Full wwPDB X-ray Structure Validation Report (i)

Feb 1, 2016 – 12:49 AM GMT

PDB ID	:	2BVA
Title	:	CRYSTAL STRUCTURE OF THE HUMAN P21-ACTIVATED KINASE 4
Authors	:	Debreczeni, J.E.; Bunkoczi, G.; Eswaran, J.; Filippakopoulos, P.; Das, S.; Fedorov, O.; Sundstrom, M.; Arrowsmith, C.; Edwards, A.; Von Delft, F.; Knapp, S.
Deposited on	:	2005-06-23
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
http://wwpdb.org/validation/2016/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The following versions of software and data (see references (1)) were used in the production of this report:

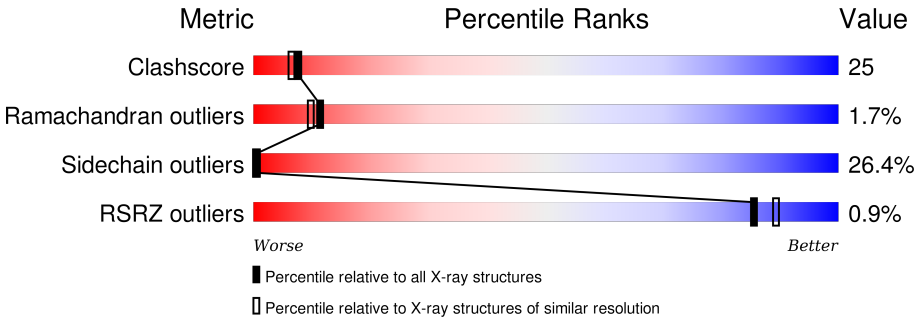
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	trunk26865

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))
Clashscore	102246	4452 (2.30-2.30)
Ramachandran outliers	100387	4410 (2.30-2.30)
Sidechain outliers	100360	4409 (2.30-2.30)
RSRZ outliers	91569	3857 (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. 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	292	42% 38% 13% • 7%
1	B	292	% 35% 42% 14% • 6%

2 Entry composition (i)

There are 2 unique types of molecules in this entry. The entry contains 4287 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 P21-ACTIVATED KINASE 4.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	273	Total	C	N	O	P	S	0	0	0
			2114	1359	362	379	1	13			
1	B	275	Total	C	N	O	P	S	0	0	0
			2137	1372	368	383	1	13			

- Molecule 2 is water.

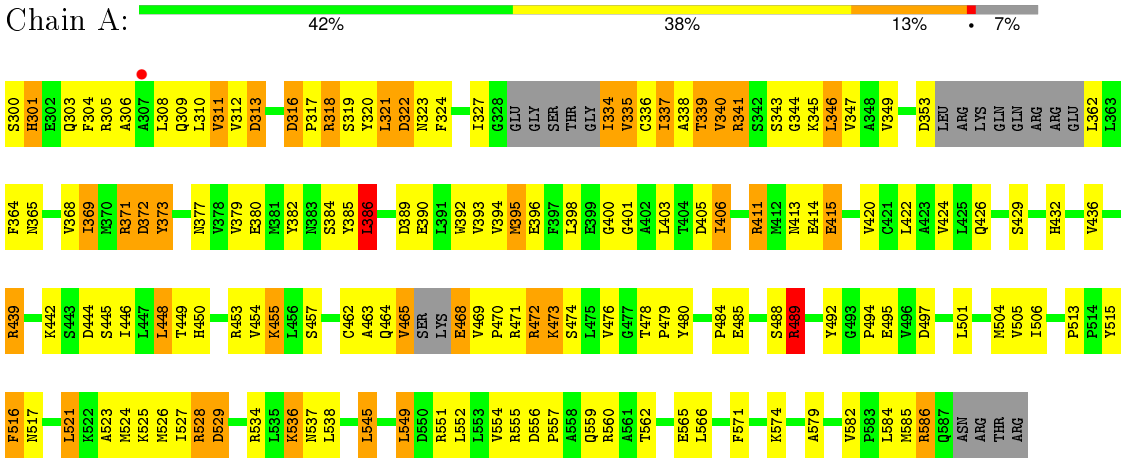
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	21	Total	O	0	0
			21	21		
2	B	15	Total	O	0	0
			15	15		

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 errors 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.

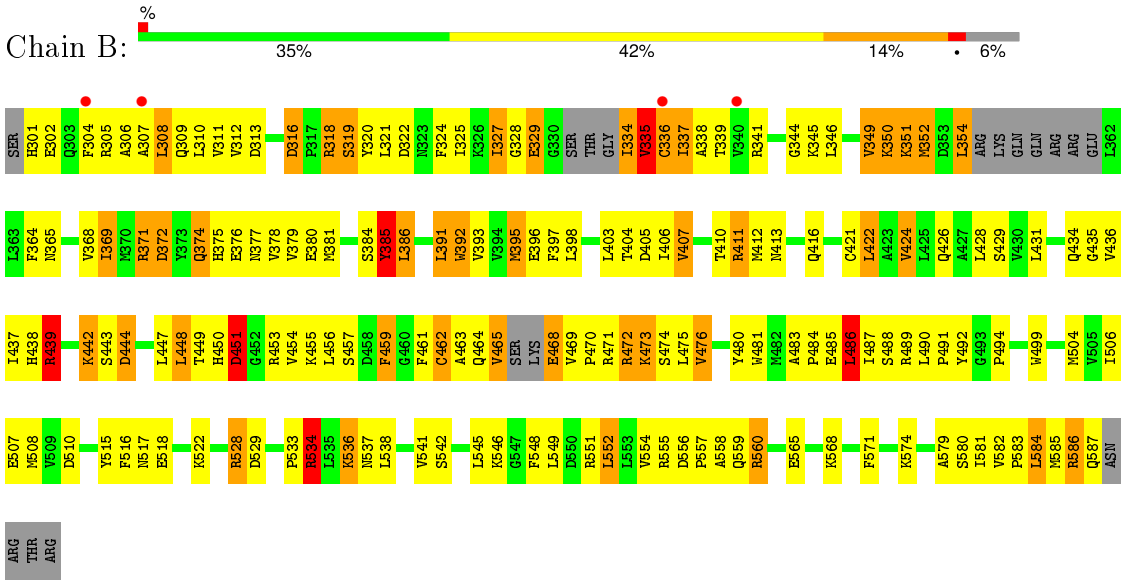
- Molecule 1: P21-ACTIVATED KINASE 4

Chain A:



- Molecule 1: P21-ACTIVATED KINASE 4

Chain B:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 32	Depositor
Cell constants a, b, c, α, β, γ	118.11Å 118.11Å 55.53Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	20.00 – 2.30 19.84 – 2.30	Depositor EDS
% Data completeness (in resolution range)	99.8 (20.00-2.30) 95.0 (19.84-2.30)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	6.98 (at 2.30Å)	Xtriage
Refinement program	SHELXL-97	Depositor
R, R_{free}	0.192 , 0.269 0.199 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	DCC
Wilson B-factor (Å^2)	15.8	Xtriage
Anisotropy	0.307	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.27 , 381.4	EDS
Estimated twinning fraction	0.079 for -h,-k,l 0.058 for h,-h-k,-l 0.075 for -k,-h,-l	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.44$, $< L^2 > = 0.27$	Xtriage
Outliers	0 of 36647 reflections	Xtriage
F_o,F_c correlation	0.89	EDS
Total number of atoms	4287	wwPDB-VP
Average B, all atoms (Å^2)	18.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.04% 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, 0.375 respectively for untwinned datasets, and 0.333, 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: SEP

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	0.41	0/2147	1.08	8/2917 (0.3%)
1	B	0.41	0/2170	1.07	12/2945 (0.4%)
All	All	0.41	0/4317	1.08	20/5862 (0.3%)

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	B	0	1

There are no bond length outliers.

All (20) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	551	ARG	CD-NE-CZ	11.04	139.05	123.60
1	B	551	ARG	NE-CZ-NH2	7.05	123.83	120.30
1	A	439	ARG	NE-CZ-NH2	-6.91	116.85	120.30
1	A	439	ARG	NE-CZ-NH1	6.87	123.73	120.30
1	B	371	ARG	NE-CZ-NH1	5.95	123.28	120.30
1	B	451	ASP	CB-CG-OD2	5.88	123.60	118.30
1	B	528	ARG	NE-CZ-NH1	5.86	123.23	120.30
1	B	468	GLU	CA-CB-CG	5.79	126.15	113.40
1	B	486	LEU	CA-CB-CG	5.68	128.36	115.30
1	A	528	ARG	NE-CZ-NH1	5.55	123.07	120.30
1	A	489	ARG	NE-CZ-NH2	-5.42	117.59	120.30
1	B	385	TYR	CA-CB-CG	5.39	123.65	113.40
1	A	411	ARG	NE-CZ-NH2	-5.30	117.65	120.30
1	B	371	ARG	NE-CZ-NH2	-5.23	117.68	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	439	ARG	CD-NE-CZ	5.21	130.89	123.60
1	B	459	PHE	CB-CG-CD1	5.15	124.41	120.80
1	A	405	ASP	CB-CG-OD2	5.14	122.93	118.30
1	A	551	ARG	NE-CZ-NH2	5.13	122.87	120.30
1	A	386	LEU	CA-CB-CG	5.07	126.96	115.30
1	B	534	ARG	NE-CZ-NH2	-5.07	117.77	120.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	469	VAL	Peptide

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	2114	0	2122	100	0
1	B	2137	0	2160	116	0
2	A	21	0	0	1	0
2	B	15	0	0	0	0
All	All	4287	0	4282	216	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 25.

All (216) 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:351:LYS:HG2	1:B:392:TRP:CH2	2.03	0.93
1:B:422:LEU:O	1:B:426:GLN:HG3	1.83	0.79
1:A:347:VAL:HG13	1:A:395:MET:O	1.83	0.79
1:A:579:ALA:O	1:A:582:VAL:HG22	1.83	0.79
1:B:472:ARG:HD2	1:B:474:SEP:O3P	1.84	0.77
1:B:541:VAL:O	1:B:546:LYS:HE2	1.83	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:528:ARG:HD2	1:A:529:ASP:OD1	1.85	0.76
1:A:337:ILE:HA	1:A:347:VAL:O	1.86	0.76
1:B:580:SER:O	1:B:583:PRO:HD2	1.87	0.75
1:B:365:ASN:O	1:B:368:VAL:HB	1.88	0.73
1:A:349:VAL:HG13	1:A:393:VAL:O	1.90	0.72
1:A:312:VAL:HG13	1:A:384:SER:O	1.89	0.71
1:B:351:LYS:HG2	1:B:392:TRP:CZ3	2.26	0.70
1:B:380:GLU:O	1:B:395:MET:HG3	1.92	0.70
1:B:351:LYS:HG2	1:B:392:TRP:CZ2	2.26	0.70
1:B:318:ARG:HG3	1:B:324:PHE:CZ	2.28	0.69
1:B:327:ILE:HB	1:B:335:VAL:O	1.92	0.69
1:A:323:ASN:HB2	1:A:339:THR:OG1	1.93	0.68
1:B:545:LEU:O	1:B:548:PHE:HB3	1.93	0.68
1:A:318:ARG:HA	1:A:321:LEU:O	1.95	0.68
1:A:318:ARG:O	1:A:318:ARG:HD3	1.94	0.67
1:B:485:GLU:O	1:B:488:SER:HB2	1.94	0.67
1:A:335:VAL:HG12	1:A:336:CYS:SG	2.36	0.66
1:B:339:THR:HG23	1:B:344:GLY:O	1.96	0.66
1:B:565:GLU:O	1:B:568:LYS:HB2	1.97	0.65
1:B:324:PHE:O	1:B:325:ILE:HG13	1.97	0.64
1:A:340:VAL:HG23	1:A:345:LYS:O	1.97	0.64
1:A:398:LEU:CD2	1:A:449:THR:HG22	2.28	0.63
1:B:322:ASP:OD2	1:B:341:ARG:HB3	1.99	0.63
1:B:449:THR:OG1	1:B:453:ARG:HG3	1.99	0.62
1:A:420:VAL:O	1:A:424:VAL:HG23	1.99	0.62
1:A:317:PRO:O	1:A:321:LEU:HD12	2.00	0.62
1:B:337:ILE:HD11	1:B:397:PHE:CD2	2.35	0.61
1:B:351:LYS:CG	1:B:392:TRP:CH2	2.81	0.61
1:A:324:PHE:HA	1:A:337:ILE:O	2.01	0.61
1:A:501:LEU:O	1:A:505:VAL:HG23	2.00	0.61
1:A:465:VAL:HG23	1:A:472:ARG:NE	2.15	0.61
1:A:305:ARG:O	1:A:305:ARG:HG2	2.01	0.60
1:B:555:ARG:O	1:B:557:PRO:HD3	2.02	0.60
1:B:325:ILE:O	1:B:336:CYS:HA	2.01	0.60
1:B:335:VAL:HG23	1:B:350:LYS:HA	1.84	0.60
1:A:365:ASN:O	1:A:369:ILE:HG13	2.02	0.59
1:A:555:ARG:O	1:A:557:PRO:HD3	2.03	0.59
1:B:582:VAL:O	1:B:586:ARG:HB2	2.03	0.59
1:B:321:LEU:HA	1:B:339:THR:O	2.03	0.58
1:B:313:ASP:O	1:B:385:TYR:HB3	2.03	0.58
1:A:308:LEU:O	1:A:311:VAL:HG22	2.04	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:533:PRO:HA	1:B:534:ARG:CZ	2.33	0.58
1:B:448:LEU:HA	1:B:453:ARG:O	2.04	0.57
1:B:483:ALA:O	1:B:487:ILE:HD12	2.04	0.57
1:B:480:TYR:HB2	1:B:481:TRP:CZ3	2.39	0.57
1:A:473:LYS:HG3	1:A:473:LYS:O	2.04	0.57
1:B:556:ASP:OD2	1:B:558:ALA:HB3	2.05	0.57
1:B:439:ARG:NH1	1:B:476:VAL:HG11	2.19	0.57
1:B:335:VAL:HG21	1:B:351:LYS:HB2	1.86	0.56
1:B:312:VAL:HG13	1:B:384:SER:O	2.04	0.56
1:A:523:ALA:O	1:A:527:ILE:HG12	2.05	0.56
1:A:338:ALA:O	1:A:346:LEU:HA	2.04	0.56
1:B:480:TYR:HB2	1:B:481:TRP:CE3	2.40	0.56
1:B:461:PHE:CD2	1:B:476:VAL:HG22	2.40	0.56
1:B:403:LEU:O	1:B:407:VAL:HG22	2.06	0.56
1:A:545:LEU:HD12	1:A:571:PHE:CE1	2.41	0.56
1:A:432:HIS:HD2	1:A:436:VAL:O	1.89	0.56
1:B:351:LYS:CG	1:B:392:TRP:CZ2	2.90	0.55
1:A:513:PRO:O	1:A:516:PHE:HB2	2.07	0.55
1:B:447:LEU:O	1:B:454:VAL:HA	2.05	0.55
1:A:554:VAL:HG12	1:A:556:ASP:O	2.07	0.55
1:A:398:LEU:HD23	1:A:449:THR:HG22	1.88	0.55
1:A:515:TYR:CZ	1:A:526:MET:HB3	2.42	0.54
1:B:306:ALA:O	1:B:310:LEU:HG	2.08	0.54
1:B:451:ASP:OD2	1:B:453:ARG:HG2	2.07	0.54
1:B:584:LEU:O	1:B:587:GLN:HG2	2.07	0.54
1:A:472:ARG:HG3	1:A:474:SEP:O3P	2.08	0.54
1:A:371:ARG:HG3	1:A:372:ASP:OD1	2.08	0.53
1:B:369:ILE:O	1:B:372:ASP:OD1	2.26	0.53
1:A:312:VAL:HG12	1:A:313:ASP:O	2.09	0.53
1:A:312:VAL:HG22	1:A:384:SER:OG	2.08	0.53
1:A:372:ASP:O	1:A:373:TYR:HB2	2.07	0.53
1:A:537:ASN:O	1:A:538:LEU:HB3	2.07	0.53
1:A:339:THR:HG22	1:A:344:GLY:O	2.08	0.53
1:A:316:ASP:OD2	1:A:318:ARG:HG3	2.08	0.53
1:B:404:THR:O	1:B:407:VAL:HG23	2.07	0.53
1:B:537:ASN:O	1:B:538:LEU:HB3	2.09	0.53
1:A:479:PRO:HB3	1:A:524:MET:SD	2.49	0.52
1:A:316:ASP:OD2	1:A:318:ARG:HD2	2.09	0.52
1:A:480:TYR:CE2	1:A:516:PHE:HA	2.44	0.52
1:A:554:VAL:O	1:A:560:ARG:HD3	2.09	0.52
1:B:305:ARG:O	1:B:308:LEU:HB2	2.09	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:468:GLU:CD	1:A:469:VAL:H	2.14	0.51
1:A:484:PRO:O	1:A:488:SER:HB2	2.10	0.51
1:B:304:PHE:O	1:B:307:ALA:HB3	2.11	0.51
1:B:375:HIS:CD2	1:B:376:GLU:HG2	2.46	0.51
1:B:312:VAL:HG12	1:B:313:ASP:O	2.10	0.51
1:A:432:HIS:CD2	1:A:494:PRO:HB3	2.46	0.51
1:B:436:VAL:HG13	1:B:463:ALA:O	2.12	0.50
1:B:483:ALA:HA	1:B:499:TRP:CD1	2.47	0.50
1:A:582:VAL:O	1:A:586:ARG:HD2	2.12	0.49
1:B:410:THR:HG21	1:B:587:GLN:NE2	2.27	0.49
1:B:510:ASP:OD2	1:B:537:ASN:OD1	2.30	0.49
1:B:312:VAL:CG1	1:B:385:TYR:HA	2.43	0.49
1:A:365:ASN:OD1	1:A:369:ILE:HD11	2.13	0.48
1:B:436:VAL:HA	1:B:463:ALA:O	2.13	0.48
1:B:407:VAL:CG1	1:B:508:MET:HA	2.43	0.48
1:A:400:GLY:HA3	1:A:448:LEU:O	2.13	0.48
1:B:381:MET:HB2	1:B:395:MET:SD	2.54	0.48
1:A:536:LYS:O	1:A:536:LYS:HG2	2.13	0.48
1:B:472:ARG:HD2	1:B:474:SEP:P	2.54	0.48
1:A:525:LYS:O	1:A:528:ARG:HB3	2.13	0.48
1:A:473:LYS:NZ	1:A:489:ARG:HA	2.28	0.48
1:B:542:SER:O	1:B:546:LYS:HG3	2.13	0.48
1:A:524:MET:O	1:A:528:ARG:HB2	2.14	0.48
1:B:443:SER:OG	1:B:507:GLU:OE2	2.29	0.47
1:B:316:ASP:OD2	1:B:318:ARG:HB2	2.15	0.47
1:B:404:THR:OG1	1:B:444:ASP:HA	2.14	0.47
1:A:303:GLN:O	1:A:306:ALA:HB3	2.15	0.47
1:A:442:LYS:CE	1:A:444:ASP:HB2	2.44	0.47
1:B:518:GLU:OE2	1:B:522:LYS:HE2	2.16	0.46
1:A:465:VAL:HG23	1:A:472:ARG:HE	1.80	0.46
1:B:465:VAL:HG22	1:B:470:PRO:O	2.14	0.46
1:A:552:LEU:HD21	1:A:566:LEU:HD11	1.96	0.46
1:A:415:GLU:HA	1:A:574:LYS:O	2.16	0.46
1:B:545:LEU:HG	1:B:571:PHE:CZ	2.50	0.46
1:B:450:HIS:CE1	1:B:586:ARG:HH12	2.33	0.46
1:B:504:MET:O	1:B:507:GLU:HB2	2.15	0.46
1:A:521:LEU:O	1:A:524:MET:HB2	2.15	0.46
1:B:352:MET:CB	1:B:391:LEU:HD23	2.46	0.46
1:A:319:SER:O	1:A:341:ARG:NH1	2.48	0.46
1:A:322:ASP:OD1	1:A:322:ASP:N	2.48	0.46
1:A:365:ASN:ND2	1:A:462:CYS:O	2.49	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:554:VAL:HG11	1:A:559:GLN:C	2.37	0.46
1:B:437:ILE:O	1:B:462:CYS:HA	2.16	0.45
1:B:313:ASP:C	1:B:385:TYR:HB3	2.37	0.45
1:A:469:VAL:O	1:A:469:VAL:HG12	2.16	0.45
1:A:562:THR:O	1:A:566:LEU:HD12	2.17	0.45
1:B:336:CYS:HB2	1:B:349:VAL:HG23	1.98	0.45
1:B:337:ILE:N	1:B:349:VAL:HG23	2.32	0.45
1:A:439:ARG:NH2	1:A:474:SEP:O3P	2.49	0.45
1:A:414:GLU:OE1	1:A:571:PHE:HE1	1.99	0.45
1:B:484:PRO:HD3	1:B:499:TRP:CE2	2.51	0.45
1:A:545:LEU:O	1:A:549:LEU:HB2	2.17	0.45
1:B:424:VAL:O	1:B:428:LEU:HG	2.17	0.45
1:A:353:ASP:HA	1:A:389:ASP:O	2.17	0.45
1:B:475:LEU:HD13	1:B:489:ARG:HD3	1.97	0.45
1:A:406:ILE:HG21	1:A:584:LEU:HD23	1.99	0.45
1:A:485:GLU:OE1	1:A:560:ARG:NH2	2.50	0.45
1:B:350:LYS:HG2	1:B:393:VAL:O	2.17	0.45
1:B:372:ASP:OD1	1:B:372:ASP:N	2.50	0.45
1:B:439:ARG:NH2	1:B:492:TYR:OH	2.50	0.45
1:A:485:GLU:OE1	1:A:560:ARG:NH1	2.49	0.45
1:B:471:ARG:NH2	1:B:491:PRO:O	2.49	0.45
1:B:319:SER:O	1:B:341:ARG:NH1	2.50	0.44
1:A:334:ILE:HG21	2:A:2002:HOH:O	2.18	0.44
1:B:411:ARG:NH1	1:B:412:MET:O	2.50	0.44
1:B:337:ILE:O	1:B:338:ALA:HB2	2.17	0.44
1:A:432:HIS:NE2	1:A:494:PRO:HB3	2.32	0.44
1:B:579:ALA:O	1:B:583:PRO:HD3	2.17	0.44
1:A:340:VAL:O	1:A:344:GLY:N	2.49	0.44
1:B:552:LEU:HD23	1:B:552:LEU:N	2.32	0.44
1:A:432:HIS:NE2	1:A:497:ASP:OD2	2.50	0.44
1:B:377:ASN:CA	1:B:455:LYS:HD3	2.48	0.44
1:B:437:ILE:O	1:B:463:ALA:N	2.50	0.44
1:B:473:LYS:HD3	1:B:473:LYS:O	2.17	0.44
1:A:347:VAL:HG11	1:A:394:VAL:CG1	2.48	0.44
1:A:377:ASN:O	1:A:455:LYS:HB3	2.17	0.44
1:B:354:LEU:N	1:B:354:LEU:HD23	2.32	0.44
1:A:365:ASN:O	1:A:369:ILE:HB	2.18	0.43
1:B:480:TYR:HE2	1:B:515:TYR:O	2.01	0.43
1:B:437:ILE:HG22	1:B:439:ARG:HG3	2.00	0.43
1:A:562:THR:O	1:A:565:GLU:HB2	2.17	0.43
1:B:434:GLN:O	1:B:464:GLN:NE2	2.49	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:554:VAL:O	1:B:560:ARG:NH2	2.50	0.43
1:A:450:HIS:CD2	1:A:586:ARG:HH22	2.37	0.43
1:B:313:ASP:O	1:B:385:TYR:HA	2.19	0.43
1:A:401:GLY:O	1:A:448:LEU:HG	2.18	0.43
1:A:377:ASN:ND2	1:A:454:VAL:O	2.50	0.43
1:A:364:PHE:CE1	1:A:368:VAL:HG21	2.54	0.43
1:B:368:VAL:HG12	1:B:369:ILE:HG12	2.01	0.43
1:B:442:LYS:HG3	1:B:444:ASP:OD2	2.19	0.43
1:B:378:VAL:HG13	1:B:459:PHE:CZ	2.54	0.43
1:B:316:ASP:OD1	1:B:316:ASP:O	2.36	0.42
1:A:470:PRO:HD2	1:A:471:ARG:HG3	2.00	0.42
1:B:352:MET:CB	1:B:391:LEU:O	2.67	0.42
1:A:365:ASN:ND2	1:A:463:ALA:HA	2.35	0.42
1:B:438:HIS:O	1:B:439:ARG:HB2	2.19	0.42
1:B:435:GLY:O	1:B:465:VAL:N	2.49	0.42
1:A:445:SER:C	1:A:446:ILE:HD13	2.40	0.42
1:A:380:GLU:HG2	1:A:382:TYR:CD2	2.54	0.42
1:B:386:LEU:HD12	1:B:386:LEU:N	2.34	0.42
1:A:469:VAL:N	1:A:470:PRO:HD3	2.34	0.42
1:A:386:LEU:HA	1:A:390:GLU:O	2.20	0.42
1:A:403:LEU:HD22	1:A:420:VAL:HG11	2.01	0.42
1:B:337:ILE:HD13	1:B:346:LEU:HB3	2.02	0.42
1:B:480:TYR:CE2	1:B:516:PHE:HA	2.54	0.42
1:B:528:ARG:O	1:B:555:ARG:NH2	2.53	0.41
1:A:464:GLN:O	1:A:472:ARG:NH2	2.49	0.41
1:B:456:LEU:HG	1:B:459:PHE:CE1	2.55	0.41
1:A:468:GLU:C	1:A:470:PRO:HD3	2.39	0.41
1:A:473:LYS:HA	1:A:492:TYR:CE1	2.55	0.41
1:B:510:ASP:OD2	1:B:536:LYS:HB3	2.20	0.41
1:B:413:ASN:OD1	1:B:416:GLN:HG3	2.21	0.41
1:B:374:GLN:HG2	1:B:374:GLN:O	2.20	0.41
1:B:485:GLU:HG2	1:B:486:LEU:N	2.35	0.41
1:B:528:ARG:C	1:B:555:ARG:HH22	2.24	0.41
1:B:421:CYS:HG	1:B:548:PHE:HZ	1.66	0.41
1:B:328:GLY:O	1:B:329:GLU:HB3	2.21	0.41
1:A:327:ILE:HG13	1:A:337:ILE:CD1	2.51	0.40
1:A:347:VAL:HG11	1:A:394:VAL:HG13	2.02	0.40
1:A:513:PRO:HG2	1:A:516:PHE:CD1	2.57	0.40
1:B:306:ALA:HA	1:B:309:GLN:CB	2.51	0.40
1:A:552:LEU:HD21	1:A:566:LEU:CD1	2.51	0.40
1:B:379:VAL:HG13	1:B:396:GLU:HB3	2.02	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:317:PRO:HB2	1:A:321:LEU:HD13	2.02	0.40
1:A:369:ILE:HD13	1:A:464:GLN:HB2	2.03	0.40
1:B:431:LEU:HD22	1:B:436:VAL:CG1	2.51	0.40
1:B:334:ILE:N	1:B:334:ILE:HD13	2.35	0.40
1:A:379:VAL:HA	1:A:396:GLU:OE1	2.21	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	264/292 (90%)	230 (87%)	30 (11%)	4 (2%)	13 12
1	B	266/292 (91%)	225 (85%)	36 (14%)	5 (2%)	10 8
All	All	530/584 (91%)	455 (86%)	66 (12%)	9 (2%)	11 10

All (9) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	335	VAL
1	B	335	VAL
1	A	301	HIS
1	A	311	VAL
1	B	352	MET
1	A	373	TYR
1	B	462	CYS
1	B	345	LYS
1	B	494	PRO

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	225/254 (89%)	168 (75%)	57 (25%)	1 0
1	B	229/254 (90%)	166 (72%)	63 (28%)	0 0
All	All	454/508 (89%)	334 (74%)	120 (26%)	0 0

All (120) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	300	SER
1	A	301	HIS
1	A	304	PHE
1	A	309	GLN
1	A	310	LEU
1	A	313	ASP
1	A	316	ASP
1	A	318	ARG
1	A	320	TYR
1	A	321	LEU
1	A	322	ASP
1	A	334	ILE
1	A	337	ILE
1	A	339	THR
1	A	340	VAL
1	A	341	ARG
1	A	343	SER
1	A	346	LEU
1	A	362	LEU
1	A	369	ILE
1	A	371	ARG
1	A	372	ASP
1	A	385	TYR
1	A	386	LEU
1	A	392	TRP
1	A	395	MET
1	A	406	ILE

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Mol	Chain	Res	Type
1	A	411	ARG
1	A	413	ASN
1	A	415	GLU
1	A	422	LEU
1	A	426	GLN
1	A	429	SER
1	A	448	LEU
1	A	453	ARG
1	A	455	LYS
1	A	457	SER
1	A	465	VAL
1	A	468	GLU
1	A	472	ARG
1	A	473	LYS
1	A	476	VAL
1	A	478	THR
1	A	489	ARG
1	A	495	GLU
1	A	504	MET
1	A	506	ILE
1	A	516	PHE
1	A	517	ASN
1	A	521	LEU
1	A	529	ASP
1	A	534	ARG
1	A	536	LYS
1	A	545	LEU
1	A	549	LEU
1	A	585	MET
1	A	586	ARG
1	B	301	HIS
1	B	302	GLU
1	B	308	LEU
1	B	311	VAL
1	B	316	ASP
1	B	318	ARG
1	B	319	SER
1	B	320	TYR
1	B	327	ILE
1	B	329	GLU
1	B	334	ILE
1	B	335	VAL

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Mol	Chain	Res	Type
1	B	336	CYS
1	B	337	ILE
1	B	349	VAL
1	B	350	LYS
1	B	351	LYS
1	B	354	LEU
1	B	364	PHE
1	B	369	ILE
1	B	371	ARG
1	B	372	ASP
1	B	374	GLN
1	B	385	TYR
1	B	386	LEU
1	B	391	LEU
1	B	392	TRP
1	B	395	MET
1	B	398	LEU
1	B	405	ASP
1	B	406	ILE
1	B	407	VAL
1	B	411	ARG
1	B	422	LEU
1	B	424	VAL
1	B	429	SER
1	B	439	ARG
1	B	442	LYS
1	B	444	ASP
1	B	448	LEU
1	B	451	ASP
1	B	457	SER
1	B	465	VAL
1	B	468	GLU
1	B	472	ARG
1	B	473	LYS
1	B	476	VAL
1	B	486	LEU
1	B	490	LEU
1	B	506	ILE
1	B	517	ASN
1	B	529	ASP
1	B	534	ARG
1	B	536	LYS

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Mol	Chain	Res	Type
1	B	549	LEU
1	B	552	LEU
1	B	559	GLN
1	B	560	ARG
1	B	574	LYS
1	B	581	ILE
1	B	584	LEU
1	B	585	MET
1	B	586	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	450	HIS
1	B	450	HIS
1	B	587	GLN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains (i)

2 non-standard protein/DNA/RNA residues 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	$\#\|Z\| > 2$
1	SEP	A	474	1	8,9,10	1.01	0	8,12,14	1.42	1 (12%)
1	SEP	B	474	1	8,9,10	0.96	0	8,12,14	1.41	2 (25%)

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
1	SEP	A	474	1	-	0/6/8/10	0/0/0/0
1	SEP	B	474	1	-	0/6/8/10	0/0/0/0

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	474	SEP	O-C-CA	-3.06	117.52	125.49
1	B	474	SEP	O-C-CA	-2.51	118.96	125.49
1	B	474	SEP	OG-CB-CA	2.71	110.58	108.27

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	A	474	SEP	2	0
1	B	474	SEP	2	0

5.5 Carbohydrates (i)

There are no carbohydrates in this entry.

5.6 Ligand geometry (i)

There are no ligands in this entry.

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, 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	272/292 (93%)	-0.26	1 (0%)	93	95	2, 16, 34, 46	0
1	B	274/292 (93%)	-0.20	4 (1%)	76	81	3, 17, 36, 49	0
All	All	546/584 (93%)	-0.23	5 (0%)	85	89	2, 17, 35, 49	0

All (5) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	336	CYS	2.6
1	B	304	PHE	2.4
1	B	340	VAL	2.2
1	B	307	ALA	2.1
1	A	307	ALA	2.0

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

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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. 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	LLDF	B-factors(Å^2)	Q<0.9
1	SEP	B	474	10/11	0.98	0.10	-	17,23,24,24	0
1	SEP	A	474	10/11	0.98	0.10	-	17,23,24,26	0

6.3 Carbohydrates

There are no carbohydrates in this entry.

6.4 Ligands

There are no ligands in this entry.

6.5 Other polymers

There are no such residues in this entry.