Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2024 – 02:30 PM EST

PDB ID	:	8EFZ
Title	:	Crystal structure of CcNikZ-II, apoprotein
Authors	:	Stogios, P.J.; Evdokimova, E.; Diep, P.; Yakunin, A.; Mahadevan, K.; Savchenko, A.
Deposited on	:	2022-09-10
Resolution	:	2.38 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:

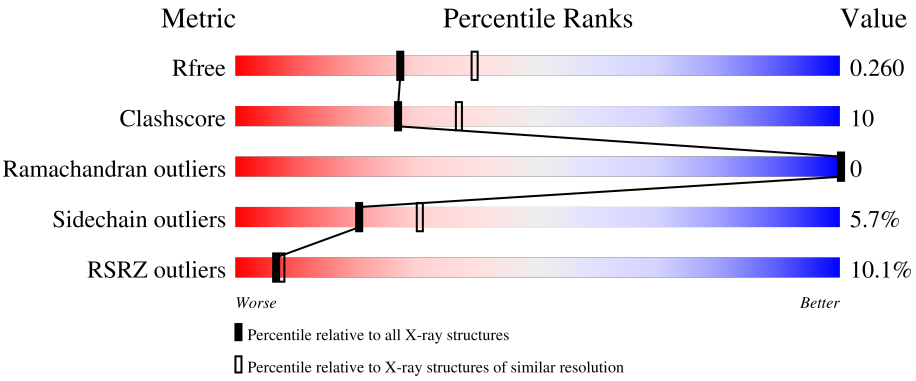
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.36
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation 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 2.38 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	5509 (2.40-2.36)
Clashscore	141614	6082 (2.40-2.36)
Ramachandran outliers	138981	5973 (2.40-2.36)
Sidechain outliers	138945	5975 (2.40-2.36)
RSRZ outliers	127900	5397 (2.40-2.36)

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	497	8% 68% 27%
1	B	497	11% 71% 25%

2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 7955 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 Extracellular solute-binding protein family 5.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	479	Total 3876	C 2494	N 630	O 742	S 10	0	0	0
1	B	483	Total 3905	C 2513	N 634	O 748	S 10	0	0	0

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	40	GLY	ALA	conflict	UNP C6PRH6
B	40	GLY	ALA	conflict	UNP C6PRH6

- Molecule 2 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	1	Total 1	Cl 1	0	0
2	B	1	Total 1	Cl 1	0	0

- Molecule 3 is water.

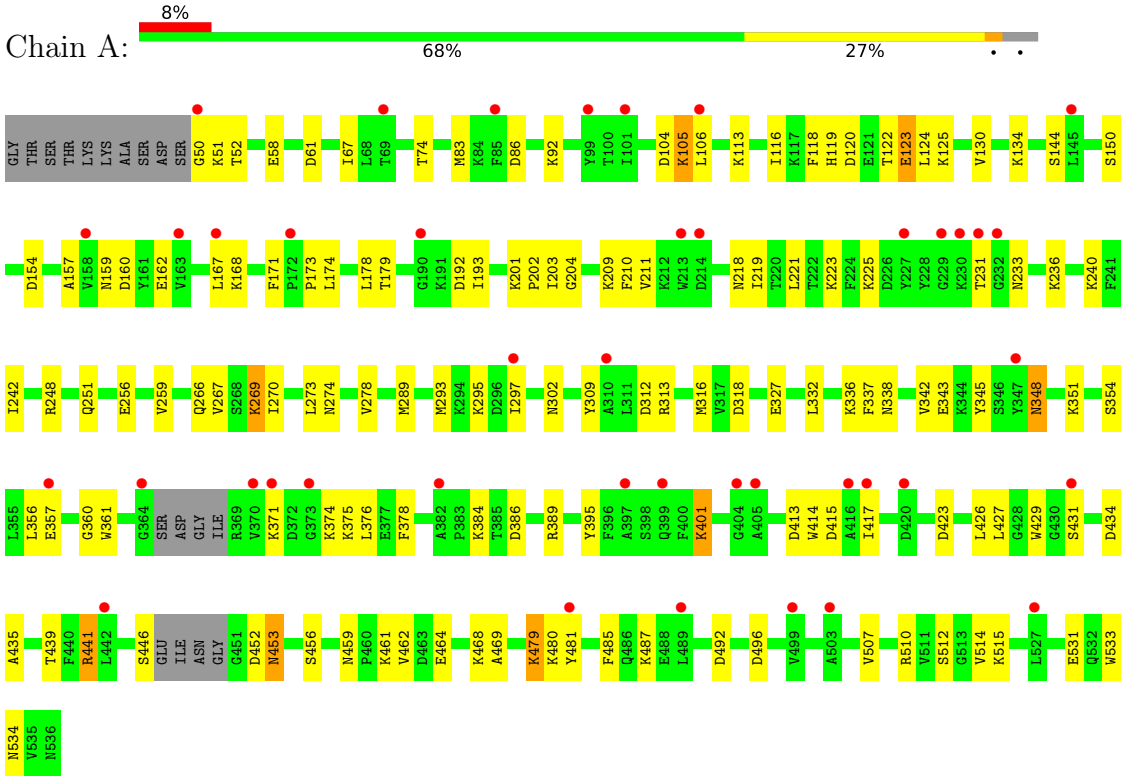
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	100	Total 100	O 100	0	0
3	B	71	Total 72	O 72	0	1

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.

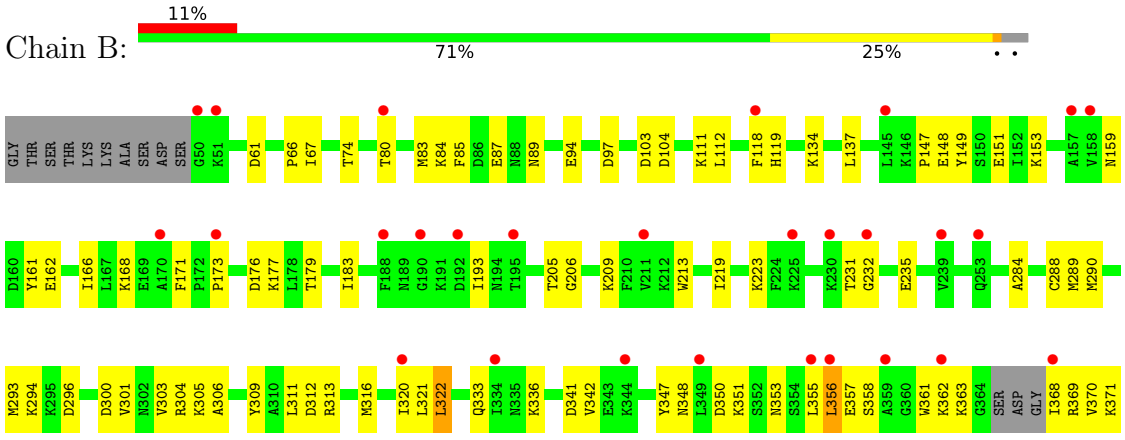
• Molecule 1: Extracellular solute-binding protein family 5

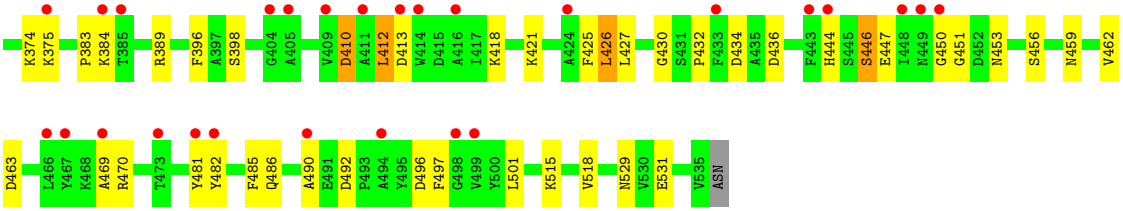
Chain A:



• Molecule 1: Extracellular solute-binding protein family 5

Chain B:




K374
K375
P383
K384
T385
R389
F396
A397
S398
G404
A405
V409
D410
A411
L412
D413
W414
D415
A416
I417
K418
K421
A424
F425
L426
L427
G430
S431
P432
F433
D434
A435
D436
F443
H444
S445
S446
E447
I448
N449
G450
G451
D452
N453
S456
N459
V462
D463
L466
Y467
K468
A469
R470
T473
Y481
Y482
F485
Q486
A490
E491
D492
P493
A494
Y495
D496
F497
G498
V499
Y500
L501
K515
V518
N529
V530
E531
V535
ASN

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	73.61Å 110.94Å 73.69Å 90.00° 113.72° 90.00°	Depositor
Resolution (Å)	29.71 – 2.38 29.71 – 2.38	Depositor EDS
% Data completeness (in resolution range)	90.0 (29.71-2.38) 90.0 (29.71-2.38)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.26 (at 2.39Å)	Xtriage
Refinement program	PHENIX 1.20_4459	Depositor
R, R_{free}	0.222 , 0.259 0.225 , 0.260	Depositor DCC
R_{free} test set	2007 reflections (4.98%)	wwPDB-VP
Wilson B-factor (Å^2)	44.9	Xtriage
Anisotropy	0.473	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.30 , 23.7	EDS
L-test for twinning[2]	$< \|L\| > = 0.44$, $< L^2 > = 0.27$	Xtriage
Estimated twinning fraction	0.438 for l,-k,h	Xtriage
F_o,F_c correlation	0.93	EDS
Total number of atoms	7955	wwPDB-VP
Average B, all atoms (Å^2)	51.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 12.86% 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

Bond lengths and bond angles in the following residue types are not validated in this section: CL

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	0.25	0/3961	0.46	0/5337
1	B	0.25	0/3991	0.45	0/5379
All	All	0.25	0/7952	0.45	0/10716

There are no bond length outliers.

There are no bond angle outliers.

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	3876	0	3830	83	0
1	B	3905	0	3862	75	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
3	A	100	0	0	4	0
3	B	72	0	0	1	0
All	All	7955	0	7692	158	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 10.

All (158) 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:159:ASN:HB3	1:A:162:GLU:HB3	1.65	0.79
1:B:356:LEU:HB3	1:B:368:ILE:HG21	1.66	0.75
1:B:418:LYS:HD2	1:B:421:LYS:HB2	1.71	0.72
1:B:469:ALA:HB2	1:B:481:TYR:HB2	1.74	0.70
1:B:316:MET:HA	1:B:320:ILE:HD13	1.74	0.70
1:A:356:LEU:HB3	1:A:361:TRP:HB2	1.74	0.69
1:A:357:GLU:N	1:A:357:GLU:OE1	2.26	0.69
1:B:313:ARG:NH1	1:B:497:PHE:O	2.27	0.67
1:A:459:ASN:HB3	1:A:462:VAL:HB	1.77	0.67
1:B:444:HIS:O	1:B:453:ASN:ND2	2.28	0.66
1:B:231:THR:HG23	1:B:531:GLU:HB2	1.79	0.65
1:A:427:LEU:HD22	1:A:429:TRP:HE1	1.64	0.63
1:A:171:PHE:CE2	1:A:173:PRO:HG2	2.35	0.62
1:A:348:ASN:HB3	1:A:351:LYS:HB2	1.80	0.62
1:B:66:PRO:HD2	1:B:183:ILE:HD11	1.82	0.61
1:B:147:PRO:HG3	1:B:450:GLY:HA2	1.82	0.61
1:B:459:ASN:HB3	1:B:462:VAL:HB	1.82	0.61
1:B:232:GLY:N	1:B:531:GLU:O	2.27	0.60
1:A:113:LYS:HB2	1:A:116:ILE:HD11	1.84	0.60
1:B:84:LYS:HB3	1:B:94:GLU:HG3	1.81	0.60
1:A:123:GLU:HG2	1:A:125:LYS:HZ3	1.67	0.59
1:B:300:ASP:HB3	1:B:303:VAL:HG23	1.84	0.59
1:A:171:PHE:CZ	1:A:173:PRO:HG2	2.38	0.59
1:A:105:LYS:NZ	3:A:710:HOH:O	2.36	0.58
1:B:425:PHE:HD2	1:B:427:LEU:HD23	1.67	0.58
1:A:223:LYS:HD3	1:A:225:LYS:HE3	1.86	0.57
1:A:348:ASN:HD22	1:A:351:LYS:HD2	1.68	0.57
1:B:432:PRO:HB3	1:B:518:VAL:HG12	1.85	0.57
1:A:469:ALA:HB2	1:A:481:TYR:HB2	1.86	0.56
1:B:322:LEU:HD12	1:B:322:LEU:O	2.04	0.56
1:B:83:MET:HB2	1:B:179:THR:HG22	1.87	0.55
1:A:360:GLY:HA3	1:A:371:LYS:HG3	1.89	0.55
1:A:515:LYS:NZ	3:A:715:HOH:O	2.40	0.55
1:B:289:MET:HB3	1:B:496:ASP:HB3	1.87	0.55
1:B:357:GLU:O	1:B:362:LYS:NZ	2.40	0.55
1:B:362:LYS:N	1:B:370:VAL:O	2.34	0.55
1:A:119:HIS:CD2	1:A:204:GLY:H	2.25	0.54
1:A:435:ALA:O	1:A:439:THR:OG1	2.22	0.54
1:A:259:VAL:HG13	1:A:507:VAL:HG22	1.88	0.54
1:A:83:MET:HB2	1:A:179:THR:HG22	1.90	0.53
1:B:363:LYS:HB3	1:B:369:ARG:HB2	1.90	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:130:VAL:HG21	1:A:157:ALA:HB2	1.91	0.53
1:B:410:ASP:N	1:B:410:ASP:OD1	2.43	0.52
1:A:342:VAL:HG12	1:A:487:LYS:HG2	1.91	0.52
1:A:223:LYS:HE2	1:A:231:THR:HG21	1.92	0.52
1:B:446:SER:O	1:B:446:SER:OG	2.27	0.52
1:A:211:VAL:HG23	1:A:221:LEU:HA	1.93	0.51
1:A:173:PRO:HB3	1:A:434:ASP:CG	2.30	0.51
1:A:267:VAL:HG13	1:A:278:VAL:HG11	1.91	0.51
1:A:202:PRO:HD2	1:A:210:PHE:CG	2.45	0.51
1:A:119:HIS:HB2	1:A:203:ILE:HG23	1.92	0.51
1:B:294:LYS:HZ2	1:B:456:SER:HG	1.54	0.51
1:A:289:MET:HB3	1:A:496:ASP:HB3	1.91	0.51
1:B:290:MET:HB2	1:B:427:LEU:HD11	1.91	0.51
1:B:348:ASN:OD1	1:B:351:LYS:HB2	2.11	0.51
1:A:74:THR:HG21	1:A:219:ILE:HG21	1.92	0.51
1:A:120:ASP:OD1	1:A:122:THR:OG1	2.29	0.51
1:A:313:ARG:NH1	1:A:345:TYR:O	2.44	0.50
1:B:213:TRP:HD1	1:B:219:ILE:HG12	1.76	0.50
1:A:361:TRP:CE3	1:A:376:LEU:HB2	2.47	0.50
1:A:50:GLY:N	1:A:233:ASN:O	2.46	0.49
1:A:354:SER:OG	1:A:354:SER:O	2.27	0.49
1:B:309:TYR:CE2	1:B:351:LYS:HG2	2.47	0.49
1:A:446:SER:CB	1:A:453:ASN:HB3	2.43	0.49
1:A:104:ASP:HB2	1:A:106:LEU:HD23	1.94	0.49
1:B:306:ALA:HB2	1:B:355:LEU:HB2	1.94	0.49
1:A:293:MET:HB2	1:A:456:SER:HB2	1.95	0.48
1:A:201:LYS:HG2	1:A:210:PHE:CD2	2.49	0.48
1:B:362:LYS:O	1:B:363:LYS:HB2	2.14	0.48
1:B:369:ARG:HG2	1:B:375:LYS:NZ	2.28	0.48
1:A:251:GLN:O	1:A:256:GLU:N	2.47	0.48
1:B:341:ASP:OD1	1:B:341:ASP:N	2.45	0.48
1:B:119:HIS:HB3	1:B:209:LYS:HG3	1.95	0.47
1:A:218:ASN:HB3	1:A:240:LYS:HD3	1.96	0.47
1:B:515:LYS:HD3	1:B:529:ASN:ND2	2.30	0.47
1:B:301:VAL:HG22	1:B:305:LYS:HD2	1.97	0.47
1:B:361:TRP:HA	1:B:371:LYS:HB2	1.96	0.47
1:B:369:ARG:NH1	3:B:711:HOH:O	2.41	0.47
1:A:105:LYS:N	1:A:105:LYS:HD3	2.30	0.47
1:B:159:ASN:HB3	1:B:162:GLU:OE1	2.15	0.47
1:B:171:PHE:CE1	1:B:173:PRO:HG2	2.49	0.47
1:B:173:PRO:HB3	1:B:434:ASP:CG	2.35	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:350:ASP:HA	1:B:353:ASN:ND2	2.30	0.47
1:B:118:PHE:CD1	1:B:205:THR:HG23	2.49	0.46
1:B:153:LYS:N	1:B:166:ILE:O	2.47	0.46
1:A:356:LEU:O	1:A:360:GLY:N	2.46	0.46
1:A:52:THR:HG23	1:A:236:LYS:HB3	1.97	0.46
1:B:383:PRO:HG2	1:B:389:ARG:HD2	1.98	0.46
1:A:332:LEU:O	1:A:338:ASN:HB2	2.16	0.46
1:A:413:ASP:O	1:A:417:ILE:HG13	2.16	0.46
1:B:159:ASN:ND2	1:B:162:GLU:OE1	2.46	0.45
1:B:436:ASP:OD1	1:B:470:ARG:HD2	2.16	0.45
1:A:297:ILE:HD12	1:A:297:ILE:H	1.81	0.45
1:A:441:ARG:H	1:A:441:ARG:HG2	1.58	0.45
1:B:223:LYS:HB2	1:B:235:GLU:HA	1.97	0.45
1:A:464:GLU:O	1:A:468:LYS:HG2	2.17	0.45
1:A:332:LEU:HD11	1:A:439:THR:HG21	1.99	0.45
1:B:67:ILE:HD11	1:B:193:ILE:HG21	1.98	0.45
1:B:288:CYS:O	1:B:426:LEU:HG	2.16	0.45
1:A:274:ASN:OD1	1:A:274:ASN:N	2.49	0.45
1:A:167:LEU:HD21	1:A:174:LEU:HD13	1.98	0.44
1:A:233:ASN:OD1	1:A:534:ASN:HA	2.16	0.44
1:B:171:PHE:CZ	1:B:173:PRO:HG2	2.52	0.44
1:A:401:LYS:HB2	1:A:401:LYS:HE2	1.50	0.44
1:B:444:HIS:CD2	1:B:463:ASP:HA	2.51	0.44
1:B:87:GLU:H	1:B:87:GLU:CD	2.20	0.44
1:A:223:LYS:HD3	1:A:225:LYS:CE	2.47	0.44
1:B:148:GLU:HB3	1:B:177:LYS:HE2	1.99	0.44
1:B:350:ASP:HA	1:B:353:ASN:HD22	1.83	0.44
1:B:482:TYR:O	1:B:486:GLN:NE2	2.46	0.44
1:A:159:ASN:OD1	1:A:160:ASP:N	2.51	0.44
1:B:183:ILE:HD13	1:B:183:ILE:HA	1.84	0.44
1:B:446:SER:O	1:B:451:GLY:HA3	2.18	0.44
1:A:178:LEU:O	3:A:701:HOH:O	2.21	0.44
1:A:309:TYR:CE2	1:A:351:LYS:HD3	2.53	0.44
1:A:134:LYS:NZ	1:A:154:ASP:OD1	2.51	0.43
1:A:242:ILE:O	1:A:248:ARG:NH1	2.49	0.43
1:A:312:ASP:HB3	1:A:395:TYR:OH	2.18	0.43
1:B:112:LEU:HB2	1:B:161:TYR:O	2.19	0.43
1:B:311:LEU:HD11	1:B:396:PHE:CE2	2.54	0.43
1:A:337:PHE:HD1	1:A:479:LYS:HG2	1.83	0.43
1:B:151:GLU:H	1:B:151:GLU:CD	2.21	0.43
1:B:284:ALA:O	1:B:430:GLY:HA3	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:444:HIS:HB3	1:B:446:SER:H	1.84	0.43
1:A:86:ASP:HB3	1:A:92:LYS:HE2	2.01	0.42
1:A:67:ILE:HD11	1:A:193:ILE:HD11	2.02	0.42
1:A:302:ASN:ND2	3:A:717:HOH:O	2.46	0.42
1:B:151:GLU:HA	1:B:168:LYS:HD2	2.02	0.42
1:B:321:LEU:HD21	1:B:501:LEU:HD23	2.02	0.42
1:A:384:LYS:C	1:A:386:ASP:H	2.22	0.42
1:B:304:ARG:NH2	1:B:492:ASP:OD1	2.45	0.42
1:B:515:LYS:HD3	1:B:529:ASN:HD21	1.83	0.42
1:A:118:PHE:CZ	1:A:124:LEU:HD12	2.55	0.42
1:A:375:LYS:HB3	1:A:375:LYS:HE2	1.45	0.42
1:A:427:LEU:HB3	1:A:429:TRP:CD1	2.55	0.42
1:A:452:ASP:OD1	1:A:452:ASP:N	2.53	0.42
1:A:459:ASN:ND2	1:A:492:ASP:OD2	2.42	0.41
1:B:85:PHE:HB3	1:B:89:ASN:HA	2.02	0.41
1:B:84:LYS:CB	1:B:94:GLU:HG3	2.49	0.41
1:B:384:LYS:HB2	1:B:412:LEU:C	2.41	0.41
1:A:514:VAL:HG22	1:A:533:TRP:CZ2	2.56	0.41
1:B:97:ASP:N	1:B:111:LYS:O	2.47	0.41
1:B:312:ASP:HB2	1:B:347:TYR:CE1	2.55	0.41
1:A:51:LYS:HE3	1:A:51:LYS:HB3	1.86	0.41
1:A:150:SER:O	1:A:168:LYS:HE2	2.20	0.41
1:A:231:THR:HG23	1:A:531:GLU:O	2.21	0.41
1:A:378:PHE:HB2	1:A:423:ASP:HB3	2.02	0.41
1:A:389:ARG:HB3	1:A:426:LEU:HD22	2.03	0.41
1:A:479:LYS:HE3	1:A:479:LYS:HB3	1.86	0.41
1:B:104:ASP:OD1	1:B:104:ASP:N	2.41	0.41
1:B:137:LEU:HD21	1:B:149:TYR:O	2.20	0.40
1:A:119:HIS:NE2	1:A:209:LYS:HA	2.36	0.40
1:A:468:LYS:HE3	1:A:468:LYS:HB3	1.89	0.40
1:B:80:THR:HG23	1:B:206:GLY:HA2	2.02	0.40
1:B:342:VAL:HB	1:B:490:ALA:HB2	2.03	0.40
1:A:52:THR:O	1:A:510:ARG:NH2	2.54	0.40
1:A:269:LYS:HA	1:A:269:LYS:HD3	1.78	0.40
1:A:270:ILE:HA	1:A:273:LEU:HG	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	473/497 (95%)	435 (92%)	38 (8%)	0	100	100
1	B	479/497 (96%)	444 (93%)	35 (7%)	0	100	100
All	All	952/994 (96%)	879 (92%)	73 (8%)	0	100	100

There are no Ramachandran outliers to report.

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	420/434 (97%)	393 (94%)	27 (6%)	17	25
1	B	423/434 (98%)	402 (95%)	21 (5%)	24	37
All	All	843/868 (97%)	795 (94%)	48 (6%)	20	30

All (48) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	58	GLU
1	A	61	ASP
1	A	105	LYS
1	A	123	GLU
1	A	144	SER
1	A	192	ASP
1	A	266	GLN
1	A	269	LYS

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Mol	Chain	Res	Type
1	A	295	LYS
1	A	316	MET
1	A	318	ASP
1	A	327	GLU
1	A	336	LYS
1	A	343	GLU
1	A	348	ASN
1	A	374	LYS
1	A	401	LYS
1	A	414	TRP
1	A	415	ASP
1	A	431	SER
1	A	441	ARG
1	A	453	ASN
1	A	461	LYS
1	A	479	LYS
1	A	480	LYS
1	A	485	PHE
1	A	512	SER
1	B	61	ASP
1	B	74	THR
1	B	103	ASP
1	B	134	LYS
1	B	176	ASP
1	B	293	MET
1	B	296	ASP
1	B	322	LEU
1	B	333	GLN
1	B	336	LYS
1	B	356	LEU
1	B	358	SER
1	B	374	LYS
1	B	398	SER
1	B	410	ASP
1	B	412	LEU
1	B	413	ASP
1	B	426	LEU
1	B	446	SER
1	B	447	GLU
1	B	485	PHE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	453	ASN
1	B	353	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 monosaccharides in this entry.

5.6 Ligand geometry

Of 2 ligands modelled in this entry, 2 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers

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	479/497 (96%)	0.81	42 (8%) 10 11	36, 48, 68, 110	0
1	B	483/497 (97%)	0.96	55 (11%) 5 5	37, 50, 80, 136	0
All	All	962/994 (96%)	0.88	97 (10%) 7 7	36, 50, 75, 136	0

All (97) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	449	ASN	10.5
1	A	364	GLY	8.6
1	B	50	GLY	8.1
1	B	368	ILE	7.6
1	B	450	GLY	6.7
1	B	448	ILE	5.0
1	A	370	VAL	4.8
1	B	190	GLY	4.5
1	A	442	LEU	4.3
1	B	344	LYS	4.1
1	B	499	VAL	4.0
1	B	411	ALA	4.0
1	B	473	THR	3.9
1	B	467	TYR	3.8
1	B	158	VAL	3.8
1	B	170	ALA	3.6
1	A	158	VAL	3.5
1	A	503	ALA	3.4
1	B	118	PHE	3.4
1	B	211	VAL	3.4
1	A	50	GLY	3.3
1	B	469	ALA	3.3
1	B	409	VAL	3.2
1	A	190	GLY	3.2

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Mol	Chain	Res	Type	RSRZ
1	B	349	LEU	3.2
1	A	489	LEU	3.2
1	B	443	PHE	3.1
1	B	405	ALA	3.1
1	B	157	ALA	3.0
1	B	253	GLN	2.9
1	B	230	LYS	2.9
1	B	239	VAL	2.9
1	A	172	PRO	2.8
1	A	373	GLY	2.8
1	B	385	THR	2.8
1	B	320	ILE	2.8
1	B	482	TYR	2.8
1	B	188	PHE	2.8
1	B	359	ALA	2.7
1	A	232	GLY	2.7
1	B	444	HIS	2.6
1	A	145	LEU	2.6
1	A	371	LYS	2.6
1	A	85	PHE	2.6
1	A	499	VAL	2.5
1	B	192	ASP	2.5
1	B	416	ALA	2.5
1	B	51	LYS	2.5
1	A	227	TYR	2.5
1	A	101	ILE	2.5
1	B	362	LYS	2.5
1	B	384	LYS	2.5
1	B	433	PHE	2.4
1	B	80	THR	2.4
1	B	195	THR	2.4
1	A	230	LYS	2.4
1	A	229	GLY	2.4
1	A	416	ALA	2.3
1	A	420	ASP	2.3
1	A	417	ILE	2.3
1	A	213	TRP	2.3
1	A	310	ALA	2.3
1	B	232	GLY	2.3
1	B	173	PRO	2.3
1	A	382	ALA	2.3
1	B	356	LEU	2.2

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Mol	Chain	Res	Type	RSRZ
1	B	498	GLY	2.2
1	A	527	LEU	2.2
1	A	481	TYR	2.2
1	A	231	THR	2.2
1	B	466	LEU	2.2
1	A	347	TYR	2.2
1	A	69	THR	2.2
1	B	414	TRP	2.2
1	A	99	TYR	2.2
1	B	413	ASP	2.2
1	B	355	LEU	2.2
1	A	297	ILE	2.2
1	B	334	ILE	2.1
1	A	167	LEU	2.1
1	B	145	LEU	2.1
1	B	490	ALA	2.1
1	A	431	SER	2.1
1	A	357	GLU	2.1
1	A	163	VAL	2.1
1	A	405	ALA	2.1
1	A	397	ALA	2.1
1	B	494	ALA	2.1
1	B	375	LYS	2.0
1	B	424	ALA	2.0
1	B	225	LYS	2.0
1	B	481	TYR	2.0
1	A	106	LEU	2.0
1	A	399	GLN	2.0
1	A	404	GLY	2.0
1	B	404	GLY	2.0
1	A	214	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

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, 95^{th} 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	CL	A	601	1/1	0.81	0.20	45,45,45,45	0
2	CL	B	601	1/1	0.99	0.13	38,38,38,38	0

6.5 Other polymers

There are no such residues in this entry.