	2.38	0.48
2:B:360:ASN:C	2:B:360:ASN:HD22	2.21	0.48
1:A:58:LEU:HD23	1:A:59:PRO:HD2	1.95	0.48
2:B:192:TYR:CZ	2:B:196:LEU:HD11	2.48	0.48
2:B:380:ASP:OD1	2:B:380:ASP:C	2.55	0.48
1:A:43:VAL:HG21	1:A:71:THR:CB	2.44	0.48
1:A:89:ILE:O	1:A:93:ILE:HD12	2.13	0.48
1:A:221:ASN:ND2	1:A:221:ASN:N	2.57	0.48
2:B:327:GLY:O	2:B:329:ILE:N	2.46	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:236:ILE:HA	2:B:239:MET:HE3	1.95	0.48
2:B:245:ASN:HB2	2:B:250:ASN:ND2	2.28	0.48
2:B:275:LEU:HD11	2:B:324:ASN:HD21	1.79	0.48
1:A:122:GLN:HE22	1:A:125:THR:HB	1.77	0.48
1:A:234:ASN:O	1:A:239:SER:HB2	2.14	0.48
2:B:329:ILE:O	2:B:329:ILE:CG1	2.55	0.48
1:A:106:GLY:O	2:B:228:ASN:HB3	2.15	0.47
1:A:156:ILE:HD12	1:A:296:ILE:CD1	2.43	0.47
2:B:135:GLN:NE2	2:B:150:LEU:CD1	2.77	0.47
2:B:360:ASN:HD21	2:B:363:GLU:CG	2.19	0.47
2:B:18:LYS:HE2	2:B:183:GLN:OE1	2.14	0.47
2:B:163:LYS:HG2	2:B:165:SER:OG	2.14	0.47
2:B:206:ASN:O	2:B:220:ASP:HB2	2.15	0.47
1:A:203:PHE:HB3	1:A:209:THR:HG21	1.96	0.47
1:A:173:THR:O	1:A:176:VAL:CG2	2.63	0.47
2:B:371:SER:HB2	2:B:373:LEU:HD12	1.95	0.47
2:B:42:GLU:HB3	2:B:108:ALA:HB3	1.96	0.47
2:B:109:LEU:HD22	2:B:211:THR:CG2	2.45	0.46
2:B:140:ILE:HG23	2:B:141:GLU:HG3	1.97	0.46
1:A:88:ALA:O	1:A:89:ILE:C	2.55	0.46
1:A:121:ARG:HG3	1:A:121:ARG:HH11	1.79	0.46
2:B:90:THR:O	2:B:92:GLN:N	2.49	0.46
2:B:163:LYS:HE3	2:B:165:SER:OG	2.16	0.46
2:B:270:VAL:HG21	2:B:279:THR:OG1	2.15	0.46
2:B:96:GLU:H	2:B:96:GLU:CD	2.24	0.46
2:B:265:ASN:OD1	2:B:266:ILE:HG13	2.15	0.46
1:A:50:LYS:O	1:A:52:GLY:N	2.48	0.46
1:A:122:GLN:HE22	1:A:125:THR:C	2.24	0.46
2:B:210:GLU:HA	2:B:215:GLN:O	2.15	0.45
2:B:301:LYS:O	2:B:302:GLU:C	2.59	0.45
2:B:361:VAL:HG12	2:B:365:GLN:OE1	2.16	0.45
2:B:307:GLN:OE1	2:B:310:LYS:HD3	2.17	0.45
2:B:330:VAL:CG1	2:B:335:ILE:CD1	2.93	0.45
1:A:122:GLN:CD	1:A:125:THR:HB	2.41	0.45
2:B:152:PHE:CE2	2:B:173:ASN:ND2	2.84	0.45
2:B:51:ALA:CB	2:B:93:THR:HG22	2.46	0.45
2:B:217:VAL:HB	2:B:219:PHE:CE1	2.51	0.45
2:B:360:ASN:CG	2:B:363:GLU:HG2	2.40	0.45
2:B:125:CYS:SG	2:B:155:GLN:NE2	2.90	0.45
1:A:156:ILE:HG21	1:A:213:ILE:HG13	1.98	0.45
2:B:45:LEU:HG	2:B:83:MET:HE1	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:385:ALA:O	2:B:389:VAL:HG23	2.17	0.45
2:B:49:ILE:O	2:B:49:ILE:HG13	2.16	0.45
1:A:32:SER:HB3	1:A:42:LEU:HD21	1.99	0.45
2:B:27:THR:HG23	2:B:30:GLU:OE2	2.17	0.45
2:B:248:ILE:HG21	2:B:259:TYR:CZ	2.52	0.45
2:B:259:TYR:O	2:B:260:ILE:HG13	2.17	0.45
1:A:127:LEU:HD23	1:A:193:GLY:CA	2.47	0.44
1:A:82:PRO:CB	1:A:83:PRO:HD3	2.47	0.44
2:B:107:GLU:O	2:B:108:ALA:O	2.36	0.44
2:B:192:TYR:CE1	2:B:196:LEU:HD11	2.53	0.44
2:B:309:PHE:O	2:B:310:LYS:C	2.60	0.44
2:B:156:ILE:HG21	2:B:192:TYR:CE2	2.52	0.44
2:B:182:ASN:H	2:B:182:ASN:ND2	2.15	0.44
2:B:116:TYR:OH	2:B:204:GLU:OE2	2.17	0.44
2:B:147:ASN:HB3	2:B:150:LEU:HG	1.99	0.44
1:A:89:ILE:HG22	1:A:93:ILE:CD1	2.36	0.44
2:B:198:ILE:HD12	2:B:225:PHE:HE1	1.83	0.44
2:B:371:SER:C	2:B:373:LEU:H	2.26	0.43
1:A:78:ILE:HG22	1:A:80:VAL:H	1.83	0.43
1:A:85:ALA:HB1	1:A:107:ILE:HD11	2.00	0.43
2:B:264:GLY:HA3	2:B:289:LYS:O	2.19	0.43
2:B:35:ALA:HB1	2:B:43:ILE:CD1	2.42	0.43
1:A:71:THR:C	1:A:73:ALA:H	2.26	0.43
2:B:1:MET:CE	2:B:2:ASN:C	2.88	0.43
2:B:241:ASP:C	2:B:243:SER:H	2.26	0.43
2:B:255:TYR:C	2:B:257:LEU:H	2.27	0.43
2:B:380:ASP:OD1	2:B:382:GLU:N	2.52	0.43
2:B:192:TYR:CD1	2:B:192:TYR:C	2.96	0.43
2:B:226:ASP:OD1	2:B:226:ASP:C	2.62	0.43
1:A:113:VAL:CG1	2:B:127:GLY:HA2	2.48	0.43
1:A:176:VAL:HG23	1:A:178:LEU:HG	2.01	0.43
2:B:1:MET:CE	2:B:3:LEU:HG	2.47	0.43
2:B:98:VAL:HG11	2:B:244:GLU:HG2	2.00	0.43
2:B:293:PHE:CD1	2:B:293:PHE:C	2.95	0.43
2:B:345:GLU:O	2:B:345:GLU:HG2	2.19	0.43
1:A:14:LYS:HG2	1:A:140:GLU:OE1	2.19	0.42
2:B:33:GLU:HB3	2:B:37:ARG:HH12	1.84	0.42
1:A:162:SER:OG	1:A:165:LEU:HB3	2.19	0.42
2:B:8:SER:O	2:B:12:MET:HG3	2.20	0.42
2:B:128:PRO:HB2	2:B:156:ILE:HB	2.01	0.42
1:A:85:ALA:CB	1:A:107:ILE:HD11	2.49	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:204:LEU:HD23	1:A:204:LEU:HA	1.78	0.42
2:B:72:ASP:O	2:B:74:GLU:N	2.52	0.42
1:A:165:LEU:O	1:A:168:GLU:HB2	2.18	0.42
2:B:45:LEU:HD21	2:B:83:MET:CE	2.50	0.42
2:B:337:ASN:HD22	2:B:337:ASN:HA	1.69	0.42
1:A:10:LEU:HD23	1:A:128:ILE:CD1	2.48	0.42
1:A:169:ALA:O	1:A:173:THR:HG23	2.19	0.42
1:A:256:ARG:HH11	1:A:256:ARG:HB3	1.85	0.42
1:A:148:GLY:O	1:A:150:ILE:N	2.53	0.42
1:A:168:GLU:O	1:A:172:GLN:HG3	2.19	0.42
2:B:122:ASP:CG	2:B:125:CYS:SG	3.02	0.42
2:B:135:GLN:NE2	2:B:150:LEU:HD13	2.33	0.42
2:B:387:LYS:O	2:B:390:ALA:N	2.52	0.42
1:A:89:ILE:CG2	1:A:93:ILE:HD11	2.37	0.42
2:B:44:VAL:HG12	2:B:46:LYS:HG2	2.01	0.42
2:B:128:PRO:C	2:B:129:VAL:CG2	2.93	0.42
1:A:218:ILE:HG23	1:A:248:GLY:HA3	2.02	0.41
2:B:44:VAL:HG22	2:B:69:LEU:CD2	2.50	0.41
2:B:93:THR:OG1	2:B:97:GLY:HA2	2.19	0.41
2:B:139:ASP:O	2:B:141:GLU:N	2.53	0.41
2:B:176:PHE:CD2	2:B:184:ALA:CB	3.03	0.41
2:B:179:PRO:CG	2:B:180:LEU:H	2.29	0.41
2:B:344:ARG:C	2:B:346:LEU:H	2.28	0.41
2:B:192:TYR:CE1	2:B:196:LEU:CD1	3.03	0.41
2:B:311:LEU:O	2:B:312:LEU:C	2.62	0.41
2:B:126:ASN:ND2	2:B:126:ASN:C	2.77	0.41
2:B:191:LEU:O	2:B:194:LEU:HB3	2.20	0.41
2:B:45:LEU:HD13	2:B:105:VAL:HG22	2.02	0.41
2:B:74:GLU:O	2:B:75:VAL:C	2.63	0.41
2:B:75:VAL:HG12	2:B:79:LEU:HD12	2.03	0.41
2:B:83:MET:HE3	2:B:103:VAL:HG11	2.02	0.41
2:B:163:LYS:HG2	2:B:165:SER:H	1.84	0.41
2:B:257:LEU:HD22	2:B:296:LEU:HD23	2.02	0.41
2:B:282:ILE:O	2:B:283:ILE:C	2.63	0.41
2:B:341:LYS:O	2:B:345:GLU:HB3	2.21	0.41
1:A:221:ASN:HD22	1:A:221:ASN:N	2.08	0.41
2:B:43:ILE:O	2:B:69:LEU:HA	2.20	0.41
2:B:307:GLN:O	2:B:310:LYS:HB3	2.21	0.41
2:B:25:ALA:O	2:B:102:LYS:HA	2.21	0.41
1:A:9:HIS:ND1	1:A:98:PRO:HB3	2.35	0.41
1:A:94:ASP:C	1:A:96:GLU:N	2.79	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:343:CYS:HB3	2:B:373:LEU:CD2	2.51	0.41
2:B:373:LEU:HB3	2:B:375:ILE:HG13	2.03	0.41
2:B:186:ASP:HB3	4:B:409:HOH:O	2.21	0.41
2:B:209:GLY:O	2:B:216:VAL:HA	2.21	0.41
2:B:356:LEU:HD23	2:B:356:LEU:HA	1.96	0.41
2:B:115:THR:C	2:B:136:GLY:HA3	2.46	0.40
2:B:133:SER:HB2	2:B:150:LEU:O	2.21	0.40
2:B:259:TYR:C	2:B:260:ILE:HG13	2.45	0.40
2:B:320:ALA:C	2:B:321:ILE:HG13	2.47	0.40
2:B:138:VAL:CG1	2:B:139:ASP:H	2.35	0.40
1:A:23:PHE:CE1	1:A:55:HIS:HD2	2.39	0.40
1:A:167:TYR:N	1:A:167:TYR:CD1	2.83	0.40
2:B:99:LYS:HG2	2:B:100:VAL:N	2.36	0.40
2:B:116:TYR:O	2:B:132:GLY:HA2	2.22	0.40
1:A:3:TYR:CE1	1:A:119:LEU:HG	2.57	0.40
1:A:61:PHE:N	1:A:61:PHE:HD1	2.17	0.40
1:A:122:GLN:CD	1:A:125:THR:H	2.30	0.40
2:B:44:VAL:HG23	2:B:108:ALA:HA	2.03	0.40
2:B:252:ALA:O	2:B:257:LEU:HB2	2.21	0.40
2:B:352:LEU:HD12	2:B:352:LEU:C	2.46	0.40
2:B:370:ASN:ND2	2:B:370:ASN:N	2.67	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%)	266 (88%)	25 (8%)	11 (4%)	2 6
2	B	391/395 (99%)	334 (85%)	43 (11%)	14 (4%)	2 6
All	All	693/700 (99%)	600 (87%)	68 (10%)	25 (4%)	2 6

All (25) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	51	GLY
1	A	67	ALA
1	A	73	ALA
2	B	140	ILE
2	B	314	ALA
2	B	330	VAL
1	A	66	GLU
2	B	39	ASN
2	B	97	GLY
2	B	126	ASN
2	B	178	GLY
2	B	328	GLY
2	B	391	SER
1	A	52	GLY
2	B	108	ALA
1	A	69	GLU
1	A	119	LEU
1	A	149	HIS
1	A	237	PRO
2	B	91	LYS
1	A	95	ALA
2	B	302	GLU
2	B	347	GLU
2	B	345	GLU
1	A	47	THR

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%)	219 (92%)	18 (8%)	12	30
2	B	317/319 (99%)	284 (90%)	33 (10%)	7	17
All	All	554/556 (100%)	503 (91%)	51 (9%)	8	22

All (51) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	4	THR
1	A	17	LYS
1	A	33	GLN
1	A	37	GLU
1	A	40	THR
1	A	41	ASN
1	A	43	VAL
1	A	61	PHE
1	A	70	GLN
1	A	124	LYS
1	A	127	LEU
1	A	181	SER
1	A	221	ASN
1	A	237	PRO
1	A	256	ARG
1	A	272	LYS
1	A	276	THR
1	A	303	ARG
2	B	1	MET
2	B	26	ASP
2	B	32	LEU
2	B	71	LYS
2	B	73	PRO
2	B	78	GLN
2	B	93	THR
2	B	96	GLU
2	B	107	GLU
2	B	109	LEU
2	B	111	ILE
2	B	113	ARG
2	B	124	SER
2	B	130	LEU
2	B	152	PHE
2	B	155	GLN
2	B	164	ASP
2	B	165	SER
2	B	246	GLU
2	B	249	GLU
2	B	269	PHE
2	B	285	LEU
2	B	293	PHE
2	B	300	VAL
2	B	330	VAL

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Mol	Chain	Res	Type
2	B	346	LEU
2	B	347	GLU
2	B	348	LEU
2	B	350	VAL
2	B	369	THR
2	B	373	LEU
2	B	379	VAL
2	B	386	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (18) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	33	GLN
1	A	55	HIS
1	A	221	ASN
1	A	225	ASN
1	A	233	HIS
2	B	4	GLN
2	B	20	GLN
2	B	135	GLN
2	B	155	GLN
2	B	168	GLN
2	B	173	ASN
2	B	181	GLN
2	B	182	ASN
2	B	183	GLN
2	B	250	ASN
2	B	324	ASN
2	B	337	ASN
2	B	370	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	1.81	3 (27%)	8,20,22	1.90	2 (25%)

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 (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	259	NEP	P-O3P	3.49	1.51	1.46
1	A	259	NEP	P-O1P	-3.22	1.48	1.56
1	A	259	NEP	P-O2P	-2.89	1.49	1.56

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	259	NEP	O1P-P-O3P	-4.11	102.84	112.95
1	A	259	NEP	CE1-ND1-CG	2.45	109.73	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
1	A	259	NEP	CA-CB-CG-ND1

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	A	259	NEP	1	0

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	SO4	B	396	-	4,4,4	0.47	0	6,6,6	0.22	0
3	SO4	A	307	-	4,4,4	0.45	0	6,6,6	0.45	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	304/305 (99%)	-0.25	4 (1%) 75 73	16, 35, 63, 75	0
2	B	393/395 (99%)	0.02	4 (1%) 79 78	18, 50, 72, 83	0
All	All	697/700 (99%)	-0.09	8 (1%) 78 76	16, 44, 70, 83	0

All (8) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	329	ILE	4.5
1	A	44	GLY	2.8
1	A	57	GLY	2.7
1	A	60	VAL	2.5
2	B	393	THR	2.2
1	A	75	ALA	2.2
2	B	126	ASN	2.1
2	B	300	VAL	2.1

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, 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
1	NEP	A	259	14/15	0.98	0.05	16,20,21,24	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, 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	SO4	B	396	5/5	0.89	0.10	71,71,72,72	0
3	SO4	A	307	5/5	0.95	0.06	50,50,51,52	0

6.5 Other polymers [i](#)

There are no such residues in this entry.