Full wwPDB X-ray Structure Validation Report (i)

Oct 12, 2021 – 10:58 AM EDT

PDB ID	:	1Z3U
Title	:	Structure of the Angiopoietin-2 Recptor Binding Domain and Identification of Surfaces Involved in Tie2 Recognition
Authors	:	Barton, W.A.; Tzvetkova, D.; Nikolov, D.B.
Deposited on	:	2005-03-14
Resolution	:	2.25 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 (i) symbol.

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

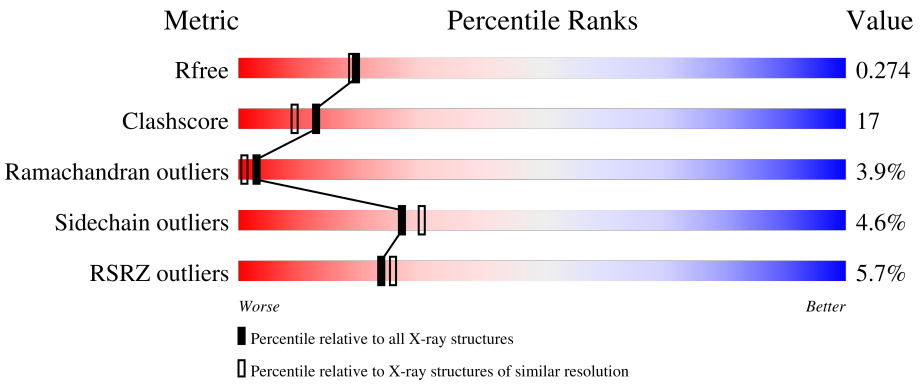
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.23.2
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.23.2

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 2.25 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	1377 (2.26-2.26)
Clashscore	141614	1487 (2.26-2.26)
Ramachandran outliers	138981	1449 (2.26-2.26)
Sidechain outliers	138945	1450 (2.26-2.26)
RSRZ outliers	127900	1356 (2.26-2.26)

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	217	5% 73% 22% • •
1	B	217	7% 69% 25% 5%
1	C	217	5% 65% 30% •
1	D	217	6% 65% 29% 5% •

2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 7259 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 Angiopoietin-2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	216	1719	1083	294	331	11	0	0	0
1	B	216	1719	1083	294	331	11	0	0	0
1	C	216	1719	1083	294	331	11	0	0	0
1	D	216	1719	1083	294	331	11	0	0	0

There are 16 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	280	SER	-	cloning artifact	UNP O15123
A	469	ALA	PHE	engineered mutation	UNP O15123
A	475	ALA	TYR	engineered mutation	UNP O15123
A	476	ALA	TYR	engineered mutation	UNP O15123
B	280	SER	-	cloning artifact	UNP O15123
B	469	ALA	PHE	engineered mutation	UNP O15123
B	475	ALA	TYR	engineered mutation	UNP O15123
B	476	ALA	TYR	engineered mutation	UNP O15123
C	280	SER	-	cloning artifact	UNP O15123
C	469	ALA	PHE	engineered mutation	UNP O15123
C	475	ALA	TYR	engineered mutation	UNP O15123
C	476	ALA	TYR	engineered mutation	UNP O15123
D	280	SER	-	cloning artifact	UNP O15123
D	469	ALA	PHE	engineered mutation	UNP O15123
D	475	ALA	TYR	engineered mutation	UNP O15123
D	476	ALA	TYR	engineered mutation	UNP O15123

- Molecule 2 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Ca		
2	A	1	1	1	0	0
2	B	1	1	1	0	0
2	C	1	1	1	0	0
2	D	1	1	1	0	0

- Molecule 3 is water.

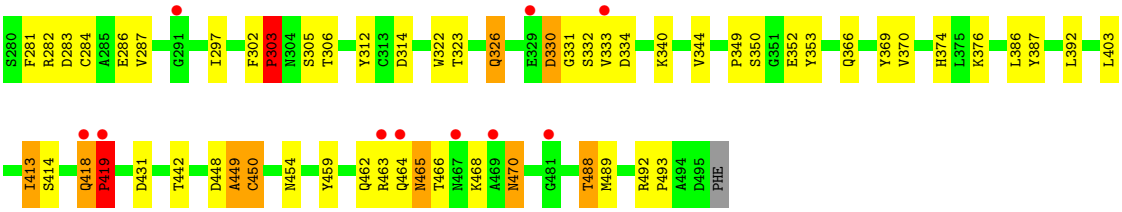
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
3	A	104	104	104	0	0
3	B	76	76	76	0	0
3	C	109	109	109	0	0
3	D	90	90	90	0	0

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.

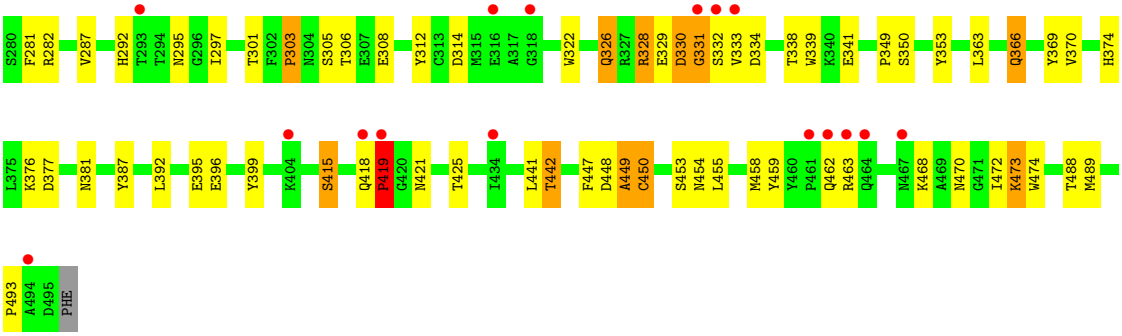
• Molecule 1: Angiopoietin-2

Chain A:



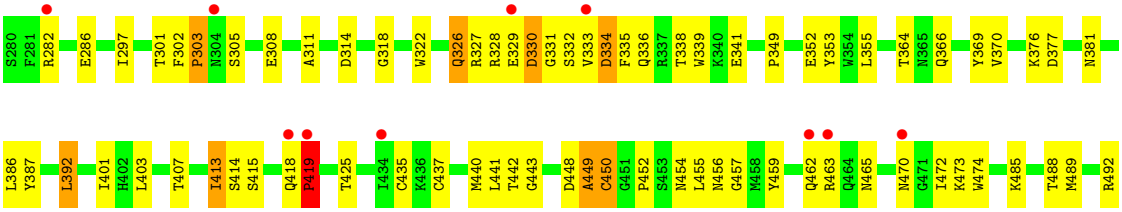
• Molecule 1: Angiopoietin-2

Chain B:



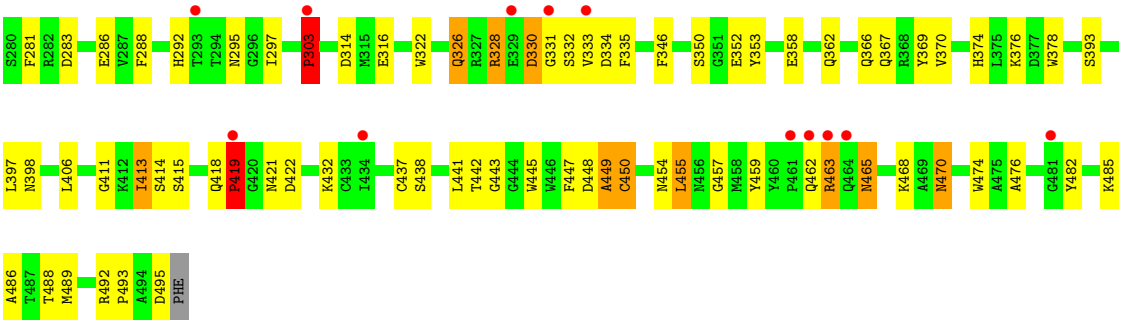
• Molecule 1: Angiopoietin-2

Chain C:



• Molecule 1: Angiopoietin-2

Chain D:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α, β, γ	140.22Å 94.47Å 84.67Å 90.00° 94.47° 90.00°	Depositor
Resolution (Å)	8.00 – 2.25 29.34 – 2.25	Depositor EDS
% Data completeness (in resolution range)	(Not available) (8.00-2.25) 98.2 (29.34-2.25)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	3.86 (at 2.24Å)	Xtriage
Refinement program	CNS 1.0	Depositor
R, R_{free}	0.246 , 0.278 0.238 , 0.274	Depositor DCC
R_{free} test set	2581 reflections (4.94%)	wwPDB-VP
Wilson B-factor (Å^2)	23.9	Xtriage
Anisotropy	0.458	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.36 , 49.4	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.91	EDS
Total number of atoms	7259	wwPDB-VP
Average B, all atoms (Å^2)	27.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.41% 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 (i)

5.1 Standard geometry (i)

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

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	0.43	0/1765	0.74	2/2384 (0.1%)
1	B	0.39	0/1765	0.69	2/2384 (0.1%)
1	C	0.43	0/1765	0.72	2/2384 (0.1%)
1	D	0.41	0/1765	0.71	2/2384 (0.1%)
All	All	0.42	0/7060	0.71	8/9536 (0.1%)

There are no bond length outliers.

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	449	ALA	N-CA-C	-7.95	89.54	111.00
1	D	331	GLY	N-CA-C	-7.48	94.40	113.10
1	A	331	GLY	N-CA-C	-7.19	95.12	113.10
1	C	449	ALA	N-CA-C	-6.89	92.39	111.00
1	B	449	ALA	N-CA-C	-6.74	92.82	111.00
1	B	331	GLY	N-CA-C	-6.30	97.36	113.10
1	C	331	GLY	N-CA-C	-6.28	97.41	113.10
1	D	449	ALA	N-CA-C	-6.15	94.40	111.00

There are no chirality outliers.

There are no planarity outliers.

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	1719	0	1610	51	0
1	B	1719	0	1610	51	0
1	C	1719	0	1610	58	0
1	D	1719	0	1610	61	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
2	C	1	0	0	0	0
2	D	1	0	0	0	0
3	A	104	0	0	0	0
3	B	76	0	0	1	0
3	C	109	0	0	1	0
3	D	90	0	0	2	0
All	All	7259	0	6440	221	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 17.

All (221) 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:418:GLN:HB3	1:C:419:PRO:HD2	1.19	1.13
1:A:418:GLN:HB3	1:A:419:PRO:HD2	1.18	1.08
1:D:418:GLN:HB3	1:D:419:PRO:HD2	1.47	0.95
1:A:374:HIS:HB3	1:A:488:THR:HG23	1.53	0.91
1:A:418:GLN:HB3	1:A:419:PRO:CD	2.03	0.87
1:D:418:GLN:CB	1:D:419:PRO:HD2	2.10	0.82
1:D:297:ILE:HD11	1:D:350:SER:HB3	1.62	0.82
1:B:418:GLN:HB3	1:B:419:PRO:HD2	1.66	0.77
1:A:418:GLN:CB	1:A:419:PRO:HD2	2.07	0.76
1:C:418:GLN:HB3	1:C:419:PRO:CD	2.09	0.75
1:D:326:GLN:HG2	1:D:489:MET:SD	2.27	0.74
1:B:418:GLN:CB	1:B:419:PRO:HD2	2.16	0.74
1:C:415:SER:O	1:C:452:PRO:HG2	1.88	0.73
1:A:370:VAL:HG23	1:A:387:TYR:O	1.88	0.72
1:C:462:GLN:HA	1:C:465:ASN:HD22	1.54	0.71
1:C:328:ARG:HH21	1:C:456:ASN:HA	1.54	0.71
1:D:442:THR:HG23	1:D:470:ASN:HD21	1.56	0.71
1:D:421:ASN:ND2	1:D:448:ASP:HA	2.07	0.70
1:B:374:HIS:HB3	1:B:488:THR:HG23	1.74	0.69
1:A:326:GLN:HG2	1:A:489:MET:SD	2.32	0.69
1:D:462:GLN:O	1:D:463:ARG:HB2	1.91	0.69
1:B:326:GLN:HG2	1:B:489:MET:SD	2.33	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:374:HIS:HB3	1:D:488:THR:CG2	2.23	0.68
1:B:448:ASP:C	1:B:450:CYS:H	1.96	0.68
1:C:418:GLN:CB	1:C:419:PRO:HD2	2.08	0.68
1:A:418:GLN:O	1:A:419:PRO:C	2.31	0.67
1:B:453:SER:HA	1:B:473:LYS:HG3	1.76	0.67
1:D:328:ARG:HB3	1:D:328:ARG:HH11	1.59	0.67
1:C:326:GLN:HG2	1:C:489:MET:SD	2.35	0.66
1:B:297:ILE:HD13	1:B:349:PRO:HB2	1.77	0.66
1:D:413:ILE:HD13	1:D:414:SER:H	1.61	0.65
1:A:448:ASP:C	1:A:450:CYS:H	1.99	0.65
1:C:413:ILE:HD13	1:C:414:SER:N	2.12	0.65
1:B:328:ARG:HH11	1:B:328:ARG:HB3	1.62	0.65
1:D:418:GLN:O	1:D:419:PRO:C	2.33	0.64
1:A:413:ILE:HD13	1:A:414:SER:H	1.61	0.64
1:D:330:ASP:HB2	1:D:459:TYR:CZ	2.33	0.63
1:B:374:HIS:HB3	1:B:488:THR:CG2	2.27	0.63
1:A:370:VAL:HG12	1:A:492:ARG:O	1.98	0.63
1:B:333:VAL:HG12	1:B:333:VAL:O	1.99	0.62
1:B:442:THR:HG21	1:B:458:MET:HE2	1.82	0.61
1:D:281:PHE:HB3	1:D:286:GLU:HB3	1.82	0.61
1:B:330:ASP:HB2	1:B:459:TYR:CZ	2.36	0.60
1:C:370:VAL:HG23	1:C:387:TYR:O	2.02	0.60
1:D:418:GLN:HB3	1:D:419:PRO:CD	2.27	0.58
1:D:328:ARG:HB3	1:D:328:ARG:NH1	2.17	0.58
1:D:413:ILE:HD13	1:D:414:SER:N	2.18	0.58
1:B:295:ASN:HB3	1:B:312:TYR:OH	2.03	0.57
1:B:282:ARG:NE	1:B:366:GLN:HE21	2.02	0.57
1:C:370:VAL:HG12	1:C:492:ARG:O	2.05	0.57
1:B:442:THR:HG23	1:B:470:ASN:HD21	1.70	0.56
1:D:448:ASP:C	1:D:450:CYS:H	2.07	0.56
1:C:448:ASP:C	1:C:450:CYS:H	2.08	0.56
1:C:282:ARG:HG2	1:C:286:GLU:OE1	2.06	0.56
1:A:413:ILE:HD13	1:A:414:SER:N	2.21	0.56
1:B:415:SER:HB2	1:B:474:TRP:CE2	2.41	0.55
1:C:418:GLN:HA	1:C:418:GLN:OE1	2.06	0.55
1:A:333:VAL:O	1:A:334:ASP:HB3	2.07	0.55
1:B:448:ASP:C	1:B:450:CYS:N	2.61	0.55
1:B:418:GLN:HG3	1:B:419:PRO:HD2	1.90	0.54
1:C:328:ARG:HH21	1:C:456:ASN:CA	2.20	0.54
1:C:376:LYS:HD2	1:C:485:LYS:HD3	1.89	0.54
1:A:374:HIS:HB3	1:A:488:THR:CG2	2.33	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:339:TRP:HA	1:B:425:THR:HG21	1.88	0.54
1:B:442:THR:HG21	1:B:458:MET:CE	2.38	0.54
1:D:465:ASN:O	1:D:482:TYR:HA	2.07	0.54
1:C:392:LEU:HD12	1:C:401:ILE:HA	1.90	0.54
1:C:318:GLY:O	1:C:492:ARG:NH2	2.40	0.53
1:A:442:THR:HG23	1:A:470:ASN:HD21	1.72	0.53
1:B:326:GLN:HA	1:B:353:TYR:O	2.08	0.53
1:B:369:TYR:CE1	1:B:493:PRO:HD3	2.43	0.53
1:C:330:ASP:HB2	1:C:459:TYR:CZ	2.44	0.53
1:A:376:LYS:HB2	1:A:376:LYS:NZ	2.24	0.53
1:B:281:PHE:CD2	1:B:287:VAL:HG22	2.43	0.53
1:B:297:ILE:HD11	1:B:350:SER:HB3	1.90	0.53
1:B:370:VAL:HG13	1:B:387:TYR:O	2.08	0.53
1:B:418:GLN:O	1:B:419:PRO:C	2.43	0.52
1:A:462:GLN:O	1:A:463:ARG:HB2	2.10	0.52
1:A:418:GLN:O	1:A:419:PRO:O	2.26	0.52
1:C:333:VAL:CG2	1:C:352:GLU:HB2	2.40	0.52
1:D:369:TYR:CE1	1:D:493:PRO:HD3	2.43	0.52
1:B:305:SER:OG	1:B:306:THR:N	2.43	0.52
1:B:442:THR:CG2	1:B:470:ASN:HD21	2.22	0.52
1:A:314:ASP:HB3	1:A:322:TRP:HB2	1.91	0.51
1:D:393:SER:HB3	1:D:397:LEU:HD12	1.93	0.51
1:A:297:ILE:HD11	1:A:350:SER:HB3	1.93	0.51
1:A:465:ASN:HD22	1:A:466:THR:N	2.08	0.51
1:B:418:GLN:CG	1:B:419:PRO:HD2	2.41	0.51
1:B:455:LEU:HA	1:B:472:ILE:HG23	1.93	0.51
1:D:288:PHE:HA	1:D:292:HIS:O	2.11	0.51
1:C:333:VAL:HG12	1:C:333:VAL:O	2.12	0.50
1:D:418:GLN:CB	1:D:419:PRO:CD	2.88	0.50
1:A:303:PRO:HB3	1:A:366:GLN:HE22	1.76	0.50
1:A:370:VAL:HG21	1:A:386:LEU:HD11	1.92	0.50
1:B:418:GLN:OE1	1:B:418:GLN:HA	2.10	0.50
1:D:378:TRP:CE3	1:D:485:LYS:HD2	2.46	0.50
1:B:472:ILE:HG12	3:B:498:HOH:O	2.12	0.50
1:C:297:ILE:HD13	1:C:349:PRO:HB2	1.91	0.50
1:B:463:ARG:HG3	1:B:463:ARG:HH11	1.76	0.50
1:D:376:LYS:HB3	1:D:486:ALA:HB3	1.93	0.50
1:A:330:ASP:HA	1:A:352:GLU:OE2	2.12	0.49
1:B:301:THR:HG22	1:B:308:GLU:HG2	1.94	0.49
1:B:333:VAL:O	1:B:333:VAL:CG1	2.59	0.49
1:D:358:GLU:O	1:D:362:GLN:HG3	2.11	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:282:ARG:NH1	1:C:286:GLU:OE1	2.46	0.49
1:C:330:ASP:HA	1:C:352:GLU:OE2	2.12	0.49
1:B:441:LEU:HD12	1:B:447:PHE:CE1	2.48	0.49
1:C:301:THR:HG22	1:C:308:GLU:HG2	1.95	0.49
1:D:374:HIS:HB3	1:D:488:THR:HG23	1.92	0.48
1:D:449:ALA:O	1:D:450:CYS:HB2	2.13	0.48
1:D:370:VAL:HG12	1:D:492:ARG:O	2.12	0.48
1:B:449:ALA:O	1:B:450:CYS:HB2	2.13	0.48
1:A:281:PHE:HD1	1:A:286:GLU:HG2	1.77	0.48
1:A:418:GLN:O	1:A:419:PRO:HB2	2.14	0.48
1:C:328:ARG:NH2	1:C:457:GLY:O	2.36	0.48
1:D:335:PHE:O	1:D:443:GLY:HA2	2.13	0.48
1:A:340:LYS:O	1:A:344:VAL:HG12	2.13	0.48
1:B:282:ARG:HG2	1:B:363:LEU:HD21	1.96	0.48
1:C:339:TRP:HA	1:C:425:THR:HG21	1.96	0.48
1:C:418:GLN:O	1:C:419:PRO:C	2.50	0.48
1:C:327:ARG:HG3	1:C:488:THR:HG22	1.95	0.47
1:D:314:ASP:HB3	1:D:322:TRP:HB2	1.95	0.47
1:D:418:GLN:CG	1:D:419:PRO:HD2	2.44	0.47
1:B:338:THR:OG1	1:B:341:GLU:HG3	2.15	0.47
1:D:328:ARG:NH2	1:D:457:GLY:O	2.46	0.47
1:D:378:TRP:CE2	1:D:485:LYS:HB2	2.49	0.47
1:D:418:GLN:OE1	1:D:418:GLN:HA	2.13	0.47
1:D:445:TRP:CH2	1:D:455:LEU:HB2	2.49	0.47
1:A:326:GLN:HA	1:A:353:TYR:O	2.15	0.47
1:C:335:PHE:O	1:C:443:GLY:HA2	2.15	0.47
1:B:421:ASN:ND2	1:B:448:ASP:HA	2.30	0.46
1:A:376:LYS:HB2	1:A:376:LYS:HZ3	1.80	0.46
1:B:441:LEU:HD11	1:B:450:CYS:HB3	1.97	0.46
1:A:414:SER:HB3	1:A:418:GLN:HE21	1.81	0.46
1:A:468:LYS:C	1:A:470:ASN:H	2.18	0.46
1:D:330:ASP:HA	1:D:352:GLU:OE2	2.15	0.46
1:D:374:HIS:HB3	1:D:488:THR:HG22	1.97	0.46
1:D:418:GLN:O	1:D:419:PRO:O	2.34	0.46
1:D:418:GLN:HG3	1:D:419:PRO:HD2	1.98	0.46
1:C:333:VAL:O	1:C:334:ASP:HB3	2.17	0.45
1:D:415:SER:HB2	1:D:474:TRP:CE2	2.51	0.45
1:A:431:ASP:HB2	1:A:448:ASP:O	2.16	0.45
1:D:398:ASN:HB2	1:D:422:ASP:HB3	1.97	0.45
1:B:462:GLN:O	1:B:463:ARG:HB2	2.16	0.45
1:D:281:PHE:HA	1:D:286:GLU:OE2	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:314:ASP:HB3	1:B:322:TRP:HB2	1.99	0.45
1:D:462:GLN:O	1:D:463:ARG:CB	2.59	0.45
1:C:418:GLN:O	1:C:419:PRO:HB2	2.16	0.45
1:D:411:GLY:HA3	1:D:476:ALA:HB1	1.98	0.45
1:A:465:ASN:ND2	1:A:466:THR:HG23	2.31	0.45
1:A:387:TYR:CG	1:A:403:LEU:HD22	2.52	0.45
1:D:295:ASN:HD21	1:D:316:GLU:HB2	1.82	0.45
1:B:297:ILE:CD1	1:B:349:PRO:HB2	2.46	0.44
1:C:328:ARG:HH21	1:C:456:ASN:C	2.21	0.44
1:C:377:ASP:OD1	1:C:381:ASN:HB2	2.17	0.44
1:D:432:LYS:HG2	3:D:562:HOH:O	2.17	0.44
1:B:376:LYS:HB2	1:B:376:LYS:NZ	2.33	0.44
1:B:418:GLN:HB3	1:B:419:PRO:CD	2.43	0.44
1:C:338:THR:OG1	1:C:341:GLU:HG3	2.17	0.44
1:C:364:THR:HA	1:C:369:TYR:CD2	2.53	0.44
1:A:302:PHE:HB2	1:A:305:SER:HB3	2.00	0.44
1:C:333:VAL:HG21	1:C:352:GLU:HB2	1.99	0.44
1:D:326:GLN:CG	1:D:489:MET:SD	3.02	0.44
1:D:441:LEU:HD12	1:D:447:PHE:HE1	1.82	0.44
1:A:442:THR:CG2	1:A:470:ASN:HD21	2.31	0.43
1:B:418:GLN:O	1:B:419:PRO:HB2	2.18	0.43
1:C:387:TYR:CD1	1:C:403:LEU:HB3	2.54	0.43
1:A:369:TYR:CE1	1:A:493:PRO:HD3	2.54	0.43
1:A:376:LYS:HZ3	1:A:376:LYS:CB	2.31	0.43
1:D:333:VAL:HG12	1:D:333:VAL:O	2.17	0.43
1:C:311:ALA:HB2	1:C:355:LEU:HD11	2.01	0.43
1:C:437:CYS:SG	1:C:450:CYS:N	2.91	0.43
1:A:284:CYS:SG	1:A:323:THR:HA	2.59	0.43
1:A:312:TYR:HB2	1:A:349:PRO:O	2.18	0.43
1:C:302:PHE:HB2	1:C:305:SER:HB3	2.00	0.43
1:C:386:LEU:HB3	1:C:407:THR:OG1	2.19	0.43
1:D:283:ASP:C	1:D:283:ASP:OD2	2.58	0.43
1:D:406:LEU:HD22	1:D:414:SER:N	2.34	0.43
1:D:492:ARG:HD3	1:D:495:ASP:OD2	2.18	0.43
1:C:327:ARG:CG	1:C:488:THR:HG22	2.49	0.42
1:D:367:GLN:HG2	3:D:543:HOH:O	2.18	0.42
1:A:448:ASP:HB3	1:A:449:ALA:H	1.65	0.42
1:A:283:ASP:O	1:A:287:VAL:HG23	2.19	0.42
1:C:415:SER:HB2	1:C:474:TRP:CE2	2.53	0.42
1:A:465:ASN:HD22	1:A:465:ASN:C	2.23	0.42
1:B:377:ASP:OD1	1:B:381:ASN:HB2	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:346:PHE:O	1:D:353:TYR:HB2	2.19	0.42
1:C:328:ARG:NH2	1:C:456:ASN:C	2.72	0.42
1:C:336:GLN:HG2	1:C:442:THR:HB	2.02	0.42
1:D:333:VAL:O	1:D:333:VAL:CG1	2.68	0.42
1:A:326:GLN:HG3	1:A:489:MET:HB2	2.01	0.42
1:C:282:ARG:CZ	1:C:286:GLU:OE1	2.68	0.42
1:C:462:GLN:O	1:C:463:ARG:HB2	2.20	0.42
1:D:468:LYS:C	1:D:470:ASN:H	2.23	0.42
1:A:282:ARG:NH1	1:A:286:GLU:OE1	2.52	0.42
1:A:305:SER:OG	1:A:306:THR:N	2.53	0.42
1:A:464:GLN:O	1:A:468:LYS:HE3	2.20	0.41
1:B:468:LYS:C	1:B:470:ASN:H	2.23	0.41
1:C:376:LYS:CD	1:C:485:LYS:HD3	2.50	0.41
1:D:421:ASN:HD21	1:D:448:ASP:HA	1.81	0.41
1:B:395:GLU:HG3	1:B:399:TYR:CE2	2.55	0.41
1:A:330:ASP:HB2	1:A:459:TYR:CZ	2.55	0.41
1:A:376:LYS:NZ	1:A:376:LYS:CB	2.84	0.41
1:D:438:SER:O	1:D:442:THR:HA	2.20	0.41
1:A:370:VAL:CG2	1:A:386:LEU:HD11	2.49	0.41
1:C:364:THR:HA	1:C:369:TYR:HD2	1.86	0.41
1:C:326:GLN:HA	1:C:353:TYR:O	2.21	0.41
1:D:303:PRO:HB3	1:D:366:GLN:OE1	2.20	0.41
1:A:492:ARG:HG2	1:A:493:PRO:N	2.35	0.41
1:C:455:LEU:HA	1:C:472:ILE:HG23	2.03	0.41
1:D:418:GLN:O	1:D:419:PRO:HB2	2.20	0.41
1:C:333:VAL:O	1:C:333:VAL:CG1	2.69	0.40
1:A:369:TYR:HA	1:A:493:PRO:HA	2.03	0.40
1:B:287:VAL:HG12	1:B:292:HIS:HB2	2.04	0.40
1:C:328:ARG:NH1	1:C:472:ILE:HD11	2.36	0.40
1:C:449:ALA:O	1:C:450:CYS:HB2	2.21	0.40
1:C:314:ASP:HB3	1:C:322:TRP:HB2	2.03	0.40
1:C:441:LEU:HD23	1:C:441:LEU:N	2.36	0.40
1:C:418:GLN:HG2	3:C:571:HOH:O	2.20	0.40
1:C:435:CYS:SG	1:C:440:MET:SD	3.20	0.40
1:D:437:CYS:SG	1:D:450:CYS:N	2.94	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	214/217 (99%)	188 (88%)	19 (9%)	7 (3%)	4 1
1	B	214/217 (99%)	190 (89%)	14 (6%)	10 (5%)	2 0
1	C	214/217 (99%)	190 (89%)	16 (8%)	8 (4%)	3 1
1	D	214/217 (99%)	192 (90%)	14 (6%)	8 (4%)	3 1
All	All	856/868 (99%)	760 (89%)	63 (7%)	33 (4%)	3 1

All (33) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	303	PRO
1	A	332	SER
1	A	419	PRO
1	B	303	PRO
1	B	332	SER
1	B	419	PRO
1	C	303	PRO
1	C	332	SER
1	C	419	PRO
1	D	332	SER
1	D	419	PRO
1	A	330	ASP
1	A	450	CYS
1	B	330	ASP
1	B	334	ASP
1	B	450	CYS
1	B	454	ASN
1	C	329	GLU
1	C	454	ASN
1	D	450	CYS
1	A	454	ASN
1	B	329	GLU

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Mol	Chain	Res	Type
1	C	330	ASP
1	C	450	CYS
1	D	303	PRO
1	D	330	ASP
1	D	454	ASN
1	D	463	ARG
1	B	442	THR
1	C	334	ASP
1	D	334	ASP
1	B	331	GLY
1	A	418	GLN

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	181/182 (100%)	173 (96%)	8 (4%)	28	32
1	B	181/182 (100%)	172 (95%)	9 (5%)	24	26
1	C	181/182 (100%)	173 (96%)	8 (4%)	28	32
1	D	181/182 (100%)	173 (96%)	8 (4%)	28	32
All	All	724/728 (100%)	691 (95%)	33 (5%)	27	30

All (33) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	303	PRO
1	A	326	GLN
1	A	392	LEU
1	A	413	ILE
1	A	419	PRO
1	A	465	ASN
1	A	470	ASN
1	A	488	THR
1	B	303	PRO
1	B	326	GLN

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Mol	Chain	Res	Type
1	B	328	ARG
1	B	366	GLN
1	B	392	LEU
1	B	396	GLU
1	B	415	SER
1	B	419	PRO
1	B	473	LYS
1	C	303	PRO
1	C	326	GLN
1	C	366	GLN
1	C	392	LEU
1	C	413	ILE
1	C	419	PRO
1	C	470	ASN
1	C	473	LYS
1	D	303	PRO
1	D	326	GLN
1	D	328	ARG
1	D	413	ILE
1	D	419	PRO
1	D	455	LEU
1	D	465	ASN
1	D	470	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (26) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	326	GLN
1	A	362	GLN
1	A	365	ASN
1	A	366	GLN
1	A	389	HIS
1	A	418	GLN
1	A	462	GLN
1	A	465	ASN
1	A	470	ASN
1	B	326	GLN
1	B	362	GLN
1	B	365	ASN
1	B	366	GLN
1	B	389	HIS
1	B	470	ASN

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Mol	Chain	Res	Type
1	C	326	GLN
1	C	362	GLN
1	C	365	ASN
1	C	389	HIS
1	C	465	ASN
1	C	470	ASN
1	D	362	GLN
1	D	421	ASN
1	D	462	GLN
1	D	465	ASN
1	D	470	ASN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 4 ligands modelled in this entry, 4 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 (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 (i)

6.1 Protein, DNA and RNA chains (i)

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, 95th 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	216/217 (99%)	0.24	10 (4%)	32	35	12, 22, 44, 60	0
1	B	216/217 (99%)	0.33	16 (7%)	14	15	12, 29, 46, 61	0
1	C	216/217 (99%)	0.29	11 (5%)	28	30	10, 24, 41, 58	0
1	D	216/217 (99%)	0.31	12 (5%)	24	26	12, 27, 44, 59	0
All	All	864/868 (99%)	0.29	49 (5%)	23	25	10, 26, 44, 61	0

All (49) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	463	ARG	5.0
1	C	419	PRO	4.8
1	D	434	ILE	4.7
1	A	463	ARG	4.4
1	B	463	ARG	4.0
1	A	467	ASN	3.9
1	C	434	ILE	3.9
1	D	463	ARG	3.8
1	D	419	PRO	3.7
1	B	419	PRO	3.6
1	D	331	GLY	3.5
1	A	464	GLN	3.4
1	D	303	PRO	3.2
1	C	304	ASN	3.1
1	B	467	ASN	3.1
1	B	404	LYS	3.0
1	C	494	ALA	3.0
1	D	329	GLU	2.9
1	A	419	PRO	2.9
1	B	332	SER	2.8
1	B	461	PRO	2.8

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Mol	Chain	Res	Type	RSRZ
1	C	329	GLU	2.7
1	B	462	GLN	2.6
1	B	333	VAL	2.6
1	A	469	ALA	2.6
1	B	331	GLY	2.6
1	D	481	GLY	2.5
1	A	333	VAL	2.5
1	A	291	GLY	2.4
1	B	418	GLN	2.4
1	B	464	GLN	2.4
1	C	418	GLN	2.4
1	D	464	GLN	2.3
1	A	329	GLU	2.3
1	D	461	PRO	2.3
1	D	333	VAL	2.2
1	D	462	GLN	2.2
1	A	418	GLN	2.2
1	B	316	GLU	2.2
1	C	282	ARG	2.1
1	B	494	ALA	2.1
1	D	293	THR	2.1
1	C	333	VAL	2.1
1	A	481	GLY	2.1
1	B	434	ILE	2.1
1	C	462	GLN	2.0
1	C	470	ASN	2.0
1	B	318	GLY	2.0
1	B	293	THR	2.0

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

There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates (i)

There are no monosaccharides in this entry.

6.4 Ligands (i)

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, 95th 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	CA	D	497	1/1	0.84	0.09	35,35,35,35	0
2	CA	C	497	1/1	0.89	0.10	40,40,40,40	0
2	CA	B	497	1/1	0.93	0.06	39,39,39,39	0
2	CA	A	497	1/1	0.97	0.07	25,25,25,25	0

6.5 Other polymers (i)

There are no such residues in this entry.