



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 04:03 AM UTC

PDB ID : 1QVT / pdb_00001qvt
Title : CRYSTAL STRUCTURE OF THE MULTIDRUG BINDING TRANSCRIPTIONAL REPRESSOR QACR BOUND TO THE DRUG PROFLAVINE
Authors : Schumacher, M.A.; Miller, M.C.; Brennan, R.G.
Deposited on : 2003-08-28
Resolution : 2.89 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:

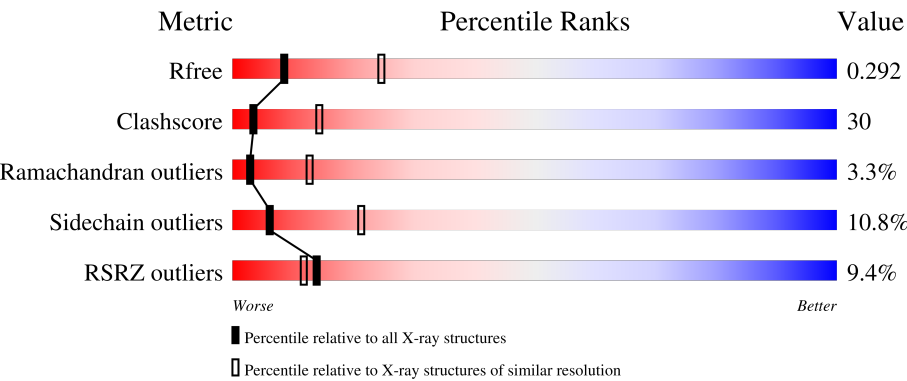
MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.89 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	2481 (2.90-2.90)
Clashscore	190562	2690 (2.90-2.90)
Ramachandran outliers	187476	2623 (2.90-2.90)
Sidechain outliers	187428	2625 (2.90-2.90)
RSRZ outliers	180081	2481 (2.90-2.90)

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	194	4% 48% 39% 8% .
1	B	194	15% 38% 45% 12% ..
1	D	194	11% 35% 53% 8% ..
1	E	194	6% 42% 46% 7% .

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	213	-	-	X	-
2	SO4	B	210	-	-	X	-
2	SO4	E	212	-	-	X	-

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 6416 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 Transcriptional regulator qacR.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	B	186	Total	C	N	O	S	0	0	0
			1547	998	252	295	2			
1	D	186	Total	C	N	O	S	0	0	0
			1547	998	252	295	2			
1	A	186	Total	C	N	O	S	0	0	0
			1547	998	252	295	2			
1	E	186	Total	C	N	O	S	0	0	0
			1547	998	252	295	2			

There are 28 discrepancies between the modelled and reference sequences:

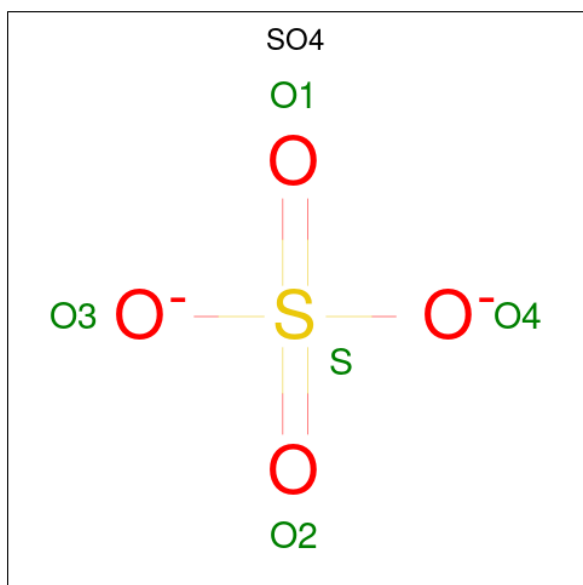
Chain	Residue	Modelled	Actual	Comment	Reference
B	141	SER	CYS	conflict	UNP P0A0N4
B	189	HIS	-	expression tag	UNP P0A0N4
B	190	HIS	-	expression tag	UNP P0A0N4
B	191	HIS	-	expression tag	UNP P0A0N4
B	192	HIS	-	expression tag	UNP P0A0N4
B	193	HIS	-	expression tag	UNP P0A0N4
B	194	HIS	-	expression tag	UNP P0A0N4
D	141	SER	CYS	conflict	UNP P0A0N4
D	189	HIS	-	expression tag	UNP P0A0N4
D	190	HIS	-	expression tag	UNP P0A0N4
D	191	HIS	-	expression tag	UNP P0A0N4
D	192	HIS	-	expression tag	UNP P0A0N4
D	193	HIS	-	expression tag	UNP P0A0N4
D	194	HIS	-	expression tag	UNP P0A0N4
A	141	SER	CYS	conflict	UNP P0A0N4
A	189	HIS	-	expression tag	UNP P0A0N4
A	190	HIS	-	expression tag	UNP P0A0N4
A	191	HIS	-	expression tag	UNP P0A0N4
A	192	HIS	-	expression tag	UNP P0A0N4
A	193	HIS	-	expression tag	UNP P0A0N4
A	194	HIS	-	expression tag	UNP P0A0N4

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Chain	Residue	Modelled	Actual	Comment	Reference
E	141	SER	CYS	conflict	UNP P0A0N4
E	189	HIS	-	expression tag	UNP P0A0N4
E	190	HIS	-	expression tag	UNP P0A0N4
E	191	HIS	-	expression tag	UNP P0A0N4
E	192	HIS	-	expression tag	UNP P0A0N4
E	193	HIS	-	expression tag	UNP P0A0N4
E	194	HIS	-	expression tag	UNP P0A0N4

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



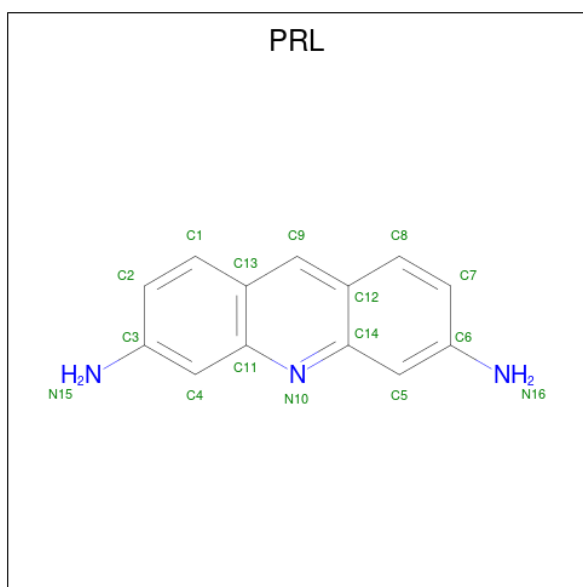
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	B	1	Total	O	S	0	0
			5	4	1		
2	B	1	Total	O	S	0	0
			5	4	1		
2	B	1	Total	O	S	0	0
			5	4	1		
2	B	1	Total	O	S	0	0
			5	4	1		
2	D	1	Total	O	S	0	0
			5	4	1		
2	D	1	Total	O	S	0	0
			5	4	1		
2	D	1	Total	O	S	0	0
			5	4	1		

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

- Molecule 3 is PROFLAVIN (CCD ID: PRL) (formula: $C_{13}H_{11}N_3$).



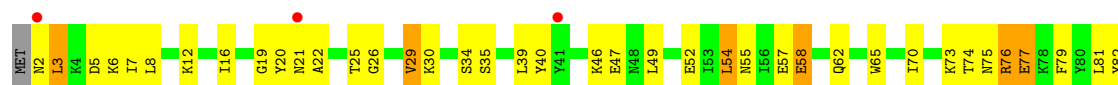
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	N	0	0
			16	13	3		

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	B	10	Total	O	0	0
			10	10		
4	D	18	Total	O	0	0
			18	18		
4	A	32	Total	O	0	0
			32	32		
4	E	22	Total	O	0	0
			22	22		



- Molecule 1: Transcriptional regulator qacR



4 Data and refinement statistics

Property	Value	Source
Space group	P 42 21 2	Depositor
Cell constants a, b, c, α , β , γ	172.30Å 172.30Å 94.75Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	47.79 – 2.89 47.79 – 2.89	Depositor EDS
% Data completeness (in resolution range)	97.6 (47.79-2.89) 97.6 (47.79-2.89)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.88 (at 2.77Å)	Xtriage
Refinement program	CNS 1.0	Depositor
R, R_{free}	0.232 , 0.291 0.234 , 0.292	Depositor DCC
R_{free} test set	3169 reflections (8.90%)	wwPDB-VP
Wilson B-factor (Å ²)	68.9	Xtriage
Anisotropy	0.011	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 75.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	6416	wwPDB-VP
Average B, all atoms (Å ²)	66.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.24% 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, PRL

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	0.51	0/1578	0.97	6/2126 (0.3%)
1	B	0.44	0/1578	0.99	9/2126 (0.4%)
1	D	0.46	0/1578	0.98	9/2126 (0.4%)
1	E	0.51	0/1578	0.93	4/2126 (0.2%)
All	All	0.48	0/6312	0.97	28/8504 (0.3%)

There are no bond length outliers.

All (28) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	161	THR	N-CA-C	8.76	120.90	111.36
1	D	6	LYS	N-CA-C	-8.05	102.58	111.36
1	E	168	ILE	N-CA-C	7.60	119.29	110.62
1	B	145	VAL	N-CA-C	7.45	118.18	110.36
1	B	118	LYS	N-CA-C	-7.18	102.86	111.69
1	A	139	GLU	N-CA-C	-6.85	103.60	112.23
1	B	161	THR	N-CA-C	6.80	120.05	111.69
1	B	90	GLU	N-CA-C	-6.78	103.38	112.94
1	D	5	ASP	N-CA-C	-6.75	105.20	113.50
1	D	165	GLU	N-CA-C	6.47	119.58	111.24
1	E	19	GLY	N-CA-C	-6.37	103.25	112.17
1	D	91	TYR	N-CA-C	6.24	120.00	109.76
1	B	7	ILE	N-CA-C	-6.18	104.61	110.42
1	B	170	GLU	N-CA-C	-6.01	104.81	111.36
1	E	139	GLU	N-CA-C	-6.00	105.45	112.89
1	B	163	THR	N-CA-C	-5.85	103.95	113.19
1	A	113	ASN	N-CA-C	-5.77	105.73	112.89
1	D	159	ILE	CB-CA-C	-5.70	104.69	111.81
1	D	161	THR	N-CA-C	5.56	119.23	112.23
1	B	122	LYS	N-CA-C	-5.38	104.84	111.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	118	LYS	N-CA-C	-5.31	105.57	111.36
1	D	76	ARG	N-CA-C	-5.25	105.03	111.75
1	A	137	ASN	N-CA-C	-5.25	105.96	114.09
1	B	67	LYS	N-CA-C	-5.24	107.18	113.21
1	A	155	ALA	N-CA-C	-5.21	105.25	111.03
1	D	122	LYS	N-CA-C	-5.16	105.34	110.97
1	D	166	GLN	N-CA-C	5.14	117.81	109.79
1	A	76	ARG	N-CA-C	-5.10	105.72	111.28

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	1547	0	1533	74	0
1	B	1547	0	1533	120	0
1	D	1547	0	1533	112	0
1	E	1547	0	1533	88	0
2	A	35	0	0	4	0
2	B	25	0	0	3	0
2	D	30	0	0	2	0
2	E	40	0	0	4	0
3	A	16	0	11	0	0
4	A	32	0	0	1	0
4	B	10	0	0	2	0
4	D	18	0	0	2	0
4	E	22	0	0	1	0
All	All	6416	0	6143	373	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 30.

All (373) 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:B:96:GLN:HG3	1:B:157:ASN:HD21	1.21	1.01
1:D:101:GLU:HG2	1:E:97:ASN:HD21	1.25	0.99
1:A:112:ILE:O	1:A:116:MET:HG3	1.64	0.98
1:B:6:LYS:HE3	1:B:6:LYS:HA	1.43	0.97
1:B:44:LYS:H	1:B:48:ASN:HD22	1.14	0.93
1:B:143:ASN:H	1:B:143:ASN:HD22	0.97	0.93
1:B:36:LYS:H	1:B:36:LYS:HD3	1.34	0.92
1:A:135:ASN:HD21	1:A:142:ILE:H	1.13	0.91
1:B:44:LYS:H	1:B:48:ASN:ND2	1.68	0.91
1:D:21:ASN:OD1	1:D:101:GLU:HB3	1.71	0.89
1:B:106:TYR:O	1:B:112:ILE:HG13	1.73	0.88
1:D:165:GLU:HB3	1:E:103:TYR:CE1	2.09	0.87
1:D:2:ASN:ND2	1:D:3:LEU:H	1.73	0.87
1:E:106:TYR:HB3	1:E:112:ILE:HG21	1.58	0.85
1:B:66:LYS:HA	1:B:69:GLN:NE2	1.91	0.84
1:B:143:ASN:HD22	1:B:143:ASN:N	1.74	0.83
1:D:14:LEU:HD12	1:D:28:ILE:HD13	1.60	0.83
1:B:18:ASN:HD22	1:B:23:THR:HG22	1.43	0.83
1:E:54:LEU:HD23	1:E:116:MET:HE1	1.58	0.82
1:D:6:LYS:HG3	1:D:32:SER:HB2	1.59	0.82
1:A:21:ASN:ND2	1:A:101:GLU:HG2	1.95	0.81
1:A:83:ASN:ND2	1:A:156:VAL:HG21	1.95	0.81
1:B:6:LYS:O	1:B:10:VAL:HG23	1.81	0.80
1:A:51:LEU:HD11	1:A:112:ILE:HG23	1.63	0.79
1:B:44:LYS:N	1:B:48:ASN:HD22	1.82	0.77
1:B:47:GLU:O	1:B:51:LEU:HB2	1.84	0.77
1:D:101:GLU:HG2	1:E:97:ASN:ND2	1.99	0.77
1:B:4:LYS:O	1:B:4:LYS:HD3	1.85	0.76
1:B:7:ILE:HD13	1:B:32:SER:OG	1.86	0.76
1:D:27:GLU:O	1:D:31:LEU:HB2	1.85	0.76
1:B:165:GLU:HG3	1:B:166:GLN:H	1.51	0.76
1:D:142:ILE:HD11	1:D:186:LEU:HD13	1.68	0.76
1:D:101:GLU:CG	1:E:97:ASN:HD21	1.99	0.75
1:B:39:LEU:O	1:B:43:PHE:HB2	1.86	0.75
1:A:109:THR:O	1:A:113:ASN:HB2	1.87	0.75
1:A:91:TYR:CE1	1:A:168:ILE:HD13	2.21	0.75
1:B:24:THR:HG23	1:B:27:GLU:H	1.51	0.74
1:D:21:ASN:ND2	1:D:105:GLU:OE2	2.20	0.74
1:D:65:TRP:O	1:D:69:GLN:HB3	1.88	0.74
1:E:100:ILE:O	1:E:104:THR:HG23	1.88	0.74
1:B:8:LEU:HD21	1:B:52:GLU:HG2	1.68	0.73
1:D:2:ASN:ND2	1:D:3:LEU:N	2.35	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:96:GLN:NE2	1:D:157:ASN:HD21	1.86	0.73
1:D:126:ALA:O	1:D:130:ILE:HD13	1.87	0.73
1:D:131:PHE:HE1	1:D:186:LEU:HD11	1.54	0.73
1:B:66:LYS:HA	1:B:69:GLN:HE21	1.53	0.73
1:B:73:LYS:H	1:B:73:LYS:HZ2	1.35	0.73
1:A:143:ASN:HD22	1:A:144:ASP:N	1.85	0.73
1:A:47:GLU:HG2	1:A:106:TYR:CZ	2.23	0.72
1:B:60:LYS:HB3	1:B:91:TYR:CE1	2.24	0.72
1:A:21:ASN:HD21	1:A:101:GLU:HG2	1.55	0.72
1:B:36:LYS:HD3	1:B:36:LYS:N	2.04	0.71
1:E:3:LEU:O	1:E:7:ILE:HG13	1.90	0.71
1:E:76:ARG:HG2	1:E:183:LEU:HD23	1.71	0.71
1:B:177:LYS:HE2	4:B:232:HOH:O	1.90	0.71
1:D:84:GLU:HG3	1:D:176:ASN:HD21	1.55	0.71
1:B:106:TYR:O	1:B:109:THR:HG23	1.91	0.70
1:D:97:ASN:OD1	1:E:101:GLU:HG3	1.91	0.70
1:B:73:LYS:H	1:B:73:LYS:NZ	1.87	0.70
1:D:2:ASN:CG	1:D:3:LEU:H	1.98	0.70
1:D:58:GLU:HG3	1:D:119:LEU:HD22	1.74	0.70
1:B:96:GLN:HG3	1:B:157:ASN:ND2	2.03	0.69
1:B:89:THR:HG22	1:B:91:TYR:H	1.57	0.69
1:D:181:ILE:O	1:E:185:GLY:HA3	1.93	0.68
1:B:58:GLU:HG3	1:B:119:LEU:HD21	1.74	0.68
1:B:4:LYS:HG3	1:B:42:HIS:ND1	2.08	0.68
1:B:89:THR:HG22	1:B:90:GLU:H	1.58	0.68
1:A:143:ASN:HD22	1:A:143:ASN:C	1.99	0.68
1:D:55:ASN:CG	1:D:119:LEU:HD21	2.18	0.68
1:A:21:ASN:ND2	1:A:101:GLU:CG	2.57	0.68
1:E:111:SER:O	1:E:115:LYS:HG3	1.95	0.67
1:E:25:THR:HG21	1:E:40:TYR:OH	1.95	0.67
1:B:3:LEU:HD21	1:B:34:SER:OG	1.95	0.66
1:B:39:LEU:H	1:B:39:LEU:HD22	1.60	0.66
1:B:96:GLN:NE2	1:B:157:ASN:OD1	2.28	0.66
1:A:168:ILE:O	1:A:172:ILE:HG12	1.96	0.66
1:B:45:THR:HG23	1:B:48:ASN:HB2	1.78	0.66
1:D:51:LEU:HD11	1:D:112:ILE:HG23	1.78	0.66
1:B:143:ASN:H	1:B:143:ASN:ND2	1.76	0.66
1:D:73:LYS:HG3	1:D:74:THR:H	1.62	0.65
1:B:35:SER:HB3	1:B:38:ASN:OD1	1.98	0.64
1:E:81:LEU:HG	1:E:85:LEU:HD21	1.79	0.64
1:E:135:ASN:C	1:E:137:ASN:H	2.06	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:93:TYR:CD2	1:A:94:PRO:HD2	2.33	0.64
1:E:20:TYR:CZ	1:E:46:LYS:HE2	2.32	0.64
1:E:163:THR:O	1:E:171:ARG:HD3	1.98	0.63
1:D:97:ASN:ND2	1:E:100:ILE:HD11	2.13	0.63
1:A:134:GLY:HA3	1:A:140:TRP:CZ2	2.33	0.63
1:B:64:GLN:O	1:B:68:GLU:HB2	1.99	0.62
1:E:105:GLU:HG2	1:E:106:TYR:CD2	2.35	0.62
1:B:126:ALA:O	1:B:130:ILE:HD13	1.99	0.62
1:A:106:TYR:CE1	1:A:112:ILE:HD12	2.35	0.62
1:D:151:ILE:HD11	1:E:177:LYS:HB3	1.80	0.62
1:B:142:ILE:HD11	1:B:186:LEU:HD13	1.81	0.61
1:B:6:LYS:HE3	1:B:6:LYS:CA	2.27	0.61
1:D:131:PHE:CE1	1:D:186:LEU:HD11	2.34	0.61
1:D:133:GLU:O	1:D:137:ASN:HB2	2.01	0.61
1:D:7:ILE:HD13	1:D:32:SER:OG	1.99	0.61
1:D:173:LYS:HE2	2:E:222:SO4:O4	2.01	0.61
1:B:106:TYR:HB3	1:B:112:ILE:HG13	1.82	0.61
1:D:147:ALA:O	1:D:151:ILE:HG13	2.00	0.61
1:A:135:ASN:ND2	1:A:142:ILE:H	1.94	0.60
1:B:15:PHE:CE1	1:B:50:PHE:HD2	2.19	0.60
1:D:165:GLU:HB3	1:E:103:TYR:HE1	1.66	0.60
1:D:22:ALA:HB2	1:E:22:ALA:HB2	1.83	0.60
1:D:168:ILE:HA	1:D:171:ARG:HD3	1.82	0.60
1:E:65:TRP:CH2	1:E:82:TYR:HB2	2.37	0.60
1:B:89:THR:HG22	1:B:90:GLU:N	2.18	0.59
1:A:25:THR:O	1:A:29:VAL:HG23	2.02	0.59
1:E:110:ASN:O	1:E:114:GLU:HG3	2.01	0.59
1:B:6:LYS:HA	1:B:6:LYS:CE	2.25	0.59
1:B:81:LEU:HG	1:B:85:LEU:HD22	1.84	0.59
1:A:114:GLU:O	1:A:118:LYS:HD2	2.03	0.59
1:B:10:VAL:O	1:B:14:LEU:HD13	2.02	0.59
1:D:43:PHE:O	1:D:44:LYS:HB2	2.03	0.59
1:E:29:VAL:HG21	1:E:35:SER:C	2.28	0.59
1:D:135:ASN:C	1:D:137:ASN:H	2.10	0.59
1:A:134:GLY:HA3	1:A:140:TRP:CE2	2.38	0.59
1:A:103:TYR:C	1:A:105:GLU:H	2.11	0.58
1:A:54:LEU:HB3	1:A:119:LEU:HD21	1.84	0.58
1:E:133:GLU:O	1:E:137:ASN:ND2	2.31	0.58
1:E:112:ILE:O	1:E:116:MET:HB2	2.04	0.58
1:E:79:PHE:CD2	1:E:183:LEU:HD13	2.38	0.57
1:D:64:GLN:O	1:D:64:GLN:HG3	2.04	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:128:HIS:HA	1:D:149:SER:OG	2.04	0.57
1:B:100:ILE:O	1:B:104:THR:HG23	2.05	0.57
1:A:142:ILE:HD11	1:A:186:LEU:HD13	1.85	0.57
1:A:106:TYR:CD1	1:A:112:ILE:HD12	2.39	0.57
1:D:151:ILE:CG2	1:E:178:PHE:HB2	2.35	0.56
1:D:151:ILE:HG21	1:E:178:PHE:HB2	1.86	0.56
1:D:100:ILE:HD11	1:E:162:PHE:CE2	2.40	0.56
1:E:21:ASN:ND2	1:E:105:GLU:OE2	2.34	0.56
1:D:73:LYS:HG3	1:D:74:THR:N	2.21	0.56
1:B:97:ASN:OD1	1:A:104:THR:HG22	2.05	0.56
1:A:112:ILE:O	1:A:116:MET:CG	2.47	0.56
1:B:66:LYS:HD3	2:B:210:SO4:S	2.46	0.56
1:B:135:ASN:HD21	1:B:142:ILE:HB	1.71	0.56
1:A:12:LYS:HD2	2:A:213:SO4:O4	2.06	0.56
1:B:119:LEU:HD23	1:B:119:LEU:O	2.06	0.55
1:B:165:GLU:HG3	1:B:166:GLN:N	2.20	0.55
1:A:79:PHE:CD2	1:A:183:LEU:HD13	2.41	0.55
1:E:158:GLY:O	1:E:162:PHE:HB2	2.06	0.55
1:E:168:ILE:O	1:E:172:ILE:HG13	2.05	0.55
1:D:168:ILE:O	1:D:172:ILE:HG12	2.05	0.55
1:A:21:ASN:OD1	1:A:105:GLU:OE2	2.25	0.55
1:A:16:ILE:HG12	1:A:94:PRO:HB2	1.87	0.55
1:B:49:LEU:O	1:B:52:GLU:HB3	2.07	0.55
1:B:3:LEU:C	1:B:5:ASP:H	2.14	0.55
1:B:177:LYS:CE	4:B:232:HOH:O	2.52	0.54
1:D:177:LYS:O	1:D:177:LYS:HD3	2.07	0.54
1:E:96:GLN:HG3	1:E:161:THR:HG21	1.89	0.54
1:B:115:LYS:C	1:B:117:ASN:H	2.14	0.54
1:B:14:LEU:HB3	1:B:23:THR:CG2	2.38	0.54
1:E:164:HIS:HA	1:E:171:ARG:NH1	2.22	0.54
1:B:58:GLU:HG3	1:B:119:LEU:CD2	2.38	0.54
1:D:17:LYS:HE2	4:D:229:HOH:O	2.08	0.54
1:A:143:ASN:ND2	1:A:144:ASP:OD1	2.41	0.53
1:A:135:ASN:HD21	1:A:142:ILE:N	1.95	0.53
1:A:144:ASP:N	1:A:144:ASP:OD1	2.40	0.53
1:D:70:ILE:C	1:D:72:CYS:H	2.15	0.53
1:D:185:GLY:HA2	1:E:184:ASN:HB3	1.90	0.53
1:A:167:ASN:ND2	1:A:169:ASN:H	2.06	0.53
1:A:143:ASN:C	1:A:143:ASN:ND2	2.64	0.53
1:A:164:HIS:HA	1:A:171:ARG:NH2	2.24	0.52
1:B:8:LEU:HD21	1:B:52:GLU:CG	2.38	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:39:LEU:H	1:B:39:LEU:CD2	2.21	0.52
1:B:95:LEU:O	1:B:99:ILE:HG13	2.09	0.52
1:D:4:LYS:HB2	2:D:205:SO4:O4	2.09	0.52
1:E:83:ASN:ND2	1:E:127:TYR:OH	2.42	0.52
1:B:120:GLU:O	1:B:124:ILE:HG23	2.10	0.52
1:B:36:LYS:H	1:B:36:LYS:CD	2.12	0.52
1:D:54:LEU:O	1:D:58:GLU:HB2	2.09	0.52
1:E:128:HIS:CE1	1:E:145:VAL:HG11	2.45	0.52
1:E:54:LEU:CD2	1:E:116:MET:HE1	2.37	0.52
1:B:31:LEU:O	1:B:31:LEU:HG	2.10	0.52
1:D:45:THR:HG23	1:D:47:GLU:HG3	1.92	0.52
1:A:118:LYS:N	1:A:118:LYS:HE2	2.25	0.52
1:E:81:LEU:O	1:E:85:LEU:HD22	2.10	0.51
1:D:167:ASN:ND2	1:D:169:ASN:H	2.07	0.51
1:B:2:ASN:HB2	2:B:216:SO4:O4	2.09	0.51
1:B:91:TYR:O	1:B:93:TYR:N	2.44	0.51
1:D:2:ASN:HD22	1:D:3:LEU:N	2.04	0.51
1:D:96:GLN:O	1:D:100:ILE:HG12	2.11	0.51
1:D:168:ILE:O	1:D:168:ILE:HG13	2.10	0.51
1:A:179:SER:O	1:A:183:LEU:HB2	2.11	0.51
1:B:14:LEU:C	1:B:23:THR:HG21	2.36	0.51
1:D:43:PHE:O	1:D:48:ASN:ND2	2.38	0.51
1:E:135:ASN:O	1:E:137:ASN:N	2.41	0.51
1:B:60:LYS:HB3	1:B:91:TYR:CD1	2.46	0.50
1:E:12:LYS:O	1:E:16:ILE:HG13	2.12	0.50
1:D:38:ASN:O	1:D:41:TYR:HB3	2.11	0.50
1:D:125:ASP:O	1:D:129:VAL:HG23	2.11	0.50
1:A:53:ILE:HG23	2:A:213:SO4:O4	2.11	0.50
1:D:81:LEU:O	1:D:85:LEU:HG	2.12	0.50
1:D:15:PHE:CD1	1:D:50:PHE:HD2	2.30	0.50
1:D:24:THR:O	1:D:28:ILE:HG12	2.12	0.49
1:B:113:ASN:O	1:B:117:ASN:HB2	2.13	0.49
1:D:124:ILE:HG23	1:D:149:SER:O	2.13	0.49
1:D:29:VAL:HG13	1:D:34:SER:C	2.37	0.49
1:E:124:ILE:HD13	1:E:150:LYS:HG2	1.94	0.49
1:D:151:ILE:CD1	1:E:177:LYS:HB3	2.43	0.49
1:B:39:LEU:HD22	1:B:39:LEU:N	2.26	0.49
1:B:80:TYR:O	1:B:84:GLU:HG3	2.12	0.48
1:E:91:TYR:O	1:E:93:TYR:N	2.44	0.48
1:D:15:PHE:CE1	1:D:50:PHE:HD2	2.30	0.48
1:B:21:ASN:HD21	1:B:105:GLU:CD	2.22	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:47:GLU:HB2	1:B:102:PHE:HE2	1.78	0.48
1:E:12:LYS:HD2	2:E:211:SO4:O3	2.13	0.48
1:E:163:THR:HA	1:E:165:GLU:OE2	2.13	0.48
1:D:76:ARG:CG	1:D:183:LEU:HD13	2.42	0.48
1:D:100:ILE:O	1:D:104:THR:HG23	2.13	0.48
1:A:74:THR:O	1:A:77:GLU:HB2	2.14	0.48
1:D:158:GLY:O	1:D:162:PHE:HD1	1.96	0.48
1:B:166:GLN:O	1:B:167:ASN:C	2.57	0.48
1:A:87:LEU:HD22	1:A:172:ILE:HD13	1.96	0.47
1:E:184:ASN:C	1:E:186:LEU:H	2.22	0.47
1:D:45:THR:CG2	1:D:47:GLU:HG3	2.44	0.47
1:E:2:ASN:HB2	1:E:5:ASP:HB2	1.96	0.47
1:E:74:THR:O	1:E:77:GLU:HB2	2.13	0.47
1:E:135:ASN:C	1:E:137:ASN:N	2.72	0.47
1:B:66:LYS:HD3	2:B:210:SO4:O1	2.14	0.47
1:D:177:LYS:HD2	1:D:181:ILE:HD11	1.96	0.47
1:A:68:GLU:HG2	1:A:85:LEU:HD21	1.96	0.47
1:D:74:THR:O	1:D:78:LYS:HG3	2.15	0.47
1:A:91:TYR:CD1	1:A:168:ILE:HD13	2.49	0.47
1:D:84:GLU:CG	1:D:176:ASN:HD21	2.27	0.47
1:E:180:GLN:O	1:E:181:ILE:C	2.56	0.47
1:D:118:LYS:O	1:D:121:ASN:HB2	2.14	0.47
1:E:5:ASP:HB3	2:E:212:SO4:O1	2.15	0.47
1:D:43:PHE:O	1:D:44:LYS:CB	2.62	0.47
1:D:171:ARG:HG2	1:D:171:ARG:HH11	1.79	0.47
1:B:27:GLU:O	1:B:28:ILE:C	2.58	0.47
1:D:103:TYR:CZ	1:E:165:GLU:HG2	2.50	0.46
1:E:76:ARG:NH2	4:E:225:HOH:O	2.29	0.46
1:B:57:GLU:HG3	1:B:95:LEU:HD12	1.96	0.46
1:B:143:ASN:N	1:B:143:ASN:ND2	2.46	0.46
1:D:185:GLY:HA3	1:E:181:ILE:O	2.15	0.46
1:E:95:LEU:O	1:E:99:ILE:HG13	2.15	0.46
1:B:11:ALA:HB3	1:B:53:ILE:HD11	1.96	0.46
1:D:10:VAL:HG11	1:D:31:LEU:HB3	1.98	0.46
1:D:11:ALA:HA	1:D:28:ILE:HD12	1.97	0.46
1:D:135:ASN:C	1:D:137:ASN:N	2.74	0.46
1:B:126:ALA:O	1:B:130:ILE:CD1	2.62	0.46
1:E:39:LEU:HD23	1:E:39:LEU:C	2.39	0.46
1:B:50:PHE:C	1:B:52:GLU:N	2.70	0.46
1:A:17:LYS:HG2	1:A:18:ASN:OD1	2.16	0.46
1:B:60:LYS:HD3	1:B:91:TYR:CZ	2.51	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:106:TYR:HB3	1:B:112:ILE:CG1	2.44	0.46
1:A:43:PHE:O	1:A:44:LYS:HB2	2.15	0.46
1:A:136:LEU:N	1:A:136:LEU:CD1	2.78	0.46
1:B:62:GLN:HG3	1:B:66:LYS:HE3	1.97	0.46
1:A:102:PHE:O	1:A:106:TYR:HB2	2.15	0.46
1:E:126:ALA:O	1:E:130:ILE:HG13	2.16	0.46
1:D:45:THR:O	1:D:48:ASN:N	2.46	0.46
1:A:110:ASN:O	1:A:114:GLU:HB2	2.16	0.46
1:E:96:GLN:NE2	1:E:157:ASN:HD21	2.14	0.46
1:D:2:ASN:CG	1:D:3:LEU:N	2.69	0.45
1:D:25:THR:HG22	1:D:46:LYS:HB2	1.97	0.45
1:B:24:THR:HG22	1:B:27:GLU:HG3	1.98	0.45
1:A:24:THR:OG1	1:A:27:GLU:HG3	2.16	0.45
1:A:96:GLN:HE21	1:A:100:ILE:HD11	1.80	0.45
1:D:103:TYR:CE1	1:E:165:GLU:HG2	2.51	0.45
1:D:60:LYS:HD3	1:D:91:TYR:CE2	2.51	0.45
1:A:163:THR:HG22	1:A:171:ARG:HD3	1.97	0.45
1:E:131:PHE:CE2	1:E:148:VAL:HG12	2.52	0.45
1:D:163:THR:C	1:D:165:GLU:H	2.24	0.45
1:B:66:LYS:C	1:B:68:GLU:H	2.24	0.45
1:E:8:LEU:HD23	1:E:8:LEU:HA	1.81	0.45
1:E:79:PHE:CE2	1:E:183:LEU:HD13	2.51	0.45
1:B:90:GLU:HG2	1:B:91:TYR:CD2	2.51	0.45
1:D:52:GLU:O	1:D:53:ILE:C	2.59	0.45
1:A:14:LEU:HD11	1:A:31:LEU:HD12	1.98	0.45
1:B:15:PHE:CD1	1:B:50:PHE:HD2	2.35	0.44
1:B:58:GLU:HG2	1:B:92:TYR:CE2	2.53	0.44
1:B:79:PHE:HD2	1:B:183:LEU:HD11	1.82	0.44
1:D:105:GLU:O	1:D:105:GLU:CG	2.66	0.44
1:A:43:PHE:O	1:A:48:ASN:HB3	2.17	0.44
1:D:25:THR:CG2	1:D:46:LYS:HB2	2.48	0.44
1:D:49:LEU:O	1:D:53:ILE:HG13	2.17	0.44
1:D:103:TYR:CE1	1:D:107:TYR:HB3	2.52	0.44
1:B:106:TYR:HB3	1:B:112:ILE:CD1	2.46	0.44
1:D:51:LEU:HD23	1:D:51:LEU:HA	1.87	0.44
1:E:96:GLN:CD	1:E:157:ASN:HD21	2.26	0.44
1:B:151:ILE:CG2	1:A:178:PHE:HB2	2.48	0.44
1:B:14:LEU:HB3	1:B:23:THR:HG21	2.00	0.44
1:D:23:THR:CG2	1:D:28:ILE:HD11	2.48	0.44
1:A:6:LYS:O	1:A:10:VAL:HG23	2.17	0.44
1:E:109:THR:HG21	1:E:112:ILE:HD13	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:45:THR:O	1:D:46:LYS:C	2.61	0.44
1:B:45:THR:CG2	1:B:48:ASN:HB2	2.47	0.44
1:B:61:TRP:CZ2	1:B:82:TYR:CE1	3.05	0.44
1:B:46:LYS:C	1:B:48:ASN:H	2.25	0.43
1:B:88:THR:O	1:B:89:THR:O	2.36	0.43
1:D:58:GLU:HB3	4:D:236:HOH:O	2.18	0.43
1:D:76:ARG:HG2	1:D:183:LEU:HD13	1.99	0.43
1:A:164:HIS:HA	1:A:171:ARG:CZ	2.48	0.43
1:B:83:ASN:ND2	1:B:127:TYR:OH	2.51	0.43
1:B:16:ILE:HG13	1:B:95:LEU:HD21	1.99	0.43
1:A:39:LEU:C	1:A:39:LEU:HD23	2.43	0.43
1:E:8:LEU:HD23	1:E:49:LEU:HD11	2.00	0.43
1:D:31:LEU:HD12	1:D:31:LEU:HA	1.81	0.43
1:D:183:LEU:HD23	1:D:183:LEU:HA	1.81	0.43
1:A:180:GLN:HE21	1:A:180:GLN:HB3	1.61	0.43
1:D:59:SER:HA	1:D:62:GLN:HB3	1.99	0.43
1:B:123:TYR:HE2	1:B:154:ASN:ND2	2.16	0.43
1:E:62:GLN:HE21	1:E:62:GLN:HB2	1.57	0.43
1:E:70:ILE:O	1:E:70:ILE:HG22	2.19	0.43
1:B:127:TYR:O	1:B:131:PHE:CD2	2.72	0.43
1:A:94:PRO:HG2	1:A:95:LEU:H	1.84	0.43
1:A:96:GLN:O	1:A:100:ILE:HG12	2.18	0.43
1:A:126:ALA:O	1:A:130:ILE:HG13	2.19	0.43
1:B:72:CYS:HA	1:B:73:LYS:HZ1	1.83	0.43
1:D:57:GLU:HG3	1:D:95:LEU:HD12	2.01	0.43
1:B:102:PHE:CD1	1:B:102:PHE:C	2.97	0.42
1:E:183:LEU:HD12	1:E:183:LEU:HA	1.81	0.42
1:A:64:GLN:NE2	4:A:329:HOH:O	2.48	0.42
1:E:29:VAL:HG22	1:E:34:SER:HB3	2.00	0.42
1:B:58:GLU:HG2	1:B:92:TYR:CD2	2.54	0.42
1:A:170:GLU:OE2	1:A:170:GLU:HA	2.19	0.42
1:A:67:LYS:HE2	1:A:67:LYS:HB3	1.82	0.42
1:A:4:LYS:N	2:A:218:SO4:O3	2.53	0.42
1:E:73:LYS:HB3	1:E:77:GLU:OE1	2.19	0.42
1:E:137:ASN:HB3	1:E:139:GLU:HG3	2.01	0.42
1:D:182:PHE:CE1	1:E:181:ILE:HG21	2.54	0.42
1:A:63:GLU:OE1	1:A:64:GLN:N	2.52	0.42
1:E:105:GLU:HG2	1:E:106:TYR:CE2	2.54	0.42
1:E:177:LYS:HA	1:E:177:LYS:HD2	1.83	0.42
1:B:50:PHE:C	1:B:52:GLU:H	2.27	0.42
1:E:12:LYS:HE3	1:E:57:GLU:CD	2.44	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:45:THR:OG1	1:B:46:LYS:N	2.53	0.42
1:B:137:ASN:O	1:B:137:ASN:CG	2.63	0.42
1:D:76:ARG:HG3	1:D:183:LEU:HD13	2.01	0.42
1:A:109:THR:HG22	1:A:111:SER:H	1.85	0.42
1:A:159:ILE:CG2	1:A:175:MET:HE2	2.49	0.42
1:A:165:GLU:HG2	1:A:166:GLN:N	2.35	0.42
1:E:82:TYR:CD2	1:E:82:TYR:C	2.98	0.42
1:D:3:LEU:HD11	1:D:34:SER:HB2	2.01	0.41
1:B:3:LEU:C	1:B:5:ASP:N	2.78	0.41
1:B:39:LEU:O	1:B:43:PHE:O	2.37	0.41
1:D:25:THR:HG21	2:D:203:SO4:O3	2.20	0.41
1:B:79:PHE:CD2	1:B:183:LEU:HD21	2.55	0.41
1:D:180:GLN:O	1:D:181:ILE:C	2.63	0.41
1:A:39:LEU:HD23	1:A:39:LEU:O	2.20	0.41
1:E:26:GLY:O	1:E:29:VAL:HG12	2.21	0.41
1:E:103:TYR:CD2	1:E:116:MET:HG2	2.56	0.41
1:B:103:TYR:CD2	1:B:116:MET:HG2	2.54	0.41
1:E:159:ILE:CG2	1:E:175:MET:HE2	2.51	0.41
1:B:89:THR:CG2	1:B:91:TYR:H	2.29	0.41
1:D:124:ILE:HG22	1:D:124:ILE:O	2.20	0.41
1:A:12:LYS:HD2	2:A:213:SO4:S	2.60	0.41
1:B:2:ASN:OD1	1:B:3:LEU:N	2.47	0.41
1:B:89:THR:HG22	1:B:91:TYR:N	2.30	0.41
1:D:57:GLU:HG3	1:D:95:LEU:CD1	2.51	0.41
1:D:95:LEU:O	1:D:99:ILE:HG13	2.20	0.41
1:B:18:ASN:ND2	1:B:23:THR:HG22	2.23	0.41
1:B:147:ALA:O	1:B:151:ILE:HG13	2.20	0.41
1:D:10:VAL:HG21	1:D:32:SER:HB3	2.03	0.41
1:D:159:ILE:HB	1:D:175:MET:HE1	2.03	0.41
1:E:75:ASN:C	1:E:77:GLU:N	2.77	0.41
1:B:24:THR:O	1:B:28:ILE:HD13	2.20	0.41
1:A:83:ASN:ND2	1:A:127:TYR:OH	2.53	0.41
1:D:55:ASN:ND2	1:D:119:LEU:HD21	2.35	0.41
1:D:64:GLN:O	1:D:68:GLU:HG3	2.21	0.41
1:E:57:GLU:O	1:E:58:GLU:C	2.64	0.41
1:E:165:GLU:CD	1:E:165:GLU:H	2.29	0.41
1:A:144:ASP:O	1:A:145:VAL:C	2.64	0.40
1:B:87:LEU:HD11	1:B:175:MET:HB2	2.03	0.40
1:A:30:LYS:HD3	1:A:30:LYS:HA	1.89	0.40
1:E:12:LYS:HE3	1:E:57:GLU:OE2	2.21	0.40
1:B:110:ASN:C	1:B:112:ILE:H	2.29	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:20:TYR:O	1:D:22:ALA:N	2.54	0.40
1:E:6:LYS:HG2	2:E:212:SO4:O2	2.22	0.40
1:E:58:GLU:HB2	1:E:123:TYR:CZ	2.57	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	184/194 (95%)	171 (93%)	11 (6%)	2 (1%)	11	36
1	B	184/194 (95%)	149 (81%)	25 (14%)	10 (5%)	1	5
1	D	184/194 (95%)	149 (81%)	27 (15%)	8 (4%)	2	8
1	E	184/194 (95%)	168 (91%)	12 (6%)	4 (2%)	5	20
All	All	736/776 (95%)	637 (86%)	75 (10%)	24 (3%)	3	13

All (24) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	89	THR
1	B	92	TYR
1	A	164	HIS
1	E	166	GLN
1	B	33	GLU
1	B	165	GLU
1	D	44	LYS
1	D	109	THR
1	D	123	TYR
1	D	3	LEU
1	E	92	TYR
1	E	136	LEU

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Mol	Chain	Res	Type
1	B	44	LYS
1	B	106	TYR
1	B	167	ASN
1	D	21	ASN
1	D	71	LYS
1	B	4	LYS
1	B	18	ASN
1	D	108	LYS
1	A	104	THR
1	D	92	TYR
1	E	181	ILE
1	B	168	ILE

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	169/178 (95%)	152 (90%)	17 (10%)	7	24
1	B	169/178 (95%)	150 (89%)	19 (11%)	6	19
1	D	169/178 (95%)	153 (90%)	16 (10%)	8	26
1	E	169/178 (95%)	148 (88%)	21 (12%)	4	15
All	All	676/712 (95%)	603 (89%)	73 (11%)	6	21

All (73) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	5	ASP
1	B	6	LYS
1	B	36	LYS
1	B	39	LEU
1	B	42	HIS
1	B	45	THR
1	B	69	GLN
1	B	73	LYS
1	B	85	LEU

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Mol	Chain	Res	Type
1	B	88	THR
1	B	97	ASN
1	B	109	THR
1	B	110	ASN
1	B	114	GLU
1	B	118	LYS
1	B	143	ASN
1	B	165	GLU
1	B	167	ASN
1	B	180	GLN
1	D	3	LEU
1	D	31	LEU
1	D	47	GLU
1	D	55	ASN
1	D	58	GLU
1	D	64	GLN
1	D	66	LYS
1	D	69	GLN
1	D	89	THR
1	D	96	GLN
1	D	117	ASN
1	D	137	ASN
1	D	143	ASN
1	D	165	GLU
1	D	170	GLU
1	D	177	LYS
1	A	25	THR
1	A	30	LYS
1	A	49	LEU
1	A	54	LEU
1	A	55	ASN
1	A	85	LEU
1	A	91	TYR
1	A	105	GLU
1	A	107	TYR
1	A	116	MET
1	A	118	LYS
1	A	136	LEU
1	A	143	ASN
1	A	167	ASN
1	A	171	ARG
1	A	173	LYS

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Mol	Chain	Res	Type
1	A	180	GLN
1	E	3	LEU
1	E	29	VAL
1	E	30	LYS
1	E	47	GLU
1	E	52	GLU
1	E	54	LEU
1	E	55	ASN
1	E	58	GLU
1	E	76	ARG
1	E	77	GLU
1	E	85	LEU
1	E	108	LYS
1	E	144	ASP
1	E	146	ASN
1	E	161	THR
1	E	164	HIS
1	E	165	GLU
1	E	167	ASN
1	E	170	GLU
1	E	179	SER
1	E	183	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (55) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	18	ASN
1	B	48	ASN
1	B	69	GLN
1	B	83	ASN
1	B	96	GLN
1	B	110	ASN
1	B	113	ASN
1	B	128	HIS
1	B	143	ASN
1	B	154	ASN
1	B	157	ASN
1	B	164	HIS
1	D	2	ASN
1	D	62	GLN
1	D	64	GLN
1	D	75	ASN

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Mol	Chain	Res	Type
1	D	83	ASN
1	D	96	GLN
1	D	97	ASN
1	D	154	ASN
1	D	164	HIS
1	D	167	ASN
1	D	176	ASN
1	D	180	GLN
1	D	184	ASN
1	A	21	ASN
1	A	62	GLN
1	A	69	GLN
1	A	83	ASN
1	A	96	GLN
1	A	110	ASN
1	A	113	ASN
1	A	117	ASN
1	A	121	ASN
1	A	135	ASN
1	A	137	ASN
1	A	143	ASN
1	A	164	HIS
1	A	166	GLN
1	A	167	ASN
1	A	169	ASN
1	A	180	GLN
1	E	18	ASN
1	E	62	GLN
1	E	64	GLN
1	E	69	GLN
1	E	83	ASN
1	E	96	GLN
1	E	97	ASN
1	E	113	ASN
1	E	117	ASN
1	E	121	ASN
1	E	166	GLN
1	E	169	ASN
1	E	184	ASN

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 ⓘ

27 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	E	207	-	4,4,4	0.37	0	6,6,6	0.09	0
2	SO4	E	211	-	4,4,4	0.36	0	6,6,6	0.09	0
2	SO4	A	218	-	4,4,4	0.38	0	6,6,6	0.07	0
2	SO4	D	223	-	4,4,4	0.37	0	6,6,6	0.06	0
2	SO4	A	208	-	4,4,4	0.37	0	6,6,6	0.11	0
2	SO4	B	210	-	4,4,4	0.38	0	6,6,6	0.09	0
2	SO4	D	205	-	4,4,4	0.37	0	6,6,6	0.09	0
2	SO4	E	212	-	4,4,4	0.37	0	6,6,6	0.15	0
2	SO4	A	213	-	4,4,4	0.38	0	6,6,6	0.09	0
2	SO4	B	217	-	4,4,4	0.36	0	6,6,6	0.07	0
2	SO4	D	203	-	4,4,4	0.37	0	6,6,6	0.08	0
2	SO4	E	222	-	4,4,4	0.36	0	6,6,6	0.12	0
2	SO4	E	220	-	4,4,4	0.37	0	6,6,6	0.06	0
2	SO4	E	214	-	4,4,4	0.37	0	6,6,6	0.07	0
2	SO4	E	219	-	4,4,4	0.37	0	6,6,6	0.08	0
2	SO4	D	209	-	4,4,4	0.39	0	6,6,6	0.07	0
2	SO4	A	200	-	4,4,4	0.36	0	6,6,6	0.10	0
2	SO4	D	221	-	4,4,4	0.36	0	6,6,6	0.11	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	PRL	A	311	-	18,18,18	1.46	3 (16%)	26,26,26	0.99	0
2	SO4	D	206	-	4,4,4	0.38	0	6,6,6	0.06	0
2	SO4	B	216	-	4,4,4	0.36	0	6,6,6	0.07	0
2	SO4	B	215	-	4,4,4	0.34	0	6,6,6	0.17	0
2	SO4	A	224	-	4,4,4	0.37	0	6,6,6	0.08	0
2	SO4	B	225	-	4,4,4	0.33	0	6,6,6	0.10	0
2	SO4	A	226	-	4,4,4	0.37	0	6,6,6	0.10	0
2	SO4	A	201	-	4,4,4	0.37	0	6,6,6	0.12	0
2	SO4	E	204	-	4,4,4	0.37	0	6,6,6	0.13	0

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
3	PRL	A	311	-	-	-	0/3/3/3

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	311	PRL	C5-C14	-3.27	1.36	1.41
3	A	311	PRL	C4-C11	-2.67	1.37	1.41
3	A	311	PRL	C8-C12	-2.29	1.37	1.42

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

9 monomers are involved in 13 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	E	211	SO4	1	0
2	A	218	SO4	1	0
2	B	210	SO4	2	0
2	D	205	SO4	1	0
2	E	212	SO4	2	0
2	A	213	SO4	3	0
2	D	203	SO4	1	0
2	E	222	SO4	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	216	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

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	186/194 (95%)	0.06	8 (4%) 40 31	28, 47, 89, 111	0
1	B	186/194 (95%)	0.85	29 (15%) 5 4	30, 70, 125, 136	0
1	D	186/194 (95%)	0.79	22 (11%) 9 7	39, 70, 103, 112	0
1	E	186/194 (95%)	0.28	11 (5%) 28 22	35, 55, 89, 99	0
All	All	744/776 (95%)	0.50	70 (9%) 14 12	28, 59, 106, 136	0

All (70) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	111	SER	8.8
1	B	45	THR	5.6
1	B	21	ASN	5.4
1	D	21	ASN	5.1
1	E	144	ASP	4.4
1	B	41	TYR	4.3
1	B	115	LYS	4.0
1	A	21	ASN	3.7
1	B	112	ILE	3.6
1	B	105	GLU	3.5
1	B	43	PHE	3.4
1	E	2	ASN	3.3
1	D	123	TYR	3.3
1	B	169	ASN	3.3
1	B	29	VAL	3.3
1	B	23	THR	3.3
1	B	3	LEU	3.2
1	D	41	TYR	3.1
1	D	2	ASN	3.1
1	A	187	SER	3.1
1	B	37	GLY	3.0

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Mol	Chain	Res	Type	RSRZ
1	B	44	LYS	3.0
1	B	117	ASN	2.9
1	D	59	SER	2.9
1	D	66	LYS	2.9
1	B	113	ASN	2.9
1	D	163	THR	2.9
1	B	42	HIS	2.8
1	E	187	SER	2.8
1	B	187	SER	2.8
1	B	134	GLY	2.8
1	D	187	SER	2.8
1	A	164	HIS	2.7
1	D	125	ASP	2.7
1	E	21	ASN	2.7
1	B	165	GLU	2.6
1	D	5	ASP	2.6
1	D	35	SER	2.6
1	B	32	SER	2.6
1	D	166	GLN	2.6
1	D	70	ILE	2.5
1	A	105	GLU	2.5
1	B	38	ASN	2.5
1	B	143	ASN	2.5
1	D	184	ASN	2.5
1	B	103	TYR	2.4
1	E	148	VAL	2.4
1	D	140	TRP	2.4
1	D	118	LYS	2.4
1	D	120	GLU	2.4
1	D	135	ASN	2.3
1	E	138	GLY	2.3
1	A	117	ASN	2.3
1	D	40	TYR	2.3
1	D	24	THR	2.3
1	E	184	ASN	2.2
1	E	41	TYR	2.2
1	E	123	TYR	2.2
1	B	170	GLU	2.2
1	D	3	LEU	2.1
1	D	144	ASP	2.1
1	E	185	GLY	2.1
1	A	103	TYR	2.1

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Mol	Chain	Res	Type	RSRZ
1	A	114	GLU	2.1
1	E	97	ASN	2.1
1	B	104	THR	2.1
1	B	35	SER	2.0
1	B	19	GLY	2.0
1	B	2	ASN	2.0
1	A	165	GLU	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
2	SO4	B	216	5/5	0.52	0.12	159,159,160,161	0
2	SO4	A	224	5/5	0.64	0.14	188,188,189,189	0
2	SO4	A	201	5/5	0.72	0.20	118,119,119,120	0
2	SO4	B	217	5/5	0.76	0.11	147,147,147,147	0
2	SO4	A	226	5/5	0.78	0.14	126,126,126,127	0
2	SO4	D	223	5/5	0.79	0.12	153,153,154,155	0
2	SO4	D	203	5/5	0.79	0.14	159,159,160,160	0
2	SO4	E	222	5/5	0.79	0.15	159,159,160,160	0
2	SO4	E	219	5/5	0.81	0.14	141,141,142,142	0
2	SO4	A	218	5/5	0.81	0.18	151,151,152,153	0
2	SO4	B	225	5/5	0.82	0.11	130,130,132,133	0
2	SO4	E	220	5/5	0.84	0.12	127,127,128,128	0
2	SO4	D	206	5/5	0.84	0.12	153,153,154,154	0
2	SO4	B	210	5/5	0.85	0.10	190,191,191,192	0
2	SO4	B	215	5/5	0.85	0.15	97,101,103,103	0
2	SO4	E	214	5/5	0.85	0.11	151,151,152,152	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	SO4	D	205	5/5	0.86	0.09	174,175,175,176	0
2	SO4	A	200	5/5	0.86	0.17	141,141,143,143	0
2	SO4	A	208	5/5	0.87	0.18	94,96,98,98	0
2	SO4	D	209	5/5	0.87	0.14	139,139,141,141	0
2	SO4	E	204	5/5	0.90	0.12	113,113,115,115	0
2	SO4	E	207	5/5	0.90	0.11	121,121,121,124	0
2	SO4	D	221	5/5	0.91	0.10	154,154,155,155	0
2	SO4	E	212	5/5	0.91	0.23	105,106,106,107	0
2	SO4	E	211	5/5	0.92	0.17	153,154,154,154	0
3	PRL	A	311	16/16	0.92	0.13	76,85,89,91	0
2	SO4	A	213	5/5	0.95	0.13	137,139,139,139	0

6.5 Other polymers [i](#)

There are no such residues in this entry.