Full wwPDB X-ray Structure Validation Report ⓘ

May 22, 2020 – 11:19 pm BST

PDB ID	:	1RF5
Title	:	Structural Studies of Streptococcus pneumoniae EPSP Synthase in Unliganded State
Authors	:	Park, H.; Hilsenbeck, J.L.; Kim, H.J.; Shuttleworth, W.A.; Park, Y.H.; Evans, J.N.; Kang, C.
Deposited on	:	2003-11-07
Resolution	:	2.30 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 following versions of software and data (see references ①) were used in the production of this report:

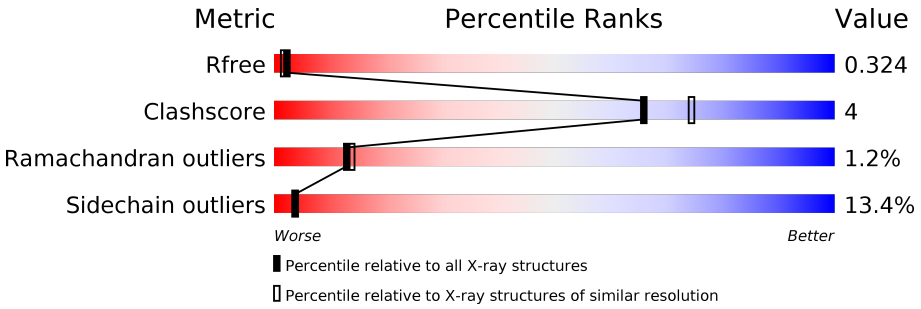
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.11
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.11

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 2.30 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	5042 (2.30-2.30)
Clashscore	141614	5643 (2.30-2.30)
Ramachandran outliers	138981	5575 (2.30-2.30)
Sidechain outliers	138945	5575 (2.30-2.30)

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 on 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%

Mol	Chain	Length	Quality of chain
1	A	427	77% 21% .
1	B	427	74% 23% .
1	C	427	78% 19% .
1	D	427	75% 22% .

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 13615 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 5-enolpyruvylshikimate-3-phosphate synthase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	427	Total	C	N	O	S	51	0	0
			3212	2019	559	619	15			
1	B	427	Total	C	N	O	S	51	0	0
			3212	2019	559	619	15			
1	C	427	Total	C	N	O	S	51	0	0
			3212	2019	559	619	15			
1	D	427	Total	C	N	O	S	51	0	0
			3212	2019	559	619	15			

- Molecule 2 is water.

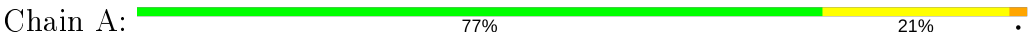
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	191	Total	O	0	0
			191	191		
2	B	172	Total	O	0	0
			172	172		
2	C	203	Total	O	0	0
			203	203		
2	D	201	Total	O	0	0
			201	201		

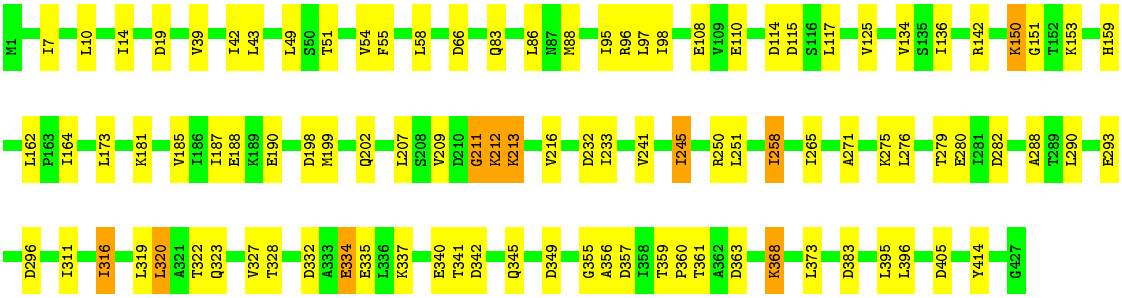
3 Residue-property plots (i)

These plots are drawn for all protein, RNA and DNA 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. 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. 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: 5-enolpyruvylshikimate-3-phosphate synthase

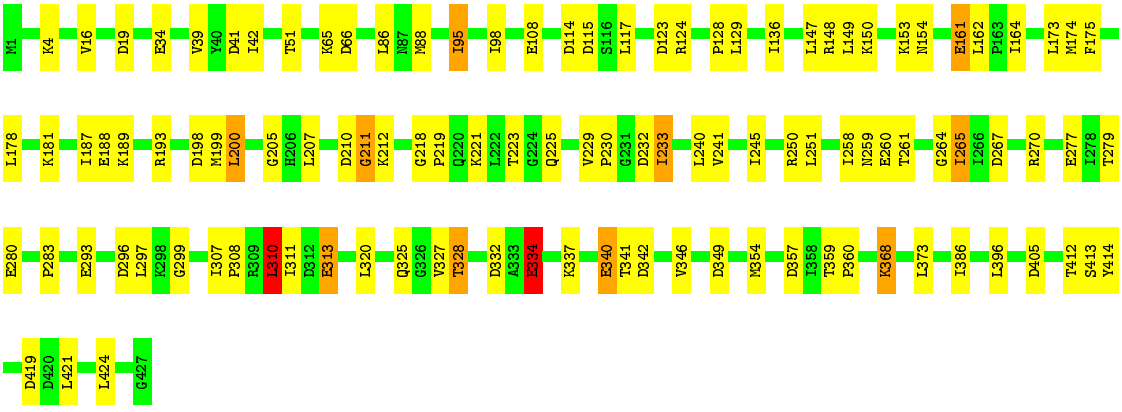
Chain A:





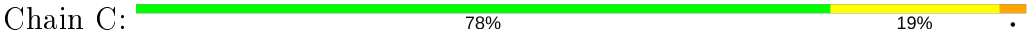
- Molecule 1: 5-enolpyruvylshikimate-3-phosphate synthase

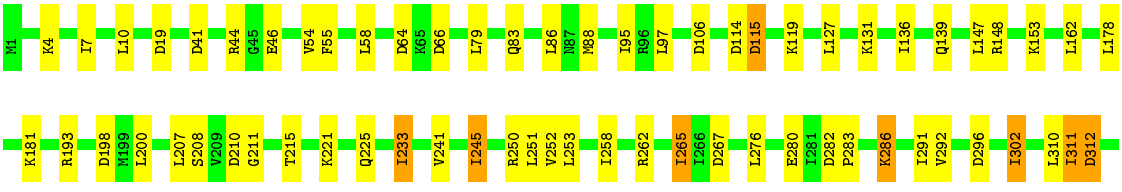
Chain B:



- Molecule 1: 5-enolpyruvylshikimate-3-phosphate synthase

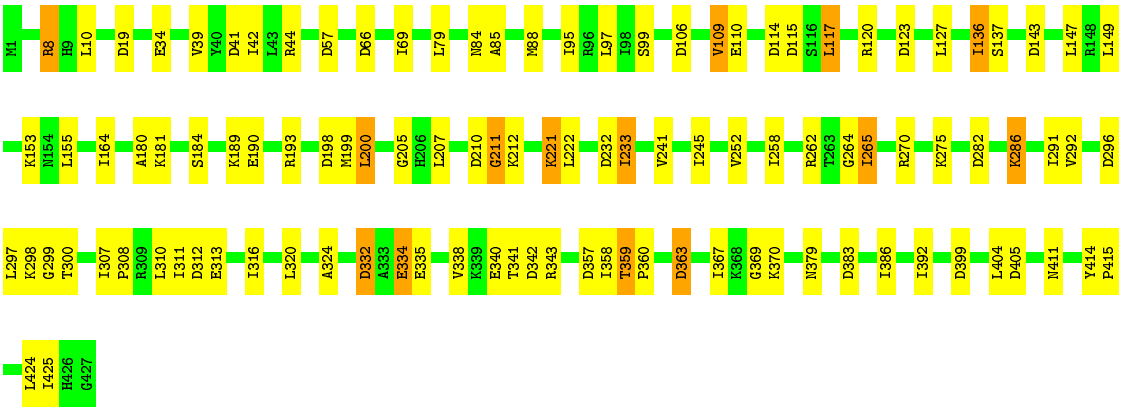
Chain C:





- Molecule 1: 5-enolpyruvylshikimate-3-phosphate synthase

Chain D:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	115.59Å 116.48Å 176.32Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	10.00 – 2.30 9.99 – 2.30	Depositor EDS
% Data completeness (in resolution range)	(Not available) (10.00-2.30) 95.7 (9.99-2.30)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	19.68 (at 2.31Å)	Xtriage
Refinement program	X-PLOR 3.851	Depositor
R, R_{free}	0.218 , 0.277 0.311 , 0.324	Depositor DCC
R_{free} test set	5011 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å^2)	29.5	Xtriage
Anisotropy	0.025	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.40 , 62.2	EDS
L-test for twinning[2]	$< \|L\| > = 0.51$, $< L^2 > = 0.35$	Xtriage
Estimated twinning fraction	0.007 for k,h,-l	Xtriage
F_o,F_c correlation	0.86	EDS
Total number of atoms	13615	wwPDB-VP
Average B, all atoms (Å^2)	39.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.43% 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	0.53	2/3252 (0.1%)	1.02	18/4391 (0.4%)
1	B	0.63	2/3252 (0.1%)	1.25	24/4391 (0.5%)
1	C	0.46	1/3251 (0.0%)	1.15	17/4388 (0.4%)
1	D	0.30	0/3252	1.35	26/4391 (0.6%)
All	All	0.50	5/13007 (0.0%)	1.20	85/17561 (0.5%)

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
1	A	0	1
1	B	0	3
1	D	0	1
All	All	0	5

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	340	GLU	C-N	-29.87	0.65	1.34
1	A	340	GLU	C-N	22.25	1.85	1.34
1	C	334	GLU	C-N	20.19	1.80	1.34
1	A	334	GLU	C-N	-11.84	1.06	1.34
1	B	334	GLU	C-N	-11.61	1.07	1.34

All (85) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	D	334	GLU	O-C-N	-64.31	19.80	122.70
1	C	334	GLU	O-C-N	-59.96	26.76	122.70
1	B	340	GLU	O-C-N	-47.90	46.05	122.70
1	A	334	GLU	O-C-N	-46.96	47.57	122.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	334	GLU	O-C-N	-42.94	54.00	122.70
1	D	340	GLU	O-C-N	-32.77	70.27	122.70
1	D	340	GLU	CA-C-N	23.30	168.47	117.20
1	B	334	GLU	CA-C-N	-18.60	76.27	117.20
1	A	340	GLU	C-N-CA	-15.83	82.12	121.70
1	B	340	GLU	CA-C-N	14.68	149.50	117.20
1	C	334	GLU	CA-C-N	-8.64	98.18	117.20
1	B	334	GLU	C-N-CA	-7.53	102.88	121.70
1	B	340	GLU	C-N-CA	-7.26	103.54	121.70
1	D	334	GLU	CA-C-N	-7.00	101.80	117.20
1	C	114	ASP	CB-CG-OD2	6.53	124.18	118.30
1	A	114	ASP	CB-CG-OD2	6.47	124.12	118.30
1	C	210	ASP	CB-CG-OD2	6.31	123.98	118.30
1	B	114	ASP	CB-CG-OD2	6.30	123.97	118.30
1	B	232	ASP	CB-CG-OD2	6.28	123.95	118.30
1	A	232	ASP	CB-CG-OD2	6.25	123.92	118.30
1	D	340	GLU	C-N-CA	6.18	137.14	121.70
1	D	106	ASP	CB-CG-OD2	6.15	123.84	118.30
1	D	210	ASP	CB-CG-OD2	6.15	123.83	118.30
1	D	114	ASP	CB-CG-OD2	6.13	123.81	118.30
1	B	198	ASP	CB-CG-OD2	6.12	123.81	118.30
1	C	106	ASP	CB-CG-OD2	6.05	123.75	118.30
1	D	198	ASP	CB-CG-OD2	5.99	123.69	118.30
1	D	357	ASP	CB-CG-OD2	5.97	123.67	118.30
1	B	123	ASP	CB-CG-OD2	5.97	123.67	118.30
1	D	399	ASP	CB-CG-OD2	5.96	123.66	118.30
1	A	198	ASP	CB-CG-OD2	5.93	123.64	118.30
1	D	57	ASP	CB-CG-OD2	5.91	123.62	118.30
1	D	123	ASP	CB-CG-OD2	5.90	123.61	118.30
1	C	64	ASP	CB-CG-OD2	5.90	123.61	118.30
1	C	282	ASP	CB-CG-OD2	5.89	123.60	118.30
1	D	312	ASP	CB-CG-OD2	5.89	123.60	118.30
1	A	349	ASP	CB-CG-OD2	5.88	123.59	118.30
1	D	232	ASP	CB-CG-OD2	5.83	123.55	118.30
1	A	363	ASP	CB-CG-OD2	5.82	123.53	118.30
1	B	419	ASP	CB-CG-OD2	5.80	123.52	118.30
1	C	41	ASP	CB-CG-OD2	5.79	123.51	118.30
1	D	342	ASP	CB-CG-OD2	5.79	123.51	118.30
1	C	198	ASP	CB-CG-OD2	5.78	123.50	118.30
1	C	267	ASP	CB-CG-OD2	5.75	123.48	118.30
1	B	357	ASP	CB-CG-OD2	5.75	123.48	118.30
1	B	349	ASP	CB-CG-OD2	5.74	123.47	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	115	ASP	CB-CG-OD2	5.70	123.43	118.30
1	D	405	ASP	CB-CG-OD2	5.70	123.43	118.30
1	C	296	ASP	CB-CG-OD2	5.60	123.34	118.30
1	D	66	ASP	CB-CG-OD2	5.58	123.32	118.30
1	D	282	ASP	CB-CG-OD2	5.58	123.32	118.30
1	A	115	ASP	CB-CG-OD2	5.55	123.29	118.30
1	A	383	ASP	CB-CG-OD2	5.49	123.24	118.30
1	C	357	ASP	CB-CG-OD2	5.49	123.24	118.30
1	D	383	ASP	CB-CG-OD2	5.44	123.19	118.30
1	C	19	ASP	CB-CG-OD2	5.41	123.17	118.30
1	D	332	ASP	CB-CG-OD2	5.41	123.17	118.30
1	A	405	ASP	CB-CG-OD2	5.36	123.12	118.30
1	D	41	ASP	CB-CG-OD2	5.31	123.08	118.30
1	B	19	ASP	CB-CG-OD2	5.29	123.06	118.30
1	B	310	LEU	CA-CB-CG	5.27	127.42	115.30
1	A	332	ASP	CB-CG-OD2	5.23	123.01	118.30
1	B	342	ASP	CB-CG-OD2	5.23	123.00	118.30
1	B	210	ASP	CB-CG-OD2	5.20	122.97	118.30
1	A	342	ASP	CB-CG-OD2	5.18	122.96	118.30
1	D	19	ASP	CB-CG-OD2	5.17	122.95	118.30
1	A	282	ASP	CB-CG-OD2	5.15	122.94	118.30
1	A	19	ASP	CB-CG-OD2	5.15	122.94	118.30
1	B	267	ASP	CB-CG-OD2	5.14	122.92	118.30
1	B	332	ASP	CB-CG-OD2	5.14	122.92	118.30
1	C	115	ASP	CB-CG-OD2	5.13	122.92	118.30
1	C	342	ASP	CB-CG-OD2	5.12	122.90	118.30
1	B	296	ASP	CB-CG-OD2	5.10	122.89	118.30
1	A	340	GLU	O-C-N	5.08	130.83	122.70
1	B	405	ASP	CB-CG-OD2	5.08	122.87	118.30
1	A	296	ASP	CB-CG-OD2	5.06	122.85	118.30
1	D	296	ASP	CB-CG-OD2	5.05	122.85	118.30
1	C	419	ASP	CB-CG-OD2	5.04	122.84	118.30
1	A	357	ASP	CB-CG-OD2	5.04	122.84	118.30
1	B	66	ASP	CB-CG-OD2	5.04	122.84	118.30
1	D	143	ASP	CB-CG-OD2	5.04	122.84	118.30
1	C	66	ASP	CB-CG-OD2	5.04	122.83	118.30
1	D	115	ASP	CB-CG-OD2	5.01	122.81	118.30
1	B	41	ASP	CB-CG-OD2	5.01	122.81	118.30
1	A	66	ASP	CB-CG-OD2	5.00	122.81	118.30

There are no chirality outliers.

All (5) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	334	GLU	Mainchain
1	B	334	GLU	Mainchain
1	B	340	GLU	Mainchain,Peptide
1	D	334	GLU	Mainchain

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	3212	0	3323	26	0
1	B	3212	0	3323	30	0
1	C	3212	0	3323	26	0
1	D	3212	0	3324	26	0
2	A	191	0	0	1	0
2	B	172	0	0	0	0
2	C	203	0	0	1	0
2	D	201	0	0	0	0
All	All	13615	0	13293	102	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 4.

All (102) 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:C:286:LYS:HG2	1:C:286:LYS:O	1.66	0.92
1:D:286:LYS:O	1:D:286:LYS:HG2	1.82	0.78
1:C:311:ILE:O	1:C:312:ASP:HB2	1.92	0.70
1:B:88:MET:HG3	1:B:95:ILE:HG23	1.74	0.68
1:B:193:ARG:HA	1:B:261:THR:HG21	1.76	0.68
1:C:241:VAL:HG22	1:C:320:LEU:HG	1.74	0.67
1:C:378:VAL:HG11	1:C:390:THR:HG21	1.79	0.63
1:A:211:GLY:O	1:A:212:LYS:HB2	1.99	0.61
1:C:193:ARG:HH21	1:C:262:ARG:HH11	1.50	0.59
1:C:397:VAL:HG11	2:C:598:HOH:O	2.03	0.58
1:D:109:VAL:HG12	1:D:149:LEU:HB3	1.84	0.58
1:A:245:ILE:HG12	1:A:323:GLN:HG3	1.85	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:352:ASN:HD21	1:C:358:ILE:H	1.52	0.57
1:D:79:LEU:H	1:D:79:LEU:HD23	1.69	0.57
1:B:245:ILE:HG22	1:B:396:LEU:HD21	1.88	0.55
1:C:302:ILE:O	1:C:302:ILE:HG13	2.05	0.55
1:A:51:THR:HG23	1:A:98:ILE:HD11	1.90	0.53
1:B:264:GLY:HA3	1:B:310:LEU:HB3	1.91	0.53
1:C:319:LEU:HD11	1:C:393:ALA:HB2	1.91	0.52
1:D:358:ILE:HG12	1:D:367:ILE:HG12	1.92	0.52
1:D:411:ASN:HD22	1:D:415:PRO:HA	1.76	0.51
1:B:108:GLU:HG3	1:B:150:LYS:HB2	1.92	0.51
1:D:332:ASP:H	1:D:363:ASP:HB2	1.75	0.51
1:B:211:GLY:O	1:B:212:LYS:HB2	2.11	0.51
1:A:188:GLU:HB2	1:A:212:LYS:HG2	1.93	0.51
1:A:96:ARG:HG2	1:A:125:VAL:HG21	1.92	0.50
1:D:39:VAL:HB	1:D:69:ILE:HB	1.94	0.50
1:A:54:VAL:HG13	1:A:86:LEU:HD22	1.93	0.50
1:D:8:ARG:HH22	1:D:425:ILE:HG23	1.77	0.49
1:D:10:LEU:HG	1:D:424:LEU:HB3	1.95	0.49
1:D:211:GLY:O	1:D:212:LYS:HB2	2.12	0.49
1:A:10:LEU:HD23	1:A:251:LEU:HD11	1.93	0.49
1:B:250:ARG:HG3	1:B:293:GLU:HB3	1.93	0.49
1:D:241:VAL:HG22	1:D:320:LEU:HD13	1.95	0.49
1:A:279:THR:HA	1:B:277:GLU:HG2	1.94	0.49
1:A:327:VAL:HG22	1:A:368:LYS:HG3	1.95	0.49
1:B:280:GLU:HG2	1:C:252:VAL:HG11	1.95	0.48
1:C:10:LEU:HB3	1:C:251:LEU:HD21	1.94	0.48
1:C:283:PRO:HG3	1:D:275:LYS:HE2	1.94	0.48
1:B:241:VAL:HG22	1:B:320:LEU:HD13	1.95	0.48
1:B:51:THR:HG23	1:B:98:ILE:HD11	1.95	0.48
1:C:311:ILE:O	1:C:312:ASP:CB	2.61	0.48
1:C:302:ILE:HG12	1:C:330:ILE:HG12	1.95	0.48
1:B:327:VAL:HG22	1:B:368:LYS:HG3	1.95	0.48
1:C:245:ILE:HD12	1:C:320:LEU:HD23	1.96	0.47
1:D:88:MET:HG3	1:D:95:ILE:HD12	1.97	0.47
1:B:251:LEU:HD22	1:B:424:LEU:HD22	1.96	0.47
1:D:265:ILE:HG12	1:D:313:GLU:HG2	1.96	0.47
1:C:241:VAL:HG21	1:C:316:ILE:HG13	1.97	0.47
1:A:39:VAL:HG11	1:A:42:ILE:HD12	1.98	0.46
1:A:134:VAL:HG13	1:A:151:GLY:HA2	1.97	0.46
1:D:307:ILE:HB	1:D:308:PRO:HD3	1.96	0.46
1:B:265:ILE:H	1:B:265:ILE:HG13	1.35	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:161:GLU:HG2	1:B:187:ILE:HB	1.97	0.46
1:D:200:LEU:HD22	1:D:205:GLY:HA3	1.98	0.45
1:C:54:VAL:HG13	1:C:86:LEU:HD22	1.99	0.45
1:A:202:GLN:HA	2:A:550:HOH:O	2.16	0.45
1:B:95:ILE:H	1:B:95:ILE:HG13	1.34	0.45
1:A:359:THR:HA	1:A:360:PRO:HD3	1.86	0.44
1:C:88:MET:HG3	1:C:95:ILE:HD12	1.99	0.44
1:A:271:ALA:HA	1:B:260:GLU:HG3	1.98	0.44
1:C:208:SER:HB3	1:C:215:THR:HB	2.00	0.44
1:D:155:LEU:HD23	1:D:180:ALA:HB2	1.99	0.44
1:B:39:VAL:HG11	1:B:42:ILE:HD12	1.99	0.44
1:A:258:ILE:HD13	1:A:288:ALA:HB3	1.99	0.43
1:B:233:ILE:HG13	1:B:233:ILE:H	1.44	0.43
1:A:108:GLU:HG3	1:A:150:LYS:HG3	2.00	0.43
1:A:55:PHE:HA	1:A:58:LEU:HD12	2.00	0.43
1:B:128:PRO:HB2	1:B:173:LEU:HD21	2.00	0.43
1:A:280:GLU:HG2	1:D:252:VAL:HG11	2.01	0.43
1:C:318:ALA:O	1:C:322:THR:HG23	2.19	0.43
1:B:200:LEU:HD22	1:B:205:GLY:HA3	2.01	0.43
1:A:159:HIS:CD2	1:A:185:VAL:HG22	2.53	0.43
1:D:39:VAL:HG11	1:D:42:ILE:HD12	2.01	0.42
1:C:233:ILE:H	1:C:233:ILE:HG13	1.43	0.42
1:D:252:VAL:HG22	1:D:291:ILE:HG12	2.02	0.42
1:D:264:GLY:HA3	1:D:310:LEU:HB3	2.01	0.42
1:B:299:GLY:HA2	1:B:328:THR:HG22	2.02	0.42
1:D:233:ILE:HD13	1:D:262:ARG:HB3	2.01	0.42
1:A:316:ILE:HG13	1:A:316:ILE:H	1.43	0.42
1:C:312:ASP:HB3	1:C:385:ARG:HH21	1.85	0.42
1:C:55:PHE:HA	1:C:58:LEU:HD12	2.01	0.42
1:A:233:ILE:HG13	1:A:233:ILE:H	1.70	0.42
1:A:355:GLY:HA3	1:A:373:LEU:HD23	2.01	0.41
1:B:175:PHE:HA	1:B:178:LEU:HD12	2.03	0.41
1:B:229:VAL:HA	1:B:230:PRO:HD3	1.89	0.41
1:B:354:MET:HB3	1:B:373:LEU:HD22	2.02	0.41
1:A:241:VAL:HG22	1:A:320:LEU:HG	2.03	0.41
1:A:187:ILE:HG12	1:A:213:LYS:HG3	2.03	0.41
1:C:265:ILE:H	1:C:265:ILE:HG13	1.57	0.41
1:A:250:ARG:HG3	1:A:293:GLU:HB3	2.02	0.41
1:A:275:LYS:HE2	1:B:283:PRO:HG3	2.03	0.41
1:B:359:THR:HA	1:B:360:PRO:HD3	1.91	0.41
1:C:252:VAL:HG22	1:C:291:ILE:HG12	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:117:LEU:HD23	1:D:120:ARG:HD3	2.03	0.41
1:D:241:VAL:HG21	1:D:316:ILE:HG22	2.01	0.41
1:D:324:ALA:O	1:D:369:GLY:HA3	2.21	0.41
1:B:218:GLY:HA3	1:B:219:PRO:HD2	1.92	0.40
1:B:307:ILE:HB	1:B:308:PRO:HD3	2.04	0.40
1:C:245:ILE:HG12	1:C:396:LEU:HD21	2.03	0.40
1:B:265:ILE:HG12	1:B:313:GLU:HG2	2.02	0.40
1:D:359:THR:HA	1:D:360:PRO:HD3	1.87	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	425/427 (100%)	401 (94%)	19 (4%)	5 (1%)	13	14
1	B	425/427 (100%)	397 (93%)	25 (6%)	3 (1%)	22	26
1	C	423/427 (99%)	395 (93%)	25 (6%)	3 (1%)	22	26
1	D	425/427 (100%)	396 (93%)	20 (5%)	9 (2%)	7	5
All	All	1698/1708 (99%)	1589 (94%)	89 (5%)	20 (1%)	13	14

All (20) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	356	ALA
1	B	341	THR
1	D	335	GLU
1	A	337	LYS
1	B	337	LYS
1	A	212	LYS
1	C	312	ASP

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Mol	Chain	Res	Type
1	D	85	ALA
1	D	338	VAL
1	D	341	THR
1	A	209	VAL
1	C	373	LEU
1	D	137	SER
1	D	221	LYS
1	D	299	GLY
1	C	211	GLY
1	D	211	GLY
1	D	136	ILE
1	A	211	GLY
1	B	211	GLY

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	350/350 (100%)	308 (88%)	42 (12%)	5 5
1	B	350/350 (100%)	301 (86%)	49 (14%)	3 3
1	C	350/350 (100%)	297 (85%)	53 (15%)	3 2
1	D	350/350 (100%)	306 (87%)	44 (13%)	4 4
All	All	1400/1400 (100%)	1212 (87%)	188 (13%)	4 4

All (188) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	7	ILE
1	A	14	ILE
1	A	43	LEU
1	A	49	LEU
1	A	83	GLN
1	A	88	MET
1	A	95	ILE
1	A	97	LEU

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Mol	Chain	Res	Type
1	A	110	GLU
1	A	117	LEU
1	A	136	ILE
1	A	142	ARG
1	A	150	LYS
1	A	153	LYS
1	A	162	LEU
1	A	164	ILE
1	A	173	LEU
1	A	181	LYS
1	A	190	GLU
1	A	199	MET
1	A	207	LEU
1	A	213	LYS
1	A	216	VAL
1	A	245	ILE
1	A	258	ILE
1	A	265	ILE
1	A	276	LEU
1	A	290	LEU
1	A	311	ILE
1	A	316	ILE
1	A	319	LEU
1	A	320	LEU
1	A	322	THR
1	A	328	THR
1	A	335	GLU
1	A	341	THR
1	A	345	GLN
1	A	361	THR
1	A	368	LYS
1	A	395	LEU
1	A	396	LEU
1	A	414	TYR
1	B	4	LYS
1	B	16	VAL
1	B	34	GLU
1	B	65	LYS
1	B	86	LEU
1	B	95	ILE
1	B	117	LEU
1	B	124	ARG

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Mol	Chain	Res	Type
1	B	129	LEU
1	B	136	ILE
1	B	147	LEU
1	B	148	ARG
1	B	149	LEU
1	B	153	LYS
1	B	154	ASN
1	B	161	GLU
1	B	162	LEU
1	B	164	ILE
1	B	174	MET
1	B	181	LYS
1	B	188	GLU
1	B	189	LYS
1	B	199	MET
1	B	200	LEU
1	B	207	LEU
1	B	221	LYS
1	B	223	THR
1	B	225	GLN
1	B	233	ILE
1	B	240	LEU
1	B	258	ILE
1	B	259	ASN
1	B	265	ILE
1	B	270	ARG
1	B	279	THR
1	B	297	LEU
1	B	310	LEU
1	B	311	ILE
1	B	313	GLU
1	B	325	GLN
1	B	328	THR
1	B	334	GLU
1	B	346	VAL
1	B	368	LYS
1	B	386	ILE
1	B	412	THR
1	B	413	SER
1	B	414	TYR
1	B	421	LEU
1	C	4	LYS

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Mol	Chain	Res	Type
1	C	7	ILE
1	C	44	ARG
1	C	46	GLU
1	C	79	LEU
1	C	83	GLN
1	C	97	LEU
1	C	115	ASP
1	C	119	LYS
1	C	127	LEU
1	C	131	LYS
1	C	136	ILE
1	C	139	GLN
1	C	147	LEU
1	C	148	ARG
1	C	153	LYS
1	C	162	LEU
1	C	178	LEU
1	C	181	LYS
1	C	200	LEU
1	C	207	LEU
1	C	221	LYS
1	C	225	GLN
1	C	233	ILE
1	C	245	ILE
1	C	250	ARG
1	C	253	LEU
1	C	258	ILE
1	C	265	ILE
1	C	276	LEU
1	C	280	GLU
1	C	286	LYS
1	C	292	VAL
1	C	302	ILE
1	C	310	LEU
1	C	311	ILE
1	C	319	LEU
1	C	320	LEU
1	C	331	LYS
1	C	340	GLU
1	C	342	ASP
1	C	343	ARG
1	C	345	GLN

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Mol	Chain	Res	Type
1	C	354	MET
1	C	368	LYS
1	C	385	ARG
1	C	392	ILE
1	C	396	LEU
1	C	401	GLU
1	C	403	GLU
1	C	408	GLU
1	C	414	TYR
1	C	419	ASP
1	D	8	ARG
1	D	34	GLU
1	D	44	ARG
1	D	84	ASN
1	D	97	LEU
1	D	99	SER
1	D	109	VAL
1	D	110	GLU
1	D	117	LEU
1	D	127	LEU
1	D	136	ILE
1	D	147	LEU
1	D	153	LYS
1	D	164	ILE
1	D	181	LYS
1	D	184	SER
1	D	189	LYS
1	D	190	GLU
1	D	193	ARG
1	D	199	MET
1	D	200	LEU
1	D	207	LEU
1	D	221	LYS
1	D	222	LEU
1	D	233	ILE
1	D	245	ILE
1	D	258	ILE
1	D	265	ILE
1	D	270	ARG
1	D	286	LYS
1	D	292	VAL
1	D	297	LEU

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Mol	Chain	Res	Type
1	D	298	LYS
1	D	300	THR
1	D	311	ILE
1	D	343	ARG
1	D	359	THR
1	D	363	ASP
1	D	370	LYS
1	D	379	ASN
1	D	386	ILE
1	D	392	ILE
1	D	404	LEU
1	D	414	TYR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (17) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	83	GLN
1	A	159	HIS
1	A	255	ASN
1	A	259	ASN
1	A	325	GLN
1	B	6	ASN
1	B	325	GLN
1	C	83	GLN
1	C	90	ASN
1	C	220	GLN
1	C	259	ASN
1	C	352	ASN
1	C	411	ASN
1	D	254	GLN
1	D	259	ASN
1	D	379	ASN
1	D	411	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 carbohydrates 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

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	B	2
1	A	2
1	C	2

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	C	340:GLU	C	341:THR	N	2.02
1	A	340:GLU	C	341:THR	N	1.85
1	C	334:GLU	C	335:GLU	N	1.80
1	B	334:GLU	C	335:GLU	N	1.07
1	A	334:GLU	C	335:GLU	N	1.06
1	B	340:GLU	C	341:THR	N	0.65

6 Fit of model and data

6.1 Protein, DNA and RNA chains

Unable to reproduce the depositors R factor - this section is therefore empty.

6.2 Non-standard residues in protein, DNA, RNA chains

Unable to reproduce the depositors R factor - this section is therefore empty.

6.3 Carbohydrates

Unable to reproduce the depositors R factor - this section is therefore empty.

6.4 Ligands

Unable to reproduce the depositors R factor - this section is therefore empty.

6.5 Other polymers

Unable to reproduce the depositors R factor - this section is therefore empty.