Full wwPDB X-ray Structure Validation Report (i)

Jan 31, 2016 – 06:30 PM GMT

PDB ID	:	1B3Q
Title	:	CRYSTAL STRUCTURE OF CHEA-289, A SIGNAL TRANSDUCING HISTIDINE KINASE
Authors	:	Bilwes, A.M.; Alex, L.A.; Crane, B.R.; Simon, M.I.
Deposited on	:	1998-12-14
Resolution	:	2.60 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:

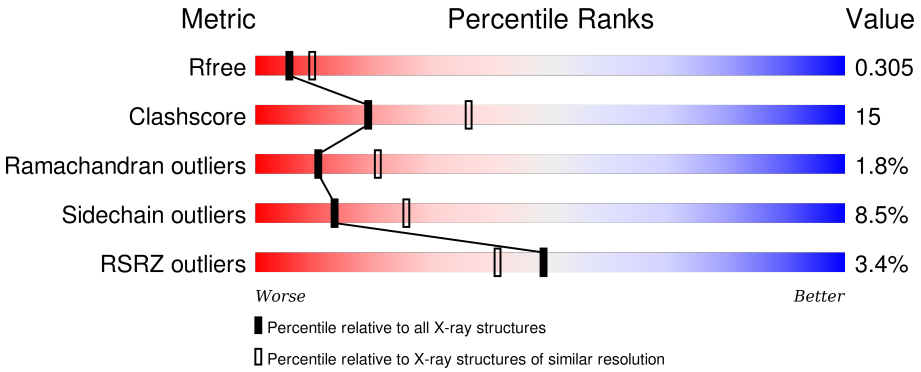
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)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

1 Overall quality at a glance

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

The reported resolution of this entry is 2.60 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}	91344	2328 (2.60-2.60)
Clashscore	102246	2679 (2.60-2.60)
Ramachandran outliers	100387	2635 (2.60-2.60)
Sidechain outliers	100360	2635 (2.60-2.60)
RSRZ outliers	91569	2334 (2.60-2.60)

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	379	2% 65% 29%
1	B	379	5% 61% 30% 6%

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 5976 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 PROTEIN (CHEMOTAXIS PROTEIN CHEA).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	368	Total	C	N	O	S	0	0	0
			2891	1837	496	547	11			
1	B	370	Total	C	N	O	S	0	0	0
			2896	1839	500	546	11			

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	521	MET	ILE	ENGINEERED	UNP Q56310
A	522	GLY	SER	ENGINEERED	UNP Q56310
A	545	CYS	GLN	ENGINEERED	UNP Q56310
B	521	MET	ILE	ENGINEERED	UNP Q56310
B	522	GLY	SER	ENGINEERED	UNP Q56310
B	545	CYS	GLN	ENGINEERED	UNP Q56310

- Molecule 2 is MERCURY (II) ION (three-letter code: HG) (formula: Hg).

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

- Molecule 3 is water.

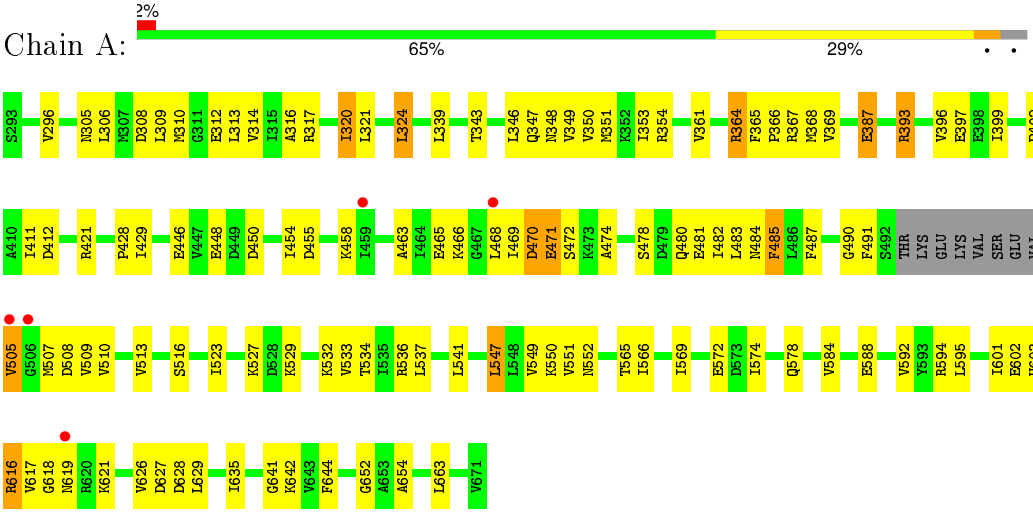
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	94	Total	O	0	0
			94	94		
3	B	93	Total	O	0	0
			93	93		

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.

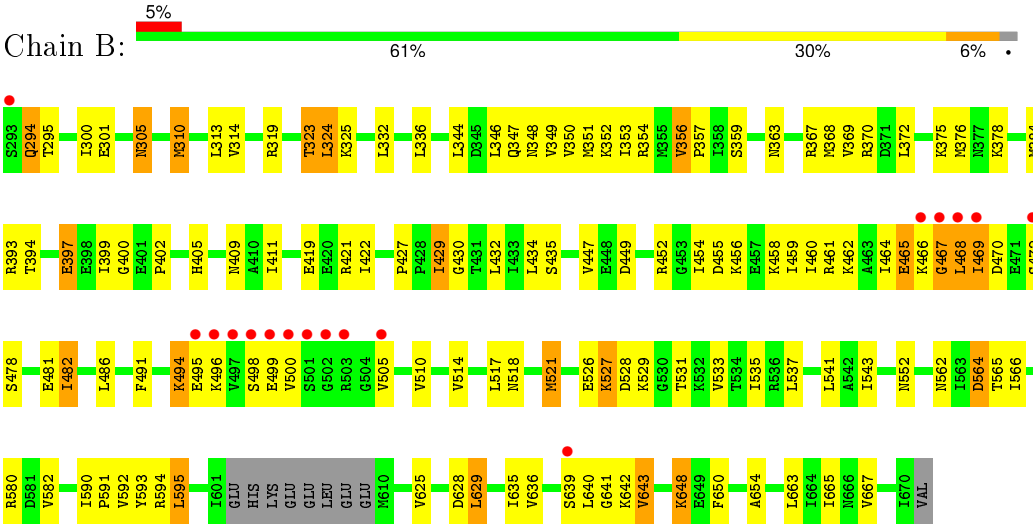
- Molecule 1: PROTEIN (CHEMOTAXIS PROTEIN CHEA)

Chain A:



- Molecule 1: PROTEIN (CHEMOTAXIS PROTEIN CHEA)

Chain B:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	61.80Å 126.50Å 75.10Å 90.00° 95.60° 90.00°	Depositor
Resolution (Å)	20.00 – 2.60 29.47 – 2.60	Depositor EDS
% Data completeness (in resolution range)	92.6 (20.00-2.60) 93.5 (29.47-2.60)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.01	Depositor
$< I/\sigma(I) >$ [1]	3.27 (at 2.61Å)	Xtriage
Refinement program	X-PLOR 3.8	Depositor
R, R_{free}	0.213 , 0.285 0.238 , 0.305	Depositor DCC
R_{free} test set	2340 reflections (7.63%)	DCC
Wilson B-factor (Å^2)	54.2	Xtriage
Anisotropy	0.320	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.31 , 59.3	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Outliers	0 of 33013 reflections	Xtriage
F_o,F_c correlation	0.93	EDS
Total number of atoms	5976	wwPDB-VP
Average B, all atoms (Å^2)	59.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.81% 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: HG

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	0/2920	0.69	1/3933 (0.0%)
1	B	0.40	0/2924	0.69	2/3937 (0.1%)
All	All	0.40	0/5844	0.69	3/7870 (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	B	495	GLU	N-CA-C	7.72	131.84	111.00
1	B	467	GLY	N-CA-C	6.02	128.14	113.10
1	A	324	LEU	CA-CB-CG	5.45	127.83	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	2891	0	3034	72	0
1	B	2896	0	3054	112	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
3	A	94	0	0	4	0
3	B	93	0	0	9	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
All	All	5976	0	6088	181	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 15.

All (181) 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:566:ILE:HG21	1:B:629:LEU:HD21	1.40	1.00
1:B:456:LYS:HB3	1:B:482:ILE:HD11	1.48	0.96
1:B:324:LEU:HD21	1:B:332:LEU:HD23	1.51	0.90
1:B:429:ILE:HD12	1:B:429:ILE:H	1.39	0.88
1:A:603:HIS:HE1	1:A:606:GLU:HB2	1.38	0.86
1:A:601:ILE:HG22	1:A:602:GLU:H	1.42	0.84
1:B:449:ASP:HB2	1:B:531:THR:H	1.41	0.83
1:B:577:VAL:HG23	1:B:578:GLN:H	1.45	0.81
1:B:459:ILE:HD11	1:B:482:ILE:HG13	1.64	0.78
1:B:454:ILE:HD11	1:B:458:LYS:HE2	1.65	0.76
1:A:365:PHE:O	1:A:369:VAL:HG23	1.89	0.73
1:B:577:VAL:HG23	1:B:578:GLN:HG2	1.72	0.72
1:B:577:VAL:HG23	1:B:578:GLN:N	2.03	0.72
1:B:369:VAL:HG13	1:B:411:ILE:HD11	1.74	0.69
1:A:387:GLU:CD	1:A:387:GLU:H	1.94	0.69
1:B:496:LYS:HE3	1:B:498:SER:HB2	1.74	0.69
1:B:500:VAL:HG13	1:B:505:VAL:HG22	1.74	0.69
1:B:456:LYS:CB	1:B:482:ILE:HD11	2.22	0.68
1:B:332:LEU:O	1:B:336:LEU:HB2	1.93	0.67
1:B:319:ARG:O	1:B:323:THR:HG22	1.95	0.67
1:A:603:HIS:CE1	1:A:606:GLU:HB2	2.28	0.67
1:B:459:ILE:HG13	1:B:460:ILE:N	2.10	0.66
1:A:313:LEU:HG	1:A:343:THR:HG23	1.79	0.65
1:B:469:ILE:HG22	1:B:470:ASP:H	1.60	0.65
1:A:454:ILE:HG21	1:A:483:LEU:HD21	1.79	0.65
1:B:349:VAL:O	1:B:353:ILE:HG13	1.98	0.64
1:A:393:ARG:O	1:A:396:VAL:HG22	1.97	0.64
1:B:460:ILE:O	1:B:464:ILE:HG12	2.00	0.62
1:B:455:ASP:HB3	1:B:527:LYS:HD3	1.81	0.62
1:A:367:ARG:HG3	3:A:1139:HOH:O	1.98	0.62
1:B:347:GLN:HE21	1:B:541:LEU:HD23	1.62	0.62
1:A:455:ASP:HB2	1:A:527:LYS:HE3	1.82	0.61
1:A:364:ARG:O	1:A:368:MET:HG3	2.00	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:494:LYS:HA	1:B:494:LYS:HE3	1.80	0.61
1:A:446:GLU:HG2	1:A:534:THR:HG23	1.82	0.61
1:A:551:VAL:HG21	1:A:595:LEU:HD23	1.82	0.61
1:B:526:GLU:HG3	3:B:1104:HOH:O	2.01	0.60
1:A:644:PHE:CD2	1:A:652:GLY:HA2	2.36	0.60
1:B:454:ILE:HD11	1:B:458:LYS:CE	2.32	0.59
1:A:487:PHE:O	1:A:508:ASP:HB3	2.00	0.59
1:A:463:ALA:HB2	1:A:491:PHE:HZ	1.68	0.59
1:B:580:ARG:HG3	3:B:1074:HOH:O	2.01	0.59
1:B:496:LYS:HB3	1:B:499:GLU:HB3	1.84	0.58
1:B:456:LYS:HB3	1:B:482:ILE:CD1	2.29	0.58
1:B:354:ARG:HD3	3:B:1169:HOH:O	2.03	0.58
1:A:305:ASN:HB3	3:A:1125:HOH:O	2.04	0.57
1:A:523:ILE:HD13	1:A:533:VAL:HG22	1.87	0.57
1:A:448:GLU:HG2	1:A:532:LYS:HG3	1.86	0.57
1:B:640:LEU:HB3	1:B:643:VAL:CG2	2.34	0.57
1:A:547:LEU:HD13	1:A:549:VAL:HG23	1.86	0.57
1:A:316:ALA:O	1:A:320:ILE:HG23	2.05	0.57
1:A:635:ILE:HD12	1:A:654:ALA:CB	2.35	0.56
1:B:347:GLN:NE2	1:B:541:LEU:HD23	2.21	0.56
1:B:405:HIS:O	1:B:409:ASN:HB2	2.06	0.56
1:B:464:ILE:HD12	1:B:470:ASP:O	2.07	0.55
1:B:640:LEU:HB3	1:B:643:VAL:HG21	1.88	0.55
1:B:301:GLU:O	1:B:305:ASN:ND2	2.40	0.55
1:A:550:LYS:HB3	1:A:628:ASP:HB2	1.89	0.55
1:B:456:LYS:N	1:B:456:LYS:HD2	2.22	0.55
1:A:616:ARG:C	1:A:616:ARG:HD2	2.28	0.54
1:B:310:MET:O	1:B:314:VAL:HG23	2.08	0.53
1:A:549:VAL:HG11	1:A:626:VAL:HG11	1.91	0.53
1:A:566:ILE:HG21	1:A:629:LEU:HD21	1.90	0.53
1:A:324:LEU:CD2	1:B:332:LEU:HD22	2.39	0.53
1:B:635:ILE:HD12	1:B:654:ALA:CB	2.39	0.53
1:B:667:VAL:HG23	3:B:1101:HOH:O	2.09	0.53
1:A:320:ILE:HG13	1:A:321:LEU:N	2.23	0.52
1:A:550:LYS:O	1:A:627:ASP:HB2	2.09	0.52
1:B:566:ILE:CG2	1:B:629:LEU:HD21	2.27	0.52
1:B:421:ARG:NH1	1:B:427:PRO:O	2.43	0.52
1:A:601:ILE:HG22	1:A:602:GLU:N	2.18	0.52
1:B:356:VAL:HG22	1:B:357:PRO:HD2	1.92	0.52
1:A:428:PRO:HG2	1:A:429:ILE:HD12	1.91	0.52
1:B:452:ARG:HD3	3:B:1108:HOH:O	2.09	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:526:GLU:HB3	1:B:529:LYS:HB2	1.92	0.51
1:B:384:MET:HA	1:B:434:LEU:O	2.10	0.51
1:A:470:ASP:O	1:A:471:GLU:HB2	2.10	0.51
1:A:396:VAL:HG23	1:A:397:GLU:N	2.25	0.51
1:B:449:ASP:HB2	1:B:531:THR:N	2.20	0.51
1:B:449:ASP:OD2	1:B:531:THR:HB	2.11	0.51
1:A:306:LEU:O	1:A:310:MET:HG2	2.11	0.50
1:B:521:MET:HG3	1:B:535:ILE:HG12	1.92	0.50
1:A:516:SER:O	1:A:641:GLY:HA3	2.11	0.50
1:B:456:LYS:HD2	1:B:456:LYS:H	1.76	0.49
1:B:368:MET:O	1:B:372:LEU:HD23	2.12	0.49
1:A:569:ILE:HD12	1:A:574:ILE:HD11	1.92	0.49
1:B:543:ILE:HG12	1:B:636:VAL:HG22	1.95	0.49
1:B:455:ASP:OD2	1:B:458:LYS:HB3	2.12	0.49
1:B:354:ARG:O	1:B:393:ARG:HG3	2.13	0.49
1:A:455:ASP:O	1:A:458:LYS:HB2	2.13	0.48
1:B:305:ASN:N	1:B:305:ASN:HD22	2.11	0.48
1:A:603:HIS:HE1	1:A:606:GLU:CB	2.18	0.48
1:B:399:ILE:C	1:B:402:PRO:HD2	2.33	0.48
1:A:617:VAL:O	1:A:619:ASN:N	2.46	0.48
1:A:308:ASP:O	1:A:312:GLU:HG3	2.13	0.48
1:A:402:PRO:HG2	1:A:513:VAL:HG11	1.95	0.48
1:B:332:LEU:HG	1:B:332:LEU:O	2.13	0.48
1:A:405:HIS:O	1:A:409:ASN:HB2	2.14	0.48
1:B:650:PHE:CZ	1:B:663:LEU:HD13	2.48	0.48
1:B:462:LYS:HA	1:B:465:GLU:HG3	1.96	0.48
1:B:641:GLY:C	1:B:643:VAL:H	2.17	0.47
1:A:366:PRO:HG2	3:A:1139:HOH:O	2.13	0.47
1:B:400:GLY:HA3	3:B:1183:HOH:O	2.14	0.47
1:A:310:MET:O	1:A:314:VAL:HG23	2.13	0.47
1:B:466:LYS:O	1:B:468:LEU:HD12	2.15	0.47
1:B:347:GLN:O	1:B:351:MET:HG2	2.14	0.47
1:B:310:MET:HE1	1:B:541:LEU:HD21	1.96	0.47
1:B:582:VAL:HG12	1:B:591:PRO:HA	1.96	0.47
1:A:481:GLU:HA	1:A:484:ASN:HB2	1.97	0.47
1:B:376:MET:SD	1:B:411:ILE:HG22	2.55	0.47
1:A:402:PRO:HB3	1:A:510:VAL:HG13	1.96	0.47
1:B:367:ARG:HG3	1:B:370:ARG:NH2	2.29	0.47
1:A:478:SER:HB3	1:A:619:ASN:HD21	1.79	0.46
1:B:564:ASP:OD1	1:B:565:THR:HG22	2.15	0.46
1:A:354:ARG:O	1:A:393:ARG:HG2	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:644:PHE:CG	1:A:652:GLY:HA2	2.51	0.46
1:A:369:VAL:HG13	1:A:411:ILE:HD11	1.96	0.46
1:A:324:LEU:HD21	1:B:332:LEU:HD22	1.97	0.46
1:B:419:GLU:O	1:B:422:ILE:HG12	2.16	0.46
1:B:394:THR:HG21	1:B:639:SER:HB3	1.97	0.46
1:A:574:ILE:HD12	1:A:592:VAL:HG21	1.97	0.45
1:B:577:VAL:HG23	1:B:578:GLN:CG	2.45	0.45
1:A:470:ASP:HB2	3:A:1210:HOH:O	2.16	0.45
1:A:347:GLN:O	1:A:351:MET:HG2	2.17	0.45
1:A:482:ILE:O	1:A:485:PHE:HB2	2.16	0.45
1:A:505:VAL:HG12	1:A:509:VAL:HG11	1.98	0.45
1:A:594:ARG:HG3	1:A:594:ARG:HH11	1.81	0.45
1:B:648:LYS:HE2	1:B:648:LYS:HB2	1.71	0.45
1:B:592:VAL:HG13	1:B:625:VAL:HG23	1.99	0.45
1:B:447:VAL:HB	1:B:533:VAL:HG13	1.98	0.45
1:B:456:LYS:CD	1:B:456:LYS:H	2.29	0.45
1:B:456:LYS:O	1:B:460:ILE:HG13	2.17	0.45
1:B:578:GLN:HG3	1:B:580:ARG:H	1.82	0.44
1:A:480:GLN:HG3	1:A:484:ASN:ND2	2.32	0.44
1:B:359:SER:HB3	1:B:387:GLU:O	2.17	0.44
1:A:603:HIS:CE1	1:A:606:GLU:N	2.85	0.44
1:B:347:GLN:HG2	3:B:1173:HOH:O	2.17	0.44
1:B:577:VAL:O	1:B:578:GLN:O	2.36	0.44
1:A:317:ARG:HH11	1:A:343:THR:CG2	2.31	0.44
1:B:562:ASN:ND2	1:B:667:VAL:HG21	2.32	0.44
1:A:421:ARG:HH22	1:A:450:ASP:CG	2.21	0.43
1:B:346:LEU:O	1:B:350:VAL:HG23	2.18	0.43
1:A:308:ASP:HA	1:A:541:LEU:HD12	1.99	0.43
1:B:594:ARG:HA	1:B:625:VAL:HB	2.01	0.43
1:A:469:ILE:HG21	1:A:474:ALA:HB2	2.00	0.43
1:B:470:ASP:HB2	1:B:473:LYS:HB2	2.00	0.43
1:B:590:ILE:HA	1:B:591:PRO:HD3	1.81	0.43
1:B:595:LEU:HD11	1:B:665:ILE:HD11	2.00	0.43
1:B:469:ILE:CG2	1:B:474:ALA:HB3	2.48	0.42
1:A:463:ALA:HB3	1:A:469:ILE:HD12	2.00	0.42
1:B:385:ARG:HB2	1:B:435:SER:HB3	2.01	0.42
1:B:496:LYS:HB3	1:B:499:GLU:CB	2.50	0.42
1:A:466:LYS:NZ	1:A:490:GLY:O	2.52	0.42
1:B:592:VAL:CG1	1:B:625:VAL:HG23	2.50	0.42
1:B:635:ILE:HD12	1:B:654:ALA:HB2	2.00	0.42
1:B:455:ASP:OD1	1:B:458:LYS:HD3	2.18	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:459:ILE:HG13	1:B:460:ILE:H	1.84	0.42
1:B:378:LYS:HB2	3:B:1106:HOH:O	2.19	0.42
1:B:397:GLU:HG2	1:B:397:GLU:H	1.57	0.42
1:B:310:MET:SD	1:B:347:GLN:HG3	2.60	0.41
1:B:452:ARG:HA	1:B:528:ASP:HA	2.01	0.41
1:B:387:GLU:H	1:B:387:GLU:CD	2.24	0.41
1:B:375:LYS:HB3	1:B:375:LYS:HE2	1.69	0.41
1:B:294:GLN:HB3	1:B:295:THR:H	1.46	0.41
1:A:399:ILE:HA	1:A:399:ILE:HD12	1.97	0.41
1:A:346:LEU:O	1:A:350:VAL:HG23	2.21	0.41
1:B:577:VAL:CG2	1:B:578:GLN:N	2.75	0.41
1:B:393:ARG:HD3	3:B:1175:HOH:O	2.21	0.41
1:B:421:ARG:NH1	1:B:430:GLY:HA2	2.35	0.41
1:B:517:LEU:O	1:B:518:ASN:HB2	2.21	0.41
1:A:565:THR:HG22	1:A:566:ILE:N	2.35	0.41
1:B:593:TYR:CD1	1:B:593:TYR:N	2.88	0.41
1:B:367:ARG:HG3	1:B:370:ARG:HH22	1.85	0.41
1:B:510:VAL:O	1:B:514:VAL:HG12	2.21	0.41
1:B:325:LYS:HE2	1:B:325:LYS:HB3	1.81	0.41
1:B:363:ASN:HD22	1:B:363:ASN:HA	1.72	0.41
1:A:296:VAL:HG23	1:B:300:ILE:CG2	2.51	0.40
1:A:663:LEU:HA	1:A:663:LEU:HD23	1.84	0.40
1:A:584:VAL:HA	1:A:588:GLU:O	2.21	0.40
1:B:473:LYS:HD3	1:B:473:LYS:HA	1.87	0.40
1:A:349:VAL:O	1:A:353:ILE:HG13	2.22	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	364/379 (96%)	332 (91%)	27 (7%)	5 (1%)	14 28

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	B	366/379 (97%)	334 (91%)	24 (7%)	8 (2%)	8 15
All	All	730/758 (96%)	666 (91%)	51 (7%)	13 (2%)	11 21

All (13) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	618	GLY
1	B	473	LYS
1	B	578	GLN
1	A	468	LEU
1	A	471	GLU
1	A	507	MET
1	B	478	SER
1	B	577	VAL
1	B	472	SER
1	B	642	LYS
1	A	578	GLN
1	B	643	VAL
1	B	467	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	327/337 (97%)	304 (93%)	23 (7%)	19 37
1	B	328/337 (97%)	295 (90%)	33 (10%)	9 17
All	All	655/674 (97%)	599 (92%)	56 (8%)	13 25

All (56) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	309	LEU
1	A	320	ILE
1	A	339	LEU

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Mol	Chain	Res	Type
1	A	348	ASN
1	A	361	VAL
1	A	364	ARG
1	A	387	GLU
1	A	393	ARG
1	A	412	ASP
1	A	465	GLU
1	A	470	ASP
1	A	472	SER
1	A	485	PHE
1	A	505	VAL
1	A	529	LYS
1	A	536	ARG
1	A	537	LEU
1	A	547	LEU
1	A	552	ASN
1	A	572	GLU
1	A	616	ARG
1	A	621	LYS
1	A	642	LYS
1	B	294	GLN
1	B	305	ASN
1	B	310	MET
1	B	313	LEU
1	B	323	THR
1	B	324	LEU
1	B	344	LEU
1	B	348	ASN
1	B	352	LYS
1	B	356	VAL
1	B	397	GLU
1	B	429	ILE
1	B	432	LEU
1	B	461	ARG
1	B	465	GLU
1	B	468	LEU
1	B	469	ILE
1	B	477	LEU
1	B	481	GLU
1	B	482	ILE
1	B	486	LEU
1	B	491	PHE

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Mol	Chain	Res	Type
1	B	494	LYS
1	B	521	MET
1	B	527	LYS
1	B	537	LEU
1	B	552	ASN
1	B	564	ASP
1	B	578	GLN
1	B	595	LEU
1	B	628	ASP
1	B	629	LEU
1	B	648	LYS

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	363	ASN
1	A	381	ASN
1	A	442	ASN
1	A	512	ASN
1	A	552	ASN
1	A	603	HIS
1	A	619	ASN
1	B	305	ASN
1	B	347	GLN
1	B	348	ASN
1	B	363	ASN
1	B	377	ASN
1	B	484	ASN
1	B	552	ASN
1	B	562	ASN
1	B	578	GLN
1	B	666	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

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	368/379 (97%)	-0.21	7 (1%) 70 64	22, 53, 98, 100	0
1	B	370/379 (97%)	-0.01	18 (4%) 33 26	24, 55, 100, 100	0
All	All	738/758 (97%)	-0.11	25 (3%) 49 41	22, 54, 99, 100	0

All (25) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	505	VAL	4.5
1	B	501	SER	4.1
1	B	498	SER	4.0
1	B	495	GLU	3.9
1	B	469	ILE	3.9
1	B	467	GLY	3.4
1	B	502	GLY	3.4
1	B	503	ARG	3.3
1	A	468	LEU	3.2
1	A	504	GLY	3.0
1	B	497	VAL	2.9
1	B	500	VAL	2.8
1	B	499	GLU	2.8
1	B	496	LYS	2.8
1	A	619	ASN	2.6
1	B	466	LYS	2.6
1	A	506	GLY	2.5
1	B	472	SER	2.5
1	B	293	SER	2.4
1	A	505	VAL	2.3
1	B	639	SER	2.2
1	B	576	ARG	2.2
1	B	468	LEU	2.2
1	A	459	ILE	2.2

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Mol	Chain	Res	Type	RSRZ
1	A	605	GLU	2.2

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 carbohydrates in this entry.

6.4 Ligands (i)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. 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
2	HG	A	998	1/1	0.99	0.10	-	78,78,78,78	0
2	HG	B	999	1/1	0.95	0.06	-	99,99,99,99	0

6.5 Other polymers (i)

There are no such residues in this entry.