Full wwPDB X-ray Structure Validation Report ⓘ

Nov 13, 2023 – 04:02 PM JST

PDB ID	:	5XKC
Title	:	Crystal structure of dibenzothiophene sulfone monooxygenase BdsA at 2.2 angstrome
Authors	:	Gu, L.; Su, T.; Liu, S.; Su, J.
Deposited on	:	2017-05-07
Resolution	:	2.21 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:

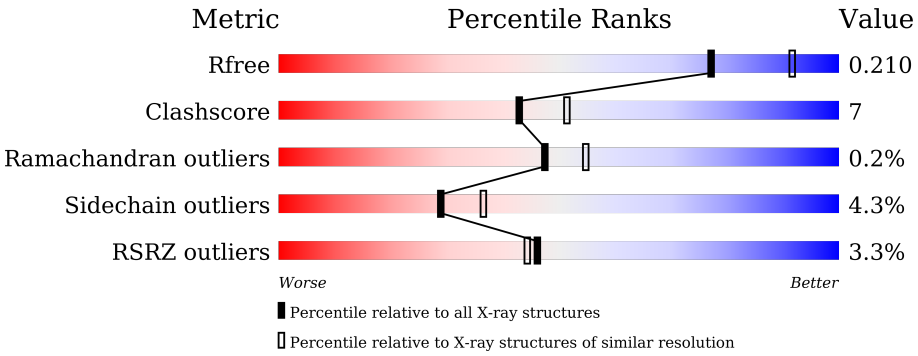
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.36
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

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 2.21 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}	130704	4898 (2.20-2.20)
Clashscore	141614	5594 (2.20-2.20)
Ramachandran outliers	138981	5503 (2.20-2.20)
Sidechain outliers	138945	5504 (2.20-2.20)
RSRZ outliers	127900	4800 (2.20-2.20)

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 <=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	453	85% 13%
1	B	453	86% 11%
1	C	453	3% 81% 16%
1	D	453	8% 78% 19%

2 Entry composition (i)

There are 2 unique types of molecules in this entry. The entry contains 14298 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 Dibenzothiophene desulfurization enzyme A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	446	Total	C	N	O	S	0	1	0
			3462	2194	615	648	5			
1	B	446	Total	C	N	O	S	0	2	0
			3473	2200	619	649	5			
1	C	446	Total	C	N	O	S	0	1	0
			3462	2194	615	648	5			
1	D	446	Total	C	N	O	S	0	0	0
			3455	2189	614	647	5			

- Molecule 2 is water.

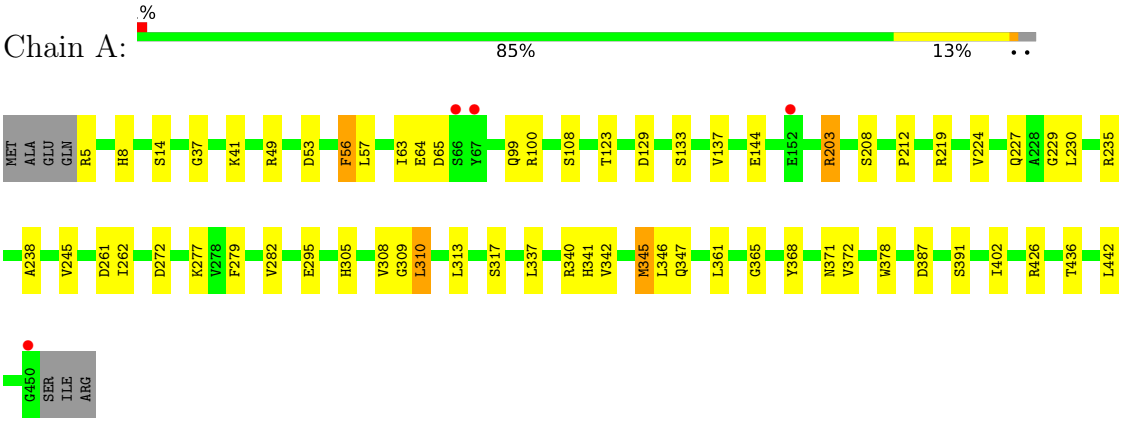
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	140	Total	O	0	0
			140	140		
2	B	120	Total	O	0	0
			120	120		
2	C	104	Total	O	0	0
			104	104		
2	D	82	Total	O	0	0
			82	82		

3 Residue-property plots (i)

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.

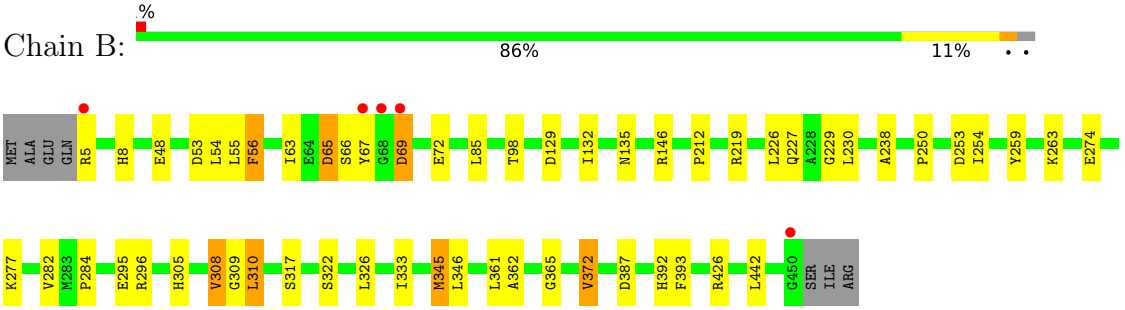
• Molecule 1: Dibenzothiophene desulfurization enzyme A

Chain A:



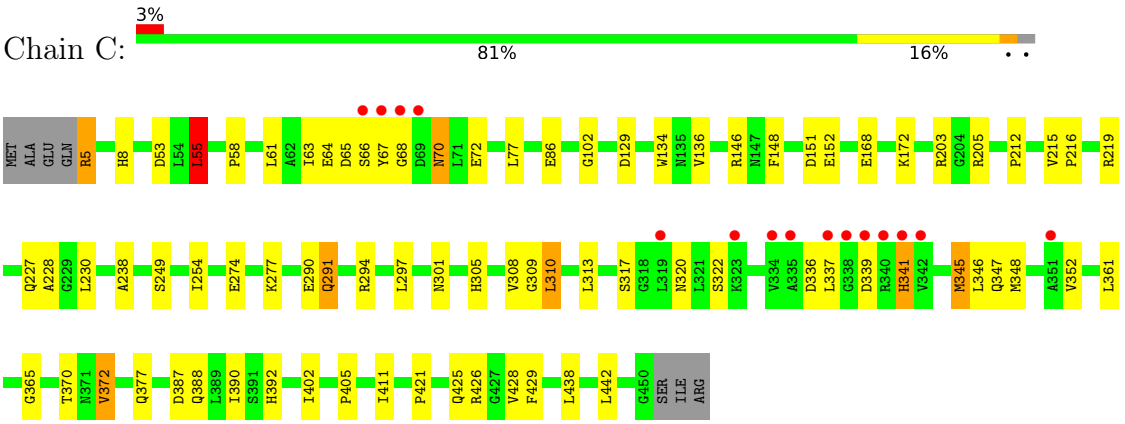
• Molecule 1: Dibenzothiophene desulfurization enzyme A

Chain B:



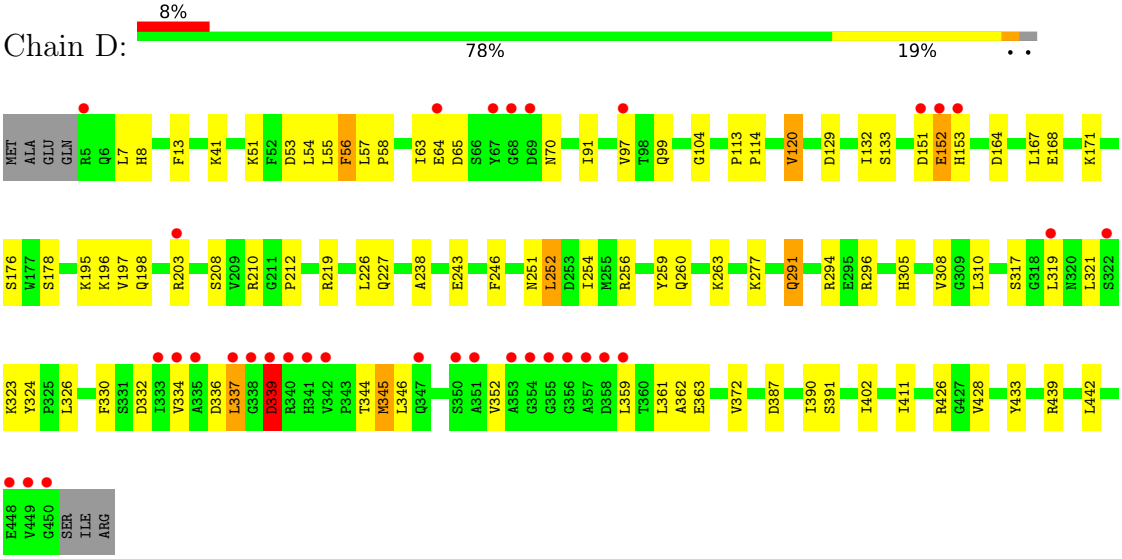
• Molecule 1: Dibenzothiophene desulfurization enzyme A

Chain C:



• Molecule 1: Dibenzothiophene desulfurization enzyme A

Chain D:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, α, β, γ	132.49Å 174.57Å 85.34Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	44.88 – 2.21 44.88 – 2.21	Depositor EDS
% Data completeness (in resolution range)	95.1 (44.88-2.21) 98.6 (44.88-2.21)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.09	Depositor
$< I/\sigma(I) >$ [1]	6.85 (at 2.20Å)	Xtriage
Refinement program	PHENIX 1.6.4_486	Depositor
R, R_{free}	0.175 , 0.213 0.174 , 0.210	Depositor DCC
R_{free} test set	4911 reflections (4.99%)	wwPDB-VP
Wilson B-factor (Å^2)	34.8	Xtriage
Anisotropy	0.430	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.37 , 43.7	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.96	EDS
Total number of atoms	14298	wwPDB-VP
Average B, all atoms (Å^2)	41.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.76% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ 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

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	0.40	0/3544	0.53	0/4818
1	B	0.41	0/3555	0.54	0/4832
1	C	0.38	0/3544	0.52	1/4818 (0.0%)
1	D	0.35	0/3537	0.49	0/4808
All	All	0.38	0/14180	0.52	1/19276 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	55	LEU	CA-CB-CG	5.40	127.71	115.30

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	3462	0	3383	47	0
1	B	3473	0	3395	35	0
1	C	3462	0	3383	50	0
1	D	3455	0	3375	66	0
2	A	140	0	0	4	0
2	B	120	0	0	3	0
2	C	104	0	0	4	0
2	D	82	0	0	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
All	All	14298	0	13536	186	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 7.

All (186) 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:99:GLN:OE1	1:D:99:GLN:NE2	1.87	1.06
1:A:340:ARG:HH11	1:A:340:ARG:HG3	1.32	0.92
1:D:246:PHE:HD2	1:D:402:ILE:HD11	1.37	0.88
1:A:108:SER:HA	1:A:137:VAL:HG23	1.54	0.88
1:D:246:PHE:CD2	1:D:402:ILE:HD11	2.09	0.87
1:A:310:LEU:HD21	1:A:361:LEU:HD22	1.59	0.84
1:B:305:HIS:HB3	1:B:308:VAL:HG22	1.64	0.79
1:C:317:SER:HB3	1:C:345:MET:HE2	1.66	0.77
1:A:144:GLU:OE1	2:A:501:HOH:O	2.03	0.76
1:A:49:ARG:NH1	2:A:503:HOH:O	2.15	0.76
1:B:333:ILE:HD11	1:B:361:LEU:HD11	1.67	0.75
1:D:152:GLU:HG2	1:D:153:HIS:N	2.03	0.73
1:C:58:PRO:O	2:C:501:HOH:O	2.06	0.72
1:A:340:ARG:HG3	1:A:340:ARG:NH1	2.03	0.72
1:A:63:ILE:HD12	1:B:212:PRO:HG2	1.72	0.70
1:C:429:PHE:O	2:C:502:HOH:O	2.10	0.70
1:C:313:LEU:HD12	1:C:345:MET:HE1	1.73	0.69
1:C:227:GLN:HG2	1:C:238:ALA:HB2	1.74	0.68
1:A:235:ARG:NH1	1:A:261:ASP:OD2	2.21	0.67
1:A:272:ASP:OD2	2:A:502:HOH:O	2.13	0.67
1:B:295:GLU:OE1	1:D:291:GLN:HG2	1.96	0.66
1:C:228:ALA:O	1:C:230:LEU:HD22	1.96	0.66
1:C:8:HIS:HD2	1:C:53:ASP:OD2	1.79	0.66
1:B:67:TYR:CD1	1:B:322:SER:HB3	2.30	0.65
1:D:41:LYS:HD3	1:D:97:VAL:HG11	1.80	0.63
1:D:8:HIS:HD2	1:D:53:ASP:OD2	1.81	0.63
1:D:203:ARG:HD2	1:D:208:SER:HB2	1.81	0.61
1:A:5:ARG:NH2	2:A:507:HOH:O	2.33	0.61
1:D:70:ASN:OD1	2:D:501:HOH:O	2.16	0.61
1:A:295:GLU:OE1	1:C:291:GLN:HG2	2.00	0.61
1:A:56:PHE:C	1:A:56:PHE:CD1	2.73	0.61
1:D:305:HIS:O	1:D:308:VAL:HG22	2.00	0.60
1:A:387:ASP:OD1	1:A:426:ARG:NH2	2.34	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:68:GLY:C	1:C:70:ASN:HD22	2.05	0.60
1:C:277:LYS:HE3	1:C:442:LEU:O	2.02	0.60
1:A:212:PRO:HG2	1:B:63:ILE:HD12	1.84	0.59
1:A:56:PHE:HD1	1:A:57:LEU:N	2.00	0.59
1:C:317:SER:HB3	1:C:345:MET:CE	2.31	0.58
1:D:317:SER:HB3	1:D:345:MET:CE	2.34	0.58
1:B:229:GLY:O	1:B:230:LEU:HD23	2.04	0.57
1:B:282[B]:VAL:HG12	1:B:284:PRO:HD3	1.87	0.57
1:A:108:SER:CA	1:A:137:VAL:HG23	2.32	0.57
1:A:99:GLN:CD	1:D:99:GLN:HE22	1.98	0.56
1:D:251:ASN:ND2	1:D:254:ILE:HD13	2.20	0.56
1:A:8:HIS:HD2	1:A:53:ASP:OD2	1.89	0.54
1:D:227:GLN:HG2	1:D:238:ALA:HB2	1.88	0.54
1:A:340:ARG:HH11	1:A:340:ARG:CG	2.12	0.54
1:A:227:GLN:HG2	1:A:238:ALA:HB2	1.87	0.54
1:D:259:TYR:CZ	1:D:263:LYS:HE3	2.43	0.54
1:B:8:HIS:HD2	1:B:53:ASP:OD2	1.91	0.54
1:B:67:TYR:HE1	1:B:310:LEU:HD13	1.72	0.54
1:D:254:ILE:HD12	1:D:254:ILE:N	2.22	0.54
1:C:337:LEU:O	1:C:341:HIS:HB2	2.08	0.53
1:D:277:LYS:HE3	1:D:442:LEU:O	2.08	0.53
1:A:317:SER:HB3	1:A:345:MET:CE	2.38	0.53
1:D:152:GLU:HG2	1:D:153:HIS:H	1.72	0.53
1:B:392:HIS:HE1	2:B:611:HOH:O	1.92	0.53
1:B:372:VAL:HG13	1:B:372:VAL:O	2.08	0.53
1:B:387:ASP:OD1	1:B:426:ARG:NH2	2.42	0.53
1:B:135:ASN:HA	1:B:226:LEU:HB2	1.92	0.52
1:A:305:HIS:HB3	1:A:308:VAL:HG22	1.91	0.52
1:A:235:ARG:HD3	1:A:261:ASP:OD2	2.10	0.52
1:D:372:VAL:O	1:D:372:VAL:HG13	2.09	0.51
1:D:55:LEU:C	1:D:55:LEU:HD23	2.29	0.51
1:D:294:ARG:NH1	1:D:294:ARG:HG2	2.25	0.51
1:C:387:ASP:OD1	1:C:426:ARG:NH2	2.43	0.51
1:B:277:LYS:HE3	1:B:442:LEU:O	2.11	0.51
1:D:319:LEU:HD23	1:D:321:LEU:HD21	1.93	0.51
1:B:253:ASP:OD2	2:B:501:HOH:O	2.18	0.50
1:C:146:ARG:HD2	2:C:503:HOH:O	2.12	0.50
1:C:372:VAL:O	1:C:372:VAL:HG13	2.12	0.50
1:A:282[A]:VAL:HG21	1:A:378:TRP:CD2	2.47	0.50
1:C:146:ARG:HD3	1:D:210:ARG:HD2	1.93	0.50
1:B:227:GLN:HG2	1:B:238:ALA:HB2	1.93	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:305:HIS:O	1:C:308:VAL:HG22	2.11	0.50
1:B:5:ARG:HG2	1:B:393:PHE:HZ	1.76	0.49
1:B:317:SER:HB3	1:B:345:MET:HE3	1.95	0.49
1:D:251:ASN:HD21	1:D:254:ILE:HD13	1.77	0.49
1:C:390:ILE:HG12	1:C:428:VAL:HG21	1.94	0.49
1:D:296:ARG:NH1	2:D:504:HOH:O	2.46	0.49
1:A:56:PHE:CD1	1:A:57:LEU:N	2.81	0.49
1:B:5:ARG:HG2	1:B:393:PHE:CZ	2.48	0.48
1:C:61:LEU:HD13	1:C:148:PHE:CE1	2.49	0.48
1:D:330:PHE:O	1:D:334:VAL:HG23	2.13	0.48
1:C:249:SER:HB3	1:C:254:ILE:HG22	1.95	0.48
1:D:198:GLN:O	1:D:212:PRO:HB3	2.14	0.48
1:C:63:ILE:HD12	1:D:212:PRO:HG2	1.96	0.48
1:C:212:PRO:HG2	1:D:63:ILE:HD12	1.96	0.48
1:A:340:ARG:NH1	1:A:340:ARG:CG	2.71	0.48
1:C:336:ASP:C	1:C:337:LEU:HD23	2.33	0.48
1:D:56:PHE:C	1:D:56:PHE:CD1	2.88	0.47
1:B:250:PRO:HG2	1:B:254:ILE:HD12	1.97	0.47
1:B:361:LEU:HA	1:B:361:LEU:HD23	1.73	0.47
1:C:313:LEU:CD1	1:C:345:MET:HE1	2.42	0.47
1:D:332:ASP:O	1:D:336:ASP:HB2	2.14	0.47
1:B:129:ASP:OD1	1:B:219:ARG:HD2	2.15	0.47
1:B:65:ASP:O	1:B:69:ASP:HA	2.14	0.47
1:A:342:VAL:CG1	1:A:347:GLN:HG3	2.45	0.47
1:D:359:LEU:HD22	1:D:363:GLU:HG2	1.96	0.46
1:C:55:LEU:C	1:C:55:LEU:HD12	2.34	0.46
1:B:296:ARG:NH1	2:B:505:HOH:O	2.48	0.46
1:B:56:PHE:CD1	1:B:56:PHE:C	2.89	0.46
1:A:282[A]:VAL:HG21	1:A:378:TRP:CE3	2.50	0.46
1:C:309:GLY:HA3	1:C:365:GLY:O	2.16	0.46
1:D:317:SER:HB3	1:D:345:MET:HE2	1.98	0.46
1:A:371:ASN:O	1:A:372:VAL:HG22	2.16	0.45
1:D:129:ASP:OD1	1:D:219:ARG:HD2	2.16	0.45
1:A:371:ASN:O	1:A:372:VAL:CG2	2.64	0.45
1:D:310:LEU:HD23	1:D:310:LEU:HA	1.83	0.45
1:A:227:GLN:NE2	1:A:229:GLY:H	2.14	0.45
1:D:56:PHE:CD1	1:D:57:LEU:N	2.84	0.45
1:D:64:GLU:HA	1:D:64:GLU:OE1	2.17	0.45
1:D:243:GLU:OE1	1:D:439:ARG:NH1	2.38	0.45
1:C:70:ASN:OD1	1:C:72:GLU:HB2	2.17	0.45
1:A:277:LYS:HE3	1:A:442:LEU:O	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:134:TRP:CE2	1:C:136:VAL:HG22	2.51	0.44
1:B:229:GLY:C	1:B:230:LEU:HD23	2.36	0.44
1:A:309:GLY:HA3	1:A:365:GLY:O	2.17	0.44
1:A:203:ARG:HD3	1:A:208:SER:OG	2.17	0.44
1:C:102:GLY:HA3	1:C:438:LEU:HD13	1.99	0.44
1:C:290:GLU:O	1:C:294:ARG:HG3	2.17	0.44
1:D:252:LEU:HD22	1:D:256:ARG:HG3	1.99	0.44
1:D:339:ASP:OD1	1:D:339:ASP:N	2.51	0.44
1:A:37:GLY:O	1:A:41:LYS:HG3	2.18	0.44
1:D:361:LEU:HD23	1:D:361:LEU:HA	1.70	0.44
1:C:168:GLU:O	1:C:172:LYS:HG3	2.18	0.43
1:B:326:LEU:HB3	1:B:362:ALA:HB2	2.00	0.43
1:D:294:ARG:HH11	1:D:294:ARG:CG	2.30	0.43
1:A:313:LEU:HD13	1:A:368:TYR:CD2	2.52	0.43
1:C:345:MET:HG3	1:C:346:LEU:N	2.33	0.43
1:C:388:GLN:O	1:C:392:HIS:HD2	2.02	0.43
1:A:361:LEU:HD23	1:A:361:LEU:HA	1.72	0.43
1:B:48:GLU:OE1	1:B:98:THR:HB	2.18	0.43
1:D:387:ASP:OD1	1:D:426:ARG:NH2	2.47	0.43
1:D:7:LEU:HD12	1:D:7:LEU:C	2.39	0.43
1:D:294:ARG:HG2	1:D:294:ARG:HH11	1.82	0.43
1:C:215:VAL:HA	1:C:216:PRO:HD3	1.84	0.43
1:C:301:ASN:ND2	1:C:370:THR:HB	2.34	0.43
1:D:57:LEU:HD12	1:D:91:ILE:HG23	2.00	0.43
1:C:146:ARG:HD3	1:D:210:ARG:CD	2.47	0.42
1:C:421:PRO:O	1:C:425:GLN:HG3	2.18	0.42
1:D:390:ILE:HG12	1:D:428:VAL:HG21	2.01	0.42
1:A:337:LEU:O	1:A:341:HIS:HB2	2.19	0.42
1:A:279:PHE:HB3	1:A:402:ILE:HG13	2.01	0.42
1:A:317:SER:HB3	1:A:345:MET:HE2	2.00	0.42
1:A:100:ARG:CZ	1:A:436:THR:HG22	2.49	0.42
1:D:104:GLY:HA2	1:D:133:SER:O	2.20	0.42
1:D:178:SER:HB2	1:D:196:LYS:HB3	2.01	0.42
1:C:129:ASP:OD1	1:C:219:ARG:CD	2.68	0.42
1:A:108:SER:HA	1:A:137:VAL:CG2	2.38	0.42
1:B:67:TYR:CE1	1:B:322:SER:HB3	2.54	0.42
1:C:68:GLY:HA3	1:C:70:ASN:ND2	2.35	0.42
1:D:113:PRO:HA	1:D:114:PRO:HD3	1.87	0.42
1:D:226:LEU:HD13	1:D:246:PHE:HE1	1.84	0.42
1:A:123:THR:HG23	1:B:85:LEU:HG	2.01	0.41
1:B:309:GLY:HA3	1:B:365:GLY:O	2.19	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:86:GLU:HG3	1:D:120:VAL:HG23	2.01	0.41
1:D:13:PHE:O	1:D:58:PRO:HD2	2.20	0.41
1:D:345:MET:HG3	1:D:346:LEU:N	2.36	0.41
1:A:129:ASP:OD1	1:A:219:ARG:CD	2.68	0.41
1:A:245:VAL:HG11	1:A:262:ILE:HD13	2.01	0.41
1:B:55:LEU:HD23	1:B:56:PHE:N	2.35	0.41
1:C:310:LEU:HD23	1:C:310:LEU:HA	1.78	0.41
1:C:336:ASP:O	1:C:337:LEU:HD23	2.19	0.41
1:D:164:ASP:O	1:D:168:GLU:HG3	2.20	0.41
1:D:254:ILE:HD12	1:D:254:ILE:H	1.85	0.41
1:A:133:SER:HB3	1:A:224:VAL:HB	2.02	0.41
1:B:129:ASP:OD1	1:B:219:ARG:CD	2.68	0.41
1:C:310:LEU:HD11	1:C:361:LEU:HB3	2.02	0.41
1:D:176:SER:O	1:D:197:VAL:HA	2.21	0.41
1:D:326:LEU:HB3	1:D:362:ALA:HB2	2.02	0.41
1:C:405:PRO:HA	1:C:411:ILE:HG21	2.03	0.41
1:D:310:LEU:HD21	1:D:361:LEU:HD22	2.03	0.41
1:C:5:ARG:NH2	2:C:511:HOH:O	2.53	0.41
1:C:77:LEU:HB2	1:C:308:VAL:CG1	2.51	0.40
1:D:51:LYS:HA	1:D:433:TYR:CZ	2.56	0.40
1:D:411:ILE:HD12	1:D:411:ILE:HA	1.97	0.40
1:B:259:TYR:CZ	1:B:263:LYS:HE3	2.56	0.40
1:C:297:LEU:HD11	1:C:377:GLN:NE2	2.36	0.40
1:C:348:MET:O	1:C:352:VAL:HG12	2.22	0.40
1:D:226:LEU:HD13	1:D:246:PHE:CE1	2.57	0.40
1:D:324:TYR:OH	1:D:337:LEU:HD21	2.21	0.40
1:C:320:ASN:OD1	1:C:320:ASN:C	2.59	0.40
1:D:167:LEU:O	1:D:171:LYS:HG3	2.21	0.40
1:C:129:ASP:OD1	1:C:219:ARG:HD3	2.21	0.40
1:D:246:PHE:HB3	1:D:402:ILE:HD11	2.03	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	445/453 (98%)	432 (97%)	13 (3%)	0	100	100
1	B	446/453 (98%)	434 (97%)	11 (2%)	1 (0%)	47	55
1	C	445/453 (98%)	427 (96%)	17 (4%)	1 (0%)	47	55
1	D	444/453 (98%)	431 (97%)	12 (3%)	1 (0%)	47	55
All	All	1780/1812 (98%)	1724 (97%)	53 (3%)	3 (0%)	47	55

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	67	TYR
1	B	69	ASP
1	D	339	ASP

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	358/363 (99%)	348 (97%)	10 (3%)	43	56
1	B	359/363 (99%)	346 (96%)	13 (4%)	35	45
1	C	358/363 (99%)	338 (94%)	20 (6%)	21	25
1	D	357/363 (98%)	339 (95%)	18 (5%)	24	30
All	All	1432/1452 (99%)	1371 (96%)	61 (4%)	29	36

All (61) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	14	SER
1	A	56	PHE
1	A	64	GLU
1	A	65	ASP
1	A	203	ARG

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Mol	Chain	Res	Type
1	A	230	LEU
1	A	310	LEU
1	A	345	MET
1	A	346	LEU
1	A	391	SER
1	B	54	LEU
1	B	56	PHE
1	B	65	ASP
1	B	66	SER
1	B	72	GLU
1	B	132	ILE
1	B	146	ARG
1	B	274	GLU
1	B	308	VAL
1	B	310	LEU
1	B	345	MET
1	B	346	LEU
1	B	372	VAL
1	C	5	ARG
1	C	55	LEU
1	C	64	GLU
1	C	65	ASP
1	C	66	SER
1	C	70	ASN
1	C	151	ASP
1	C	152	GLU
1	C	203	ARG
1	C	205	ARG
1	C	274	GLU
1	C	291	GLN
1	C	310	LEU
1	C	322	SER
1	C	339	ASP
1	C	341	HIS
1	C	345	MET
1	C	347	GLN
1	C	372	VAL
1	C	402	ILE
1	D	54	LEU
1	D	56	PHE
1	D	65	ASP
1	D	120	VAL

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Mol	Chain	Res	Type
1	D	132	ILE
1	D	151	ASP
1	D	152	GLU
1	D	195	LYS
1	D	252	LEU
1	D	260	GLN
1	D	291	GLN
1	D	323	LYS
1	D	337	LEU
1	D	339	ASP
1	D	344	THR
1	D	345	MET
1	D	352	VAL
1	D	391	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (35) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	8	HIS
1	A	99	GLN
1	A	153	HIS
1	A	227	GLN
1	A	265	HIS
1	A	291	GLN
1	A	301	ASN
1	A	377	GLN
1	A	392	HIS
1	A	425	GLN
1	B	8	HIS
1	B	99	GLN
1	B	153	HIS
1	B	265	HIS
1	B	291	GLN
1	B	301	ASN
1	B	377	GLN
1	B	392	HIS
1	B	425	GLN
1	C	8	HIS
1	C	99	GLN
1	C	301	ASN
1	C	377	GLN
1	C	392	HIS

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Mol	Chain	Res	Type
1	C	425	GLN
1	C	446	HIS
1	D	8	HIS
1	D	99	GLN
1	D	198	GLN
1	D	265	HIS
1	D	301	ASN
1	D	377	GLN
1	D	392	HIS
1	D	425	GLN
1	D	446	HIS

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 monosaccharides in this entry.

5.6 Ligand geometry

There are no ligands in this entry.

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

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, 95^{th} 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	446/453 (98%)	-0.36	4 (0%)	84	83	23, 33, 56, 86	0
1	B	446/453 (98%)	-0.33	5 (1%)	80	79	24, 34, 58, 92	0
1	C	446/453 (98%)	-0.19	15 (3%)	45	43	25, 37, 72, 118	0
1	D	446/453 (98%)	0.15	34 (7%)	13	12	28, 44, 88, 120	0
All	All	1784/1812 (98%)	-0.18	58 (3%)	46	44	23, 37, 69, 120	0

All (58) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	67	TYR	9.2
1	B	67	TYR	6.7
1	D	355	GLY	6.4
1	C	340	ARG	6.2
1	B	68	GLY	6.1
1	D	67	TYR	5.7
1	D	356	GLY	5.5
1	D	333	ILE	5.2
1	C	341	HIS	4.8
1	D	354	GLY	4.6
1	C	334	VAL	4.5
1	A	67	TYR	4.5
1	D	69	ASP	4.5
1	D	448	GLU	4.3
1	D	351	ALA	4.1
1	D	319	LEU	4.1
1	D	153	HIS	4.1
1	D	203	ARG	3.9
1	C	338	GLY	3.8
1	C	339	ASP	3.8
1	D	358	ASP	3.6

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Mol	Chain	Res	Type	RSRZ
1	A	66	SER	3.6
1	D	342	VAL	3.6
1	D	339	ASP	3.5
1	D	340	ARG	3.5
1	C	337	LEU	3.4
1	C	342	VAL	3.4
1	C	323	LYS	3.3
1	D	337	LEU	3.2
1	D	334	VAL	3.1
1	C	68	GLY	2.9
1	B	5	ARG	2.9
1	D	450	GLY	2.9
1	B	69	ASP	2.8
1	C	319	LEU	2.8
1	D	341	HIS	2.7
1	D	68	GLY	2.7
1	A	152	GLU	2.7
1	D	347	GLN	2.6
1	D	357	ALA	2.6
1	C	335	ALA	2.6
1	A	450	GLY	2.6
1	D	359	LEU	2.5
1	D	152	GLU	2.5
1	D	353	ALA	2.5
1	D	322	SER	2.5
1	C	69	ASP	2.5
1	D	97	VAL	2.4
1	D	64	GLU	2.4
1	D	449	VAL	2.4
1	D	338	GLY	2.3
1	D	5	ARG	2.2
1	B	450	GLY	2.1
1	C	66	SER	2.1
1	C	351	ALA	2.1
1	D	335	ALA	2.1
1	D	350	SER	2.1
1	D	151	ASP	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 monosaccharides in this entry.

6.4 Ligands (i)

There are no ligands in this entry.

6.5 Other polymers (i)

There are no such residues in this entry.