



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 09:48 AM UTC

PDB ID : 2VCY / pdb_00002vcy
Title : Crystal Structure of 2-Enoyl Thioester Reductase of Human FAS II
Authors : Haapalainen, A.M.; Pudas, R.; Smart, O.S.; Wierenga, R.K.
Deposited on : 2007-09-28
Resolution : 2.41 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

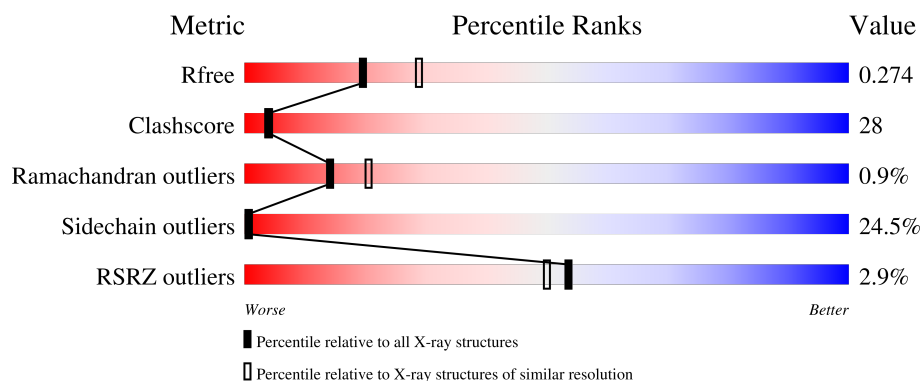
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.41 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	6062 (2.44-2.40)
Clashscore	190562	6562 (2.44-2.40)
Ramachandran outliers	187476	6481 (2.44-2.40)
Sidechain outliers	187428	6482 (2.44-2.40)
RSRZ outliers	180081	6066 (2.44-2.40)

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	344	
1	B	344	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	SO4	A	1378	-	-	X	-

2 Entry composition [i](#)

There are 3 unique types of molecules in this entry. The entry contains 5401 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 TRANS-2-ENOYL-COA REDUCTASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	332	Total	C	N	O	S	0	0	0
			2528	1596	448	470	14			
1	B	332	Total	C	N	O	S	0	0	0
			2528	1596	448	470	14			

- Molecule 2 is SULFATE ION (CCD ID: SO4) (formula: O₄S).



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

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

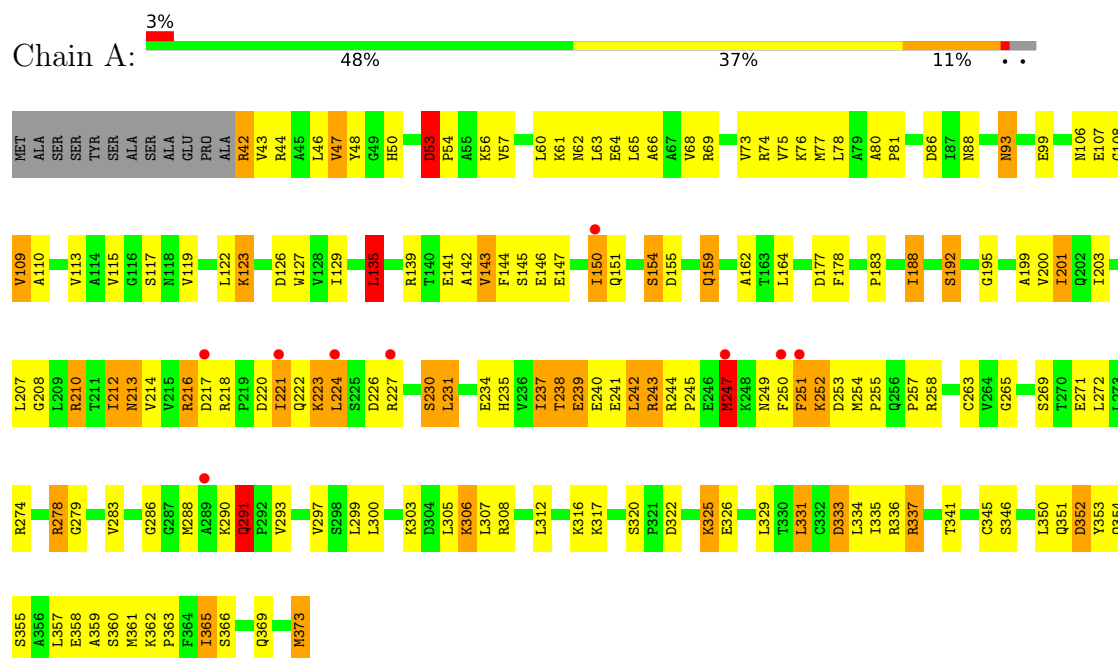
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	153	Total	O	0	0
			153	153		
3	B	137	Total	O	0	0
			137	137		

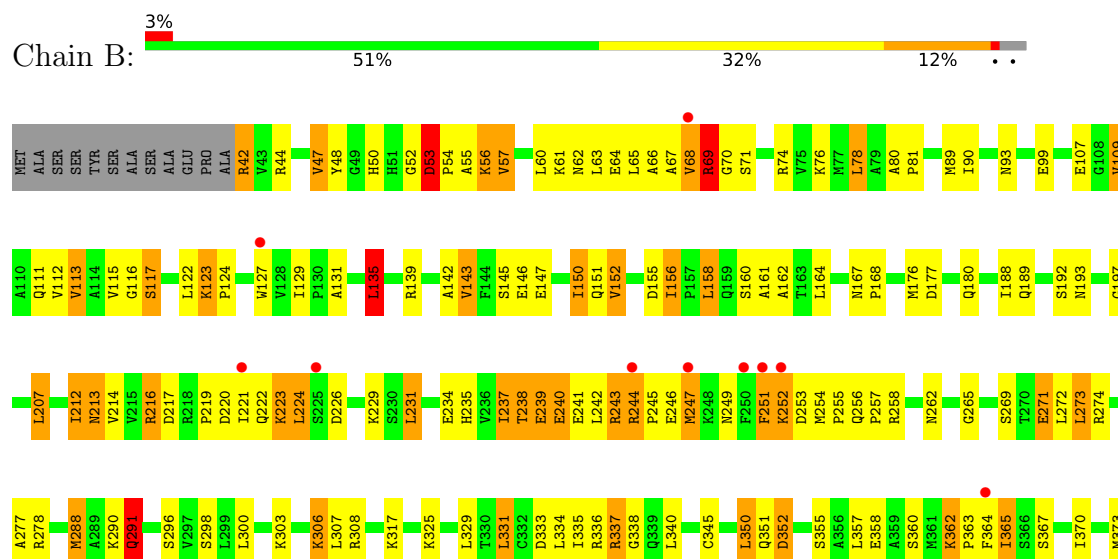
3 Residue-property plots

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: TRANS-2-ENOYL-COA REDUCTASE



• Molecule 1: TRANS-2-ENOYL-COA REDUCTASE



4 Data and refinement statistics

Property	Value	Source
Space group	P 42 21 2	Depositor
Cell constants a, b, c, α , β , γ	104.62Å 104.62Å 146.56Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	33.79 – 2.41 33.79 – 2.41	Depositor EDS
% Data completeness (in resolution range)	84.4 (33.79-2.41) 84.6 (33.79-2.41)	Depositor EDS
R_{merge}	0.05	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.01 (at 2.42Å)	Xtriage
Refinement program	BUSTER-TNT 2.1.1	Depositor
R, R_{free}	0.207 , 0.267 0.212 , 0.274	Depositor DCC
R_{free} test set	1391 reflections (5.12%)	wwPDB-VP
Wilson B-factor (Å ²)	49.9	Xtriage
Anisotropy	0.208	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 54.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.51$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	5401	wwPDB-VP
Average B, all atoms (Å ²)	56.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.42% 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: 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	0.50	0/2572	1.04	14/3486 (0.4%)
1	B	0.52	0/2572	1.04	20/3486 (0.6%)
All	All	0.51	0/5144	1.04	34/6972 (0.5%)

There are no bond length outliers.

All (34) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	291	GLN	CA-C-N	10.38	131.03	119.92
1	A	291	GLN	C-N-CA	10.38	131.03	119.92
1	B	156	ILE	CA-C-N	-10.02	109.73	119.85
1	B	156	ILE	C-N-CA	-10.02	109.73	119.85
1	A	247	MET	N-CA-C	-8.29	105.17	114.62
1	A	135	LEU	N-CA-C	7.71	119.68	111.28
1	A	80	ALA	CA-C-N	-7.53	112.98	120.21
1	A	80	ALA	C-N-CA	-7.53	112.98	120.21
1	B	247	MET	N-CA-C	-7.44	106.14	114.62
1	B	135	LEU	N-CA-C	7.26	119.19	111.28
1	B	291	GLN	CA-C-N	7.23	128.87	119.84
1	B	291	GLN	C-N-CA	7.23	128.87	119.84
1	B	362	LYS	CA-C-N	6.97	126.60	119.56
1	B	362	LYS	C-N-CA	6.97	126.60	119.56
1	A	320	SER	CA-C-N	6.95	126.76	119.05
1	A	320	SER	C-N-CA	6.95	126.76	119.05
1	B	272	LEU	N-CA-C	-6.39	104.40	111.36
1	B	239	GLU	N-CA-C	-6.28	104.44	111.28
1	A	177	ASP	N-CA-C	6.20	120.45	113.01
1	B	80	ALA	CA-C-N	-6.14	114.32	120.21
1	B	80	ALA	C-N-CA	-6.14	114.32	120.21
1	A	47	VAL	N-CA-C	6.03	117.44	108.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	53	ASP	CA-C-N	5.80	127.09	119.84
1	A	53	ASP	C-N-CA	5.80	127.09	119.84
1	B	262	ASN	N-CA-C	5.71	118.55	109.24
1	B	213	ASN	N-CA-C	5.40	117.53	108.73
1	A	250	PHE	N-CA-C	-5.37	105.33	111.07
1	B	152	VAL	CA-C-N	-5.32	114.30	119.78
1	B	152	VAL	C-N-CA	-5.32	114.30	119.78
1	B	258	ARG	N-CA-C	-5.30	106.81	113.28
1	B	177	ASP	N-CA-C	5.27	119.56	113.18
1	A	239	GLU	N-CA-C	-5.12	105.19	111.75
1	B	53	ASP	CA-C-N	5.00	126.10	119.84
1	B	53	ASP	C-N-CA	5.00	126.10	119.84

There are no chirality outliers.

There are no planarity outliers.

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	2528	0	2596	150	0
1	B	2528	0	2596	138	0
2	A	25	0	0	3	0
2	B	30	0	0	0	0
3	A	153	0	0	14	0
3	B	137	0	0	13	0
All	All	5401	0	5192	285	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 28.

All (285) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:42:ARG:HD3	1:A:62:ASN:HB3	1.28	1.10
1:B:74:ARG:HE	1:B:113:VAL:HG21	1.14	1.05

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:188:ILE:HG13	1:A:212:ILE:HG13	1.37	1.04
1:A:74:ARG:HE	1:A:113:VAL:HG21	1.27	0.95
1:B:288:MET:HB2	1:B:291:GLN:HB2	1.45	0.94
1:A:288:MET:HB2	1:A:291:GLN:HB2	1.49	0.93
1:B:251:PHE:CZ	1:B:257:PRO:HD3	2.04	0.93
1:A:188:ILE:HG13	1:A:212:ILE:CG1	1.99	0.91
1:A:48:TYR:HB2	1:A:57:VAL:HG12	1.54	0.88
1:A:350:LEU:HD22	1:A:373:MET:CE	2.04	0.87
1:A:308:ARG:HD2	1:B:306:LYS:HG3	1.58	0.85
1:A:237:ILE:HD11	1:A:242:LEU:HB2	1.58	0.85
1:A:42:ARG:HD3	1:A:62:ASN:CB	2.06	0.85
1:A:242:LEU:HD21	1:A:271:GLU:HB3	1.59	0.83
1:A:150:ILE:HD12	1:A:151:GLN:N	1.94	0.81
1:B:237:ILE:HD11	1:B:242:LEU:HB2	1.62	0.81
1:B:150:ILE:HD12	1:B:151:GLN:N	1.95	0.81
1:A:42:ARG:HG3	1:A:43:VAL:N	1.95	0.80
1:A:234:GLU:HG2	1:A:235:HIS:CD2	2.16	0.80
1:B:66:ALA:HB3	1:B:143:VAL:HG11	1.64	0.80
1:B:193:ASN:OD1	1:B:224:LEU:HD21	1.82	0.80
1:B:249:ASN:O	1:B:252:LYS:HB2	1.81	0.79
1:A:249:ASN:O	1:A:252:LYS:HB2	1.83	0.79
1:B:254:MET:HB2	1:B:255:PRO:HD2	1.62	0.79
1:B:127:TRP:CH2	1:B:158:LEU:HB2	2.18	0.78
1:B:333:ASP:O	1:B:337:ARG:HG3	1.83	0.78
1:B:188:ILE:HG13	1:B:212:ILE:HG13	1.65	0.78
1:B:81:PRO:CG	1:B:107:GLU:HG2	2.14	0.78
1:B:242:LEU:O	1:B:247:MET:HG3	1.84	0.77
1:B:74:ARG:HB3	1:B:113:VAL:HG22	1.66	0.77
1:B:109:VAL:HG22	1:B:162:ALA:HB2	1.67	0.77
1:A:308:ARG:CD	1:B:306:LYS:HG3	2.15	0.76
1:B:74:ARG:HE	1:B:113:VAL:CG2	1.97	0.76
1:A:123:LYS:HE2	1:A:126:ASP:OD1	1.87	0.75
1:A:251:PHE:CE2	1:A:257:PRO:HD3	2.22	0.74
1:B:192:SER:OG	1:B:213:ASN:HB3	1.88	0.73
1:B:78:LEU:HD23	1:B:158:LEU:HD12	1.71	0.73
1:A:150:ILE:HD13	1:A:325:LYS:HE2	1.71	0.72
1:A:254:MET:HB2	1:A:255:PRO:HD2	1.71	0.72
1:B:192:SER:CB	1:B:213:ASN:HB3	2.19	0.72
1:B:338:GLY:HA2	3:B:2121:HOH:O	1.89	0.70
1:A:48:TYR:HB2	1:A:57:VAL:CG1	2.21	0.70
1:A:46:LEU:HD23	1:A:60:LEU:HD12	1.72	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:81:PRO:CG	1:A:107:GLU:HG2	2.23	0.69
1:A:74:ARG:HE	1:A:113:VAL:CG2	2.05	0.69
1:B:220:ASP:OD2	1:B:223:LYS:HG3	1.92	0.69
1:A:66:ALA:HB3	1:A:143:VAL:HG11	1.75	0.69
1:B:242:LEU:HD21	1:B:271:GLU:HB3	1.75	0.68
1:B:300:LEU:HD21	1:B:307:LEU:CD1	2.23	0.68
1:B:139:ARG:HD2	1:B:142:ALA:HB2	1.76	0.68
1:A:62:ASN:O	1:A:63:LEU:HD12	1.93	0.68
1:A:333:ASP:O	1:A:337:ARG:HG3	1.93	0.68
1:B:62:ASN:O	1:B:63:LEU:HD12	1.93	0.67
1:A:239:GLU:O	1:A:243:ARG:HG2	1.95	0.67
1:B:155:ASP:OD2	1:B:336:ARG:NH1	2.28	0.67
1:B:238:THR:OG1	1:B:241:GLU:HG3	1.95	0.66
1:B:352:ASP:OD1	1:B:352:ASP:N	2.25	0.66
1:B:193:ASN:HB2	1:B:224:LEU:HD11	1.77	0.66
1:A:74:ARG:NE	1:A:113:VAL:HG21	2.08	0.65
1:A:155:ASP:OD2	1:A:336:ARG:NH1	2.29	0.65
1:B:78:LEU:HD23	1:B:158:LEU:CD1	2.25	0.65
1:A:258:ARG:HG2	3:A:2094:HOH:O	1.95	0.65
1:A:192:SER:CB	1:A:213:ASN:HB3	2.26	0.65
1:A:243:ARG:NH1	1:A:243:ARG:HG3	2.12	0.65
1:A:150:ILE:HD12	1:A:151:GLN:H	1.62	0.64
1:A:150:ILE:HD13	1:A:325:LYS:CE	2.27	0.64
1:A:312:LEU:HG	1:A:316:LYS:HE3	1.80	0.64
1:B:76:LYS:HD3	3:B:2014:HOH:O	1.98	0.64
1:A:61:LYS:NZ	3:A:2011:HOH:O	2.30	0.63
1:B:156:ILE:CD1	1:B:161:ALA:HB2	2.28	0.63
1:B:150:ILE:HD12	1:B:151:GLN:H	1.61	0.63
1:A:86:ASP:OD1	1:A:106:ASN:ND2	2.30	0.63
1:B:74:ARG:NE	1:B:113:VAL:HG21	2.00	0.63
1:B:135:LEU:HB2	3:B:2044:HOH:O	1.99	0.63
1:A:192:SER:OG	1:A:213:ASN:HB3	1.97	0.63
1:A:369:GLN:HB2	3:A:2146:HOH:O	1.98	0.63
1:A:117:SER:HB2	3:A:2039:HOH:O	1.99	0.62
1:B:156:ILE:HD11	1:B:161:ALA:HB2	1.79	0.62
1:A:155:ASP:CG	1:A:336:ARG:HH12	2.06	0.62
1:B:240:GLU:HG3	1:B:241:GLU:N	2.14	0.62
1:A:50:HIS:O	1:A:57:VAL:HG11	1.98	0.62
1:B:42:ARG:HD2	1:B:62:ASN:HB3	1.79	0.62
1:B:351:GLN:HB3	1:B:352:ASP:OD1	1.99	0.62
1:A:109:VAL:HG22	1:A:162:ALA:HA	1.81	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:242:LEU:HD21	1:A:271:GLU:CB	2.28	0.62
1:A:243:ARG:HG3	1:A:243:ARG:HH11	1.65	0.62
1:A:42:ARG:CD	1:A:62:ASN:HB3	2.18	0.61
1:B:251:PHE:CE2	1:B:257:PRO:HD3	2.34	0.61
1:A:242:LEU:O	1:A:247:MET:HG3	2.00	0.61
1:A:242:LEU:CD2	1:A:271:GLU:HB3	2.30	0.61
1:A:278:ARG:NH1	3:A:2099:HOH:O	2.29	0.60
1:A:127:TRP:CE3	1:A:154:SER:HA	2.36	0.60
1:A:123:LYS:NZ	3:A:2041:HOH:O	2.30	0.60
1:B:129:ILE:HG13	1:B:150:ILE:HG23	1.84	0.60
1:A:306:LYS:HD3	3:B:2135:HOH:O	2.02	0.59
1:B:239:GLU:O	1:B:243:ARG:HG2	2.03	0.59
1:A:195:GLY:N	2:A:1377:SO4:O2	2.29	0.59
1:A:352:ASP:OD1	1:A:352:ASP:N	2.36	0.59
1:B:66:ALA:HA	3:B:2010:HOH:O	2.02	0.58
1:B:288:MET:HE2	3:B:2094:HOH:O	2.02	0.58
1:A:48:TYR:CB	1:A:57:VAL:HG12	2.28	0.58
1:A:188:ILE:HD13	1:A:272:LEU:CD2	2.33	0.58
1:A:212:ILE:C	1:A:212:ILE:HD12	2.29	0.58
1:B:78:LEU:HB3	1:B:158:LEU:HD11	1.86	0.58
1:A:254:MET:HB2	1:A:255:PRO:CD	2.34	0.58
1:B:243:ARG:NH1	1:B:243:ARG:HG3	2.19	0.58
1:B:306:LYS:NZ	3:B:2100:HOH:O	2.30	0.58
1:A:210:ARG:HB3	1:A:234:GLU:OE1	2.04	0.57
1:A:325:LYS:O	1:A:329:LEU:HG	2.04	0.57
1:A:244:ARG:HB3	1:A:245:PRO:CD	2.34	0.57
1:A:331:LEU:O	1:A:335:ILE:HG13	2.04	0.57
1:A:258:ARG:NH1	3:A:2095:HOH:O	2.30	0.57
1:B:265:GLY:HA2	1:B:269:SER:HB3	1.86	0.57
1:A:46:LEU:HD23	1:A:60:LEU:CD1	2.34	0.56
1:B:131:ALA:HB3	3:B:2046:HOH:O	2.05	0.56
1:A:109:VAL:HG22	1:A:162:ALA:CA	2.36	0.56
1:A:115:VAL:HG11	1:A:122:LEU:O	2.06	0.56
1:A:139:ARG:HD2	1:A:142:ALA:HB2	1.88	0.56
1:B:350:LEU:HD12	1:B:350:LEU:O	2.06	0.56
1:A:322:ASP:O	1:A:326:GLU:HG3	2.06	0.55
1:A:350:LEU:HD22	1:A:373:MET:HE2	1.86	0.55
1:A:222:GLN:O	1:A:226:ASP:OD1	2.24	0.55
1:B:278:ARG:HA	1:B:303:LYS:HG3	1.88	0.55
1:A:220:ASP:OD2	1:A:223:LYS:HG3	2.07	0.55
1:A:238:THR:OG1	1:A:241:GLU:HG3	2.07	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:129:ILE:HG13	1:A:150:ILE:HG23	1.89	0.54
1:B:164:LEU:HD11	1:B:331:LEU:HB3	1.90	0.54
1:B:336:ARG:HG3	1:B:336:ARG:HH11	1.71	0.54
1:A:188:ILE:CG1	1:A:212:ILE:HG13	2.25	0.53
1:B:237:ILE:HG12	1:B:238:THR:N	2.20	0.53
1:B:81:PRO:HG2	1:B:107:GLU:HG2	1.88	0.53
1:B:336:ARG:NH1	1:B:336:ARG:HG3	2.24	0.53
1:A:243:ARG:HH11	1:A:243:ARG:CG	2.21	0.53
1:B:53:ASP:O	1:B:57:VAL:HG22	2.09	0.53
1:B:212:ILE:HD12	1:B:212:ILE:C	2.33	0.53
1:A:288:MET:HG3	3:A:2096:HOH:O	2.08	0.53
1:B:112:VAL:HG12	1:B:124:PRO:HA	1.91	0.53
1:B:222:GLN:O	1:B:226:ASP:OD1	2.27	0.53
1:B:188:ILE:HG13	1:B:212:ILE:CG1	2.36	0.52
1:B:109:VAL:HG22	1:B:162:ALA:CB	2.38	0.52
1:A:213:ASN:N	1:A:213:ASN:ND2	2.58	0.52
1:B:193:ASN:CG	1:B:224:LEU:HD21	2.35	0.52
1:B:123:LYS:NZ	3:B:2038:HOH:O	2.42	0.52
1:A:44:ARG:HD2	3:A:2003:HOH:O	2.10	0.52
1:A:150:ILE:HD11	1:A:325:LYS:CG	2.40	0.52
1:A:46:LEU:HG	1:A:350:LEU:HD11	1.91	0.51
1:A:216:ARG:N	2:A:1378:SO4:O2	2.34	0.51
1:B:300:LEU:HD21	1:B:307:LEU:HD11	1.91	0.51
1:B:243:ARG:CG	1:B:243:ARG:HH11	2.22	0.51
1:A:192:SER:HB3	1:A:213:ASN:HB3	1.92	0.51
1:A:265:GLY:HA2	1:A:269:SER:HB3	1.93	0.51
1:B:50:HIS:O	1:B:57:VAL:HG11	2.11	0.51
1:B:109:VAL:CG2	1:B:162:ALA:HB2	2.39	0.51
1:B:335:ILE:HG13	1:B:340:LEU:HD23	1.93	0.51
1:B:234:GLU:OE2	1:B:235:HIS:NE2	2.44	0.50
1:B:325:LYS:O	1:B:329:LEU:HG	2.11	0.50
1:B:127:TRP:HH2	1:B:158:LEU:HB2	1.71	0.50
1:B:47:VAL:HG23	1:B:48:TYR:N	2.27	0.50
1:B:127:TRP:HB3	1:B:152:VAL:CG2	2.42	0.50
1:B:192:SER:HB3	1:B:213:ASN:HB3	1.93	0.50
1:B:256:GLN:HB3	1:B:277:ALA:HB2	1.92	0.50
1:A:75:VAL:O	1:A:141:GLU:HG3	2.12	0.50
1:B:242:LEU:CD2	1:B:271:GLU:HB3	2.42	0.50
1:B:245:PRO:HD2	1:B:246:GLU:H	1.76	0.49
1:B:214:VAL:HG22	1:B:237:ILE:HD13	1.93	0.49
1:B:244:ARG:HB3	1:B:245:PRO:CD	2.43	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:336:ARG:HH11	1:A:336:ARG:CG	2.25	0.49
1:A:201:ILE:HG21	1:A:231:LEU:HB3	1.94	0.49
1:B:243:ARG:HG3	1:B:243:ARG:HH11	1.77	0.49
1:A:150:ILE:CD1	1:A:325:LYS:HG3	2.43	0.48
1:B:127:TRP:HB3	1:B:152:VAL:HG22	1.95	0.48
1:B:278:ARG:HG3	1:B:303:LYS:HE3	1.95	0.48
1:A:218:ARG:H	1:A:221:ILE:HD13	1.76	0.48
1:A:373:MET:HE3	1:A:373:MET:HB3	1.70	0.48
1:B:155:ASP:CG	1:B:336:ARG:HH12	2.20	0.48
1:B:265:GLY:CA	1:B:269:SER:HB3	2.44	0.48
1:A:150:ILE:HD12	1:A:150:ILE:C	2.39	0.48
1:A:188:ILE:HD13	1:A:272:LEU:HD23	1.94	0.48
1:A:42:ARG:HD3	1:A:62:ASN:CG	2.39	0.48
1:A:231:LEU:HD12	1:A:231:LEU:HA	1.78	0.48
1:B:254:MET:HB2	1:B:255:PRO:CD	2.37	0.48
1:A:135:LEU:HA	1:A:135:LEU:HD23	1.72	0.47
1:A:336:ARG:HD2	3:A:2131:HOH:O	2.13	0.47
1:A:81:PRO:HG3	1:A:107:GLU:HG2	1.96	0.47
1:A:234:GLU:HB2	3:A:2086:HOH:O	2.13	0.47
1:A:242:LEU:HA	1:A:247:MET:HG3	1.95	0.47
1:B:61:LYS:NZ	3:B:2005:HOH:O	2.29	0.47
1:B:212:ILE:HG13	1:B:212:ILE:O	2.13	0.47
1:B:78:LEU:HD21	1:B:127:TRP:NE1	2.29	0.47
1:A:242:LEU:HA	1:A:247:MET:CG	2.44	0.47
1:A:336:ARG:HH11	1:A:336:ARG:HG2	1.80	0.47
1:B:216:ARG:HE	1:B:216:ARG:HB2	1.52	0.47
1:A:243:ARG:HG2	1:A:243:ARG:H	1.59	0.47
1:A:217:ASP:HA	1:A:221:ILE:HD13	1.96	0.46
1:B:217:ASP:OD1	1:B:238:THR:HG21	2.15	0.46
1:B:245:PRO:CD	1:B:246:GLU:H	2.29	0.46
1:A:50:HIS:O	1:A:57:VAL:CG1	2.62	0.46
1:A:214:VAL:HG22	1:A:237:ILE:HD13	1.98	0.46
1:B:129:ILE:HG23	1:B:152:VAL:HG11	1.96	0.46
1:A:359:ALA:O	1:A:365:ILE:HG13	2.15	0.46
1:A:224:LEU:HD23	1:A:224:LEU:HA	1.73	0.46
1:A:263:CYS:SG	1:A:286:GLY:HA3	2.56	0.46
1:A:299:LEU:HB3	1:A:305:LEU:HD12	1.98	0.46
1:B:231:LEU:HD12	1:B:231:LEU:HA	1.67	0.46
1:A:316:LYS:NZ	3:A:2119:HOH:O	2.49	0.45
1:B:188:ILE:CG1	1:B:212:ILE:HG13	2.40	0.45
1:B:234:GLU:HB2	3:B:2073:HOH:O	2.15	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:365:ILE:HD11	1:B:367:SER:O	2.17	0.45
1:A:115:VAL:HB	1:A:119:VAL:HB	1.99	0.45
1:A:243:ARG:CD	1:A:271:GLU:HG3	2.47	0.45
1:A:288:MET:HE2	1:A:288:MET:HB3	1.71	0.45
1:B:244:ARG:CB	1:B:245:PRO:CD	2.95	0.45
1:B:67:ALA:C	1:B:69:ARG:H	2.23	0.45
1:B:189:GLN:OE1	1:B:197:GLY:HA2	2.17	0.45
1:B:193:ASN:CB	1:B:224:LEU:HD11	2.44	0.45
1:A:199:ALA:O	1:A:203:ILE:HD12	2.16	0.45
1:A:353:TYR:CE2	1:A:354:GLN:HG2	2.52	0.45
1:B:52:GLY:O	1:B:57:VAL:HG21	2.16	0.45
1:B:243:ARG:NH1	1:B:243:ARG:CG	2.78	0.45
1:A:265:GLY:CA	1:A:269:SER:HB3	2.47	0.44
1:A:252:LYS:HE3	3:A:2091:HOH:O	2.17	0.44
1:A:243:ARG:HD3	1:A:271:GLU:HG3	2.00	0.44
1:B:81:PRO:HG3	1:B:107:GLU:HG2	1.97	0.44
1:B:167:ASN:HB2	1:B:168:PRO:HD3	1.99	0.44
1:B:224:LEU:HA	1:B:224:LEU:HD23	1.65	0.44
1:A:53:ASP:HA	1:A:54:PRO:HD3	1.88	0.44
1:B:67:ALA:O	1:B:69:ARG:HG3	2.18	0.44
1:A:88:ASN:HB3	1:A:93:ASN:O	2.17	0.44
1:B:65:LEU:HD11	1:B:143:VAL:HG12	1.99	0.44
1:B:81:PRO:CD	1:B:107:GLU:HG2	2.48	0.44
1:B:158:LEU:HD23	3:B:2051:HOH:O	2.18	0.44
1:A:365:ILE:O	1:A:365:ILE:HG23	2.18	0.43
1:A:279:GLY:O	1:A:306:LYS:HE2	2.19	0.43
1:B:109:VAL:HG11	1:B:161:ALA:CB	2.48	0.43
1:A:362:LYS:HA	1:A:363:PRO:HD2	1.84	0.43
1:B:65:LEU:CD1	1:B:143:VAL:HG12	2.49	0.43
1:B:115:VAL:HG11	1:B:122:LEU:O	2.18	0.43
1:A:278:ARG:HA	1:A:303:LYS:HG3	1.99	0.43
1:A:230:SER:HB2	3:A:2085:HOH:O	2.19	0.43
1:A:350:LEU:HD22	1:A:373:MET:HE3	1.97	0.43
1:B:219:PRO:HB2	3:B:2074:HOH:O	2.18	0.43
1:A:308:ARG:NE	1:B:306:LYS:HG3	2.33	0.43
1:B:345:CYS:HB2	1:B:370:ILE:HG13	2.01	0.43
1:B:362:LYS:HA	1:B:363:PRO:HD2	1.87	0.43
1:A:183:PRO:HA	1:A:208:GLY:O	2.18	0.42
1:A:251:PHE:CZ	1:A:257:PRO:HG3	2.54	0.42
1:A:65:LEU:HD12	1:A:65:LEU:HA	1.83	0.42
1:A:216:ARG:HB2	2:A:1378:SO4:O2	2.18	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:54:PRO:C	1:B:56:LYS:H	2.27	0.42
1:B:69:ARG:H	1:B:69:ARG:HG3	1.52	0.42
1:A:123:LYS:HG3	1:A:126:ASP:OD2	2.19	0.42
1:B:78:LEU:CD2	1:B:158:LEU:CD1	2.96	0.42
1:B:151:GLN:HG3	1:B:152:VAL:N	2.33	0.42
1:B:247:MET:C	1:B:249:ASN:H	2.27	0.42
1:B:109:VAL:HG11	1:B:161:ALA:HB1	2.00	0.42
1:B:150:ILE:HD12	1:B:150:ILE:C	2.45	0.41
1:A:73:VAL:N	1:A:144:PHE:O	2.48	0.41
1:A:159:GLN:H	1:A:159:GLN:HG2	1.63	0.41
1:A:178:PHE:CD2	1:A:283:VAL:HG21	2.56	0.41
1:B:70:GLY:O	1:B:116:GLY:HA3	2.20	0.41
1:A:251:PHE:CZ	1:A:257:PRO:HD3	2.56	0.41
1:A:77:MET:HE2	1:A:110:ALA:HB2	2.01	0.41
1:A:75:VAL:HB	1:A:110:ALA:HB1	2.02	0.41
1:A:81:PRO:CD	1:A:107:GLU:HG2	2.50	0.41
1:A:164:LEU:HD11	1:A:331:LEU:HB3	2.01	0.41
1:B:78:LEU:CG	1:B:158:LEU:HD11	2.50	0.41
1:B:112:VAL:CG1	1:B:124:PRO:HA	2.50	0.41
1:B:243:ARG:HD2	1:B:271:GLU:HG2	2.02	0.41
1:B:247:MET:C	1:B:249:ASN:N	2.78	0.41
1:A:188:ILE:HG13	1:A:212:ILE:CD1	2.48	0.41
1:A:214:VAL:HG22	1:A:237:ILE:CD1	2.51	0.41
1:A:336:ARG:NH1	1:A:336:ARG:CG	2.83	0.41
1:A:345:CYS:O	1:A:345:CYS:SG	2.79	0.41
1:B:176:MET:CE	1:B:207:LEU:HD21	2.50	0.41
1:A:150:ILE:HD11	1:A:325:LYS:HG2	2.03	0.40
1:A:220:ASP:C	1:A:222:GLN:N	2.79	0.40
1:A:251:PHE:CE2	1:A:257:PRO:CD	2.98	0.40
1:B:67:ALA:O	1:B:69:ARG:N	2.49	0.40
1:A:300:LEU:HD21	1:A:307:LEU:CD1	2.51	0.40
1:B:48:TYR:CE2	1:B:90:ILE:HA	2.55	0.40
1:B:135:LEU:HA	1:B:135:LEU:HD23	1.78	0.40
1:B:273:LEU:HD12	1:B:273:LEU:HA	1.82	0.40
1:A:150:ILE:CD1	1:A:325:LYS:CG	2.99	0.40
1:A:107:GLU:HG3	1:A:108:GLY:N	2.36	0.40
1:B:364:PHE:N	1:B:364:PHE:CD1	2.90	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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	330/344 (96%)	307 (93%)	23 (7%)	0	100	100
1	B	330/344 (96%)	305 (92%)	19 (6%)	6 (2%)	6	8
All	All	660/688 (96%)	612 (93%)	42 (6%)	6 (1%)	14	20

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	68	VAL
1	B	69	ARG
1	B	117	SER
1	B	55	ALA
1	B	350	LEU
1	B	244	ARG

5.3.2 Protein sidechains

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	275/283 (97%)	205 (74%)	70 (26%)	0	0
1	B	275/283 (97%)	210 (76%)	65 (24%)	1	1
All	All	550/566 (97%)	415 (76%)	135 (24%)	1	1

All (135) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	42	ARG
1	A	47	VAL
1	A	53	ASP
1	A	56	LYS
1	A	64	GLU
1	A	68	VAL
1	A	69	ARG
1	A	76	LYS
1	A	78	LEU
1	A	93	ASN
1	A	99	GLU
1	A	109	VAL
1	A	123	LYS
1	A	135	LEU
1	A	143	VAL
1	A	145	SER
1	A	146	GLU
1	A	147	GLU
1	A	150	ILE
1	A	154	SER
1	A	159	GLN
1	A	188	ILE
1	A	192	SER
1	A	200	VAL
1	A	201	ILE
1	A	207	LEU
1	A	210	ARG
1	A	212	ILE
1	A	213	ASN
1	A	216	ARG
1	A	221	ILE
1	A	223	LYS
1	A	224	LEU
1	A	227	ARG
1	A	230	SER
1	A	231	LEU
1	A	237	ILE
1	A	238	THR
1	A	240	GLU
1	A	242	LEU
1	A	243	ARG
1	A	247	MET
1	A	251	PHE

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Mol	Chain	Res	Type
1	A	252	LYS
1	A	253	ASP
1	A	274	ARG
1	A	278	ARG
1	A	290	LYS
1	A	291	GLN
1	A	293	VAL
1	A	297	VAL
1	A	306	LYS
1	A	317	LYS
1	A	325	LYS
1	A	331	LEU
1	A	333	ASP
1	A	334	LEU
1	A	337	ARG
1	A	341	THR
1	A	346	SER
1	A	351	GLN
1	A	352	ASP
1	A	355	SER
1	A	357	LEU
1	A	358	GLU
1	A	360	SER
1	A	361	MET
1	A	365	ILE
1	A	366	SER
1	A	373	MET
1	B	42	ARG
1	B	44	ARG
1	B	47	VAL
1	B	53	ASP
1	B	56	LYS
1	B	57	VAL
1	B	60	LEU
1	B	64	GLU
1	B	68	VAL
1	B	69	ARG
1	B	71	SER
1	B	78	LEU
1	B	89	MET
1	B	93	ASN
1	B	99	GLU

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Mol	Chain	Res	Type
1	B	109	VAL
1	B	111	GLN
1	B	113	VAL
1	B	117	SER
1	B	123	LYS
1	B	135	LEU
1	B	143	VAL
1	B	145	SER
1	B	146	GLU
1	B	147	GLU
1	B	150	ILE
1	B	158	LEU
1	B	160	SER
1	B	180	GLN
1	B	207	LEU
1	B	212	ILE
1	B	216	ARG
1	B	221	ILE
1	B	223	LYS
1	B	224	LEU
1	B	229	LYS
1	B	231	LEU
1	B	237	ILE
1	B	238	THR
1	B	240	GLU
1	B	243	ARG
1	B	251	PHE
1	B	252	LYS
1	B	253	ASP
1	B	271	GLU
1	B	273	LEU
1	B	274	ARG
1	B	288	MET
1	B	290	LYS
1	B	291	GLN
1	B	296	SER
1	B	298	SER
1	B	306	LYS
1	B	308	ARG
1	B	317	LYS
1	B	331	LEU
1	B	334	LEU

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Mol	Chain	Res	Type
1	B	337	ARG
1	B	352	ASP
1	B	355	SER
1	B	357	LEU
1	B	358	GLU
1	B	360	SER
1	B	365	ILE
1	B	373	MET

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (14) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	88	ASN
1	A	111	GLN
1	A	235	HIS
1	A	249	ASN
1	A	256	GLN
1	A	291	GLN
1	A	351	GLN
1	A	369	GLN
1	B	88	ASN
1	B	93	ASN
1	B	111	GLN
1	B	256	GLN
1	B	351	GLN
1	B	354	GLN

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 oligosaccharides in this entry.

5.6 Ligand geometry

11 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
2	SO4	B	1377	-	4,4,4	0.39	0	6,6,6	0.10	0
2	SO4	B	1378	-	4,4,4	0.38	0	6,6,6	0.13	0
2	SO4	A	1375	-	4,4,4	0.33	0	6,6,6	0.25	0
2	SO4	A	1374	-	4,4,4	0.40	0	6,6,6	0.23	0
2	SO4	A	1376	-	4,4,4	0.46	0	6,6,6	0.18	0
2	SO4	B	1375	-	4,4,4	0.46	0	6,6,6	0.09	0
2	SO4	B	1376	-	4,4,4	0.30	0	6,6,6	0.08	0
2	SO4	B	1379	-	4,4,4	0.38	0	6,6,6	0.21	0
2	SO4	A	1378	-	4,4,4	0.49	0	6,6,6	0.29	0
2	SO4	A	1377	-	4,4,4	0.35	0	6,6,6	0.27	0
2	SO4	B	1374	-	4,4,4	0.47	0	6,6,6	0.22	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.

2 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	1378	SO4	2	0
2	A	1377	SO4	1	0

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

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	332/344 (96%)	0.14	9 (2%) 56 52	31, 51, 92, 129	0
1	B	332/344 (96%)	0.14	10 (3%) 52 49	30, 50, 91, 128	0
All	All	664/688 (96%)	0.14	19 (2%) 53 50	30, 51, 92, 129	0

All (19) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	251	PHE	4.4
1	A	251	PHE	4.1
1	B	221	ILE	3.1
1	A	250	PHE	3.0
1	A	221	ILE	2.5
1	A	247	MET	2.5
1	B	364	PHE	2.4
1	B	68	VAL	2.4
1	A	217	ASP	2.4
1	B	127	TRP	2.4
1	B	247	MET	2.3
1	A	289	ALA	2.1
1	A	224	LEU	2.1
1	A	227	ARG	2.1
1	B	225	SER	2.1
1	B	252	LYS	2.1
1	B	244	ARG	2.0
1	B	250	PHE	2.0
1	A	150	ILE	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($\text{\AA}^2$)	Q<0.9
2	SO4	B	1377	5/5	0.63	0.21	71,75,76,77	5
2	SO4	B	1376	5/5	0.83	0.13	93,98,99,99	5
2	SO4	B	1374	5/5	0.83	0.13	70,74,75,76	5
2	SO4	A	1375	5/5	0.84	0.09	72,76,77,78	5
2	SO4	A	1376	5/5	0.86	0.11	67,72,73,73	5
2	SO4	B	1375	5/5	0.88	0.14	75,79,80,82	5
2	SO4	A	1374	5/5	0.91	0.10	64,67,68,69	5
2	SO4	B	1378	5/5	0.91	0.10	81,85,86,87	0
2	SO4	B	1379	5/5	0.91	0.12	57,61,63,64	0
2	SO4	A	1377	5/5	0.94	0.12	65,68,70,70	0
2	SO4	A	1378	5/5	0.96	0.10	57,61,62,63	0

6.5 Other polymers [i](#)

There are no such residues in this entry.