Full wwPDB X-ray Structure Validation Report (i)

Nov 2, 2023 – 01:10 AM EDT

PDB ID	:	3T6B
Title	:	Structure of human DPPIII in complex with the opioid peptide Tynorphin, at 2.4 Angstroms
Authors	:	Bezerra, G.A.; Gruber, K.
Deposited on	:	2011-07-28
Resolution	:	2.40 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 types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

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

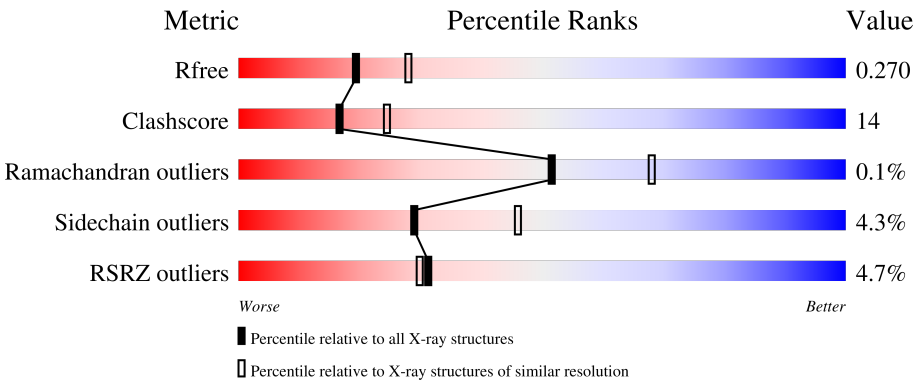
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.36
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation 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 2.40 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	3907 (2.40-2.40)
Clashscore	141614	4398 (2.40-2.40)
Ramachandran outliers	138981	4318 (2.40-2.40)
Sidechain outliers	138945	4319 (2.40-2.40)
RSRZ outliers	127900	3811 (2.40-2.40)

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	726	3%, 72%, 26%, •
1	B	726	6%, 69%, 29%, •
2	C	5	60%, 40%
2	D	5	40%, 60%

2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 11875 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 Dipeptidyl peptidase 3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	724	5748	3664	971	1100	13	0	0	0
1	B	724	5748	3664	971	1100	13	0	0	0

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	451	ALA	GLU	engineered mutation	UNP Q9NY33
B	451	ALA	GLU	engineered mutation	UNP Q9NY33

- Molecule 2 is a protein called Tynorphin.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
2	C	5	48	35	6	7	0	0	0
2	D	5	48	35	6	7	0	0	0

- Molecule 3 is water.

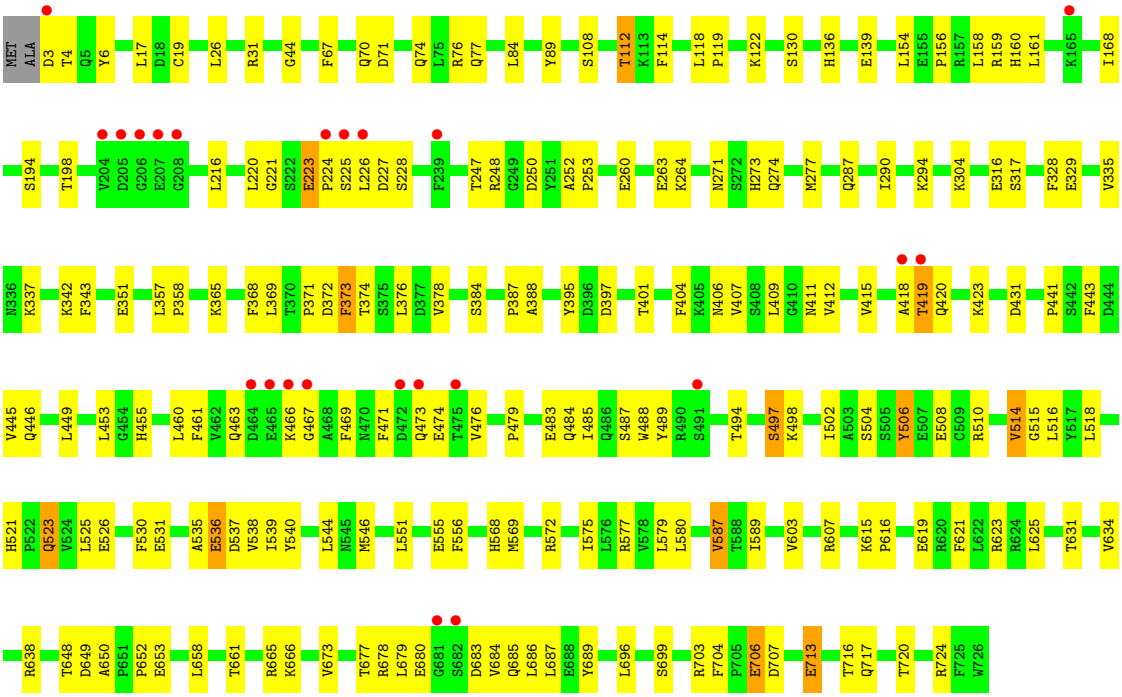
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
3	A	154	154	154	0	0
3	C	2	2	2	0	0
3	B	127	127	127	0	0

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.

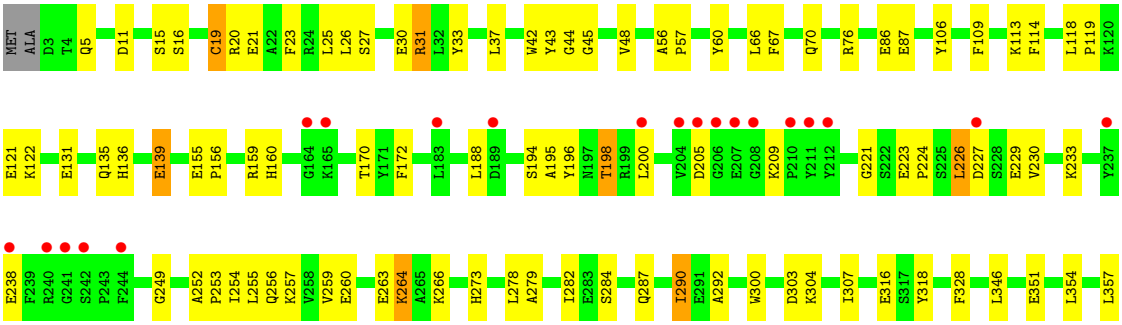
• Molecule 1: Dipeptidyl peptidase 3

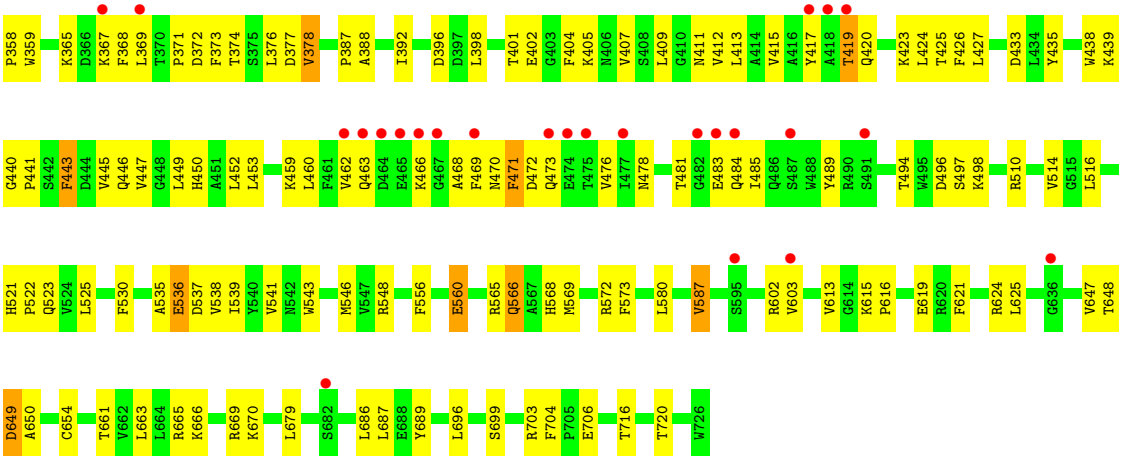
Chain A:



• Molecule 1: Dipeptidyl peptidase 3

Chain B:





- Molecule 2: Tynorphin

Chain C: 60% 40%

- Molecule 2: Tynorphin

Chain D: 40% 60%

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	61.97Å 107.55Å 119.10Å 90.00° 90.67° 90.00°	Depositor
Resolution (Å)	54.71 – 2.40 54.71 – 2.40	Depositor EDS
% Data completeness (in resolution range)	78.6 (54.71-2.40) 90.6 (54.71-2.40)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.12	Depositor
$< I/\sigma(I) >$ [1]	2.68 (at 2.40Å)	Xtriage
Refinement program	PHENIX 1.7_650	Depositor
R, R_{free}	0.197 , 0.258 0.207 , 0.270	Depositor DCC
R_{free} test set	2806 reflections (5.07%)	wwPDB-VP
Wilson B-factor (Å^2)	28.6	Xtriage
Anisotropy	0.496	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.39 , 59.7	EDS
L-test for twinning[2]	$< \|L\| > = 0.46$, $< L^2 > = 0.29$	Xtriage
Estimated twinning fraction	0.054 for h,-k,-l	Xtriage
F_o,F_c correlation	0.93	EDS
Total number of atoms	11875	wwPDB-VP
Average B, all atoms (Å^2)	35.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 43.83 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 1.6656e-04. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

[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)

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	0.28	0/5880	0.47	0/7966
1	B	0.27	0/5880	0.45	0/7966
2	C	0.31	0/51	0.44	0/70
2	D	0.23	0/51	0.49	0/70
All	All	0.27	0/11862	0.46	0/16072

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 (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	5748	0	5620	162	0
1	B	5748	0	5620	165	0
2	C	48	0	46	4	0
2	D	48	0	46	4	0
3	A	154	0	0	9	0
3	B	127	0	0	9	0
3	C	2	0	0	0	0
All	All	11875	0	11332	325	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 14.

All (325) 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:223:GLU:HB2	1:A:224:PRO:HD2	1.32	1.10
1:A:526:GLU:HB3	3:A:889:HOH:O	1.74	0.88
1:A:455:HIS:CE1	2:C:1:VAL:HG11	2.09	0.87
1:A:466:LYS:HG2	1:A:467:GLY:H	1.41	0.84
1:A:365:LYS:HE2	1:A:368:PHE:HA	1.60	0.83
1:B:304:LYS:HE3	1:B:372:ASP:HB2	1.65	0.79
1:A:494:THR:HG22	1:A:497:SER:HB3	1.62	0.79
1:A:271:ASN:HD21	1:A:273:HIS:HB2	1.46	0.78
1:A:194:SER:HB3	1:A:290:ILE:HG21	1.67	0.77
1:A:223:GLU:HB2	1:A:224:PRO:CD	2.14	0.75
1:B:205:ASP:OD1	1:B:209:LYS:HB3	1.86	0.75
1:A:409:LEU:O	1:A:412:VAL:HG12	1.86	0.75
1:A:418:ALA:O	1:A:419:THR:HG22	1.86	0.74
1:B:420:GLN:HB3	1:B:423:LYS:HE2	1.67	0.74
1:A:615:LYS:HB3	1:A:616:PRO:HD3	1.69	0.73
1:A:623:ARG:HD2	3:A:859:HOH:O	1.88	0.72
1:B:260:GLU:O	1:B:264:LYS:HD2	1.88	0.72
1:B:365:LYS:HE2	1:B:368:PHE:HA	1.71	0.72
1:B:376:LEU:HD13	1:B:407:VAL:HG13	1.71	0.72
1:B:21:GLU:O	1:B:25:LEU:HD13	1.91	0.71
1:A:108:SER:OG	1:A:384:SER:HB2	1.92	0.70
1:B:438:TRP:HB2	1:B:541:VAL:HG21	1.73	0.69
1:B:565:ARG:HD2	3:B:846:HOH:O	1.91	0.69
1:A:483:GLU:HG2	1:A:484:GLN:H	1.58	0.68
1:A:463:GLN:HE21	1:A:467:GLY:HA2	1.59	0.68
1:A:716:THR:O	1:A:720:THR:HG23	1.94	0.68
1:A:466:LYS:HG2	1:A:467:GLY:N	2.09	0.68
1:B:525:LEU:HD23	1:B:535:ALA:HB1	1.77	0.67
1:A:494:THR:HG23	1:A:497:SER:H	1.60	0.67
1:B:27:SER:O	1:B:31:ARG:HG2	1.95	0.66
1:B:358:PRO:HB3	1:B:619:GLU:HG3	1.77	0.66
1:B:19:CYS:O	1:B:686:LEU:HD21	1.95	0.66
1:A:225:SER:HB3	1:A:248:ARG:NH2	2.12	0.65
1:B:378:VAL:HG22	1:B:409:LEU:HD22	1.79	0.65
1:A:77:GLN:NE2	1:B:687:LEU:HD22	2.12	0.65
1:A:108:SER:HB2	3:A:880:HOH:O	1.97	0.64
1:A:31:ARG:HB3	1:A:684:VAL:HG11	1.80	0.64
1:A:494:THR:CG2	1:A:497:SER:H	2.10	0.64
1:B:441:PRO:HB3	1:B:530:PHE:CZ	2.33	0.64
1:A:198:THR:HG22	1:A:216:LEU:HD22	1.80	0.64
1:B:369:LEU:HD22	1:B:402:GLU:O	1.98	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:371:PRO:HB3	1:A:404:PHE:CE1	2.32	0.63
1:A:225:SER:HB3	1:A:248:ARG:HH22	1.64	0.63
1:B:435:TYR:O	1:B:439:LYS:HB2	1.98	0.63
1:B:546:MET:SD	1:B:572:ARG:HG2	2.39	0.63
1:B:425:THR:H	1:B:548:ARG:HH21	1.47	0.62
1:A:446:GLN:HE22	1:A:515:GLY:HA3	1.64	0.62
1:A:696:LEU:O	1:A:696:LEU:HD23	1.99	0.62
1:B:615:LYS:HB3	1:B:616:PRO:HD3	1.80	0.62
1:A:419:THR:HG23	1:A:419:THR:O	1.99	0.62
1:A:26:LEU:HB2	1:A:31:ARG:HD3	1.82	0.61
1:B:445:VAL:O	1:B:449:LEU:HD13	2.00	0.61
1:A:551:LEU:HD11	1:A:658:LEU:HD13	1.82	0.61
1:A:536:GLU:HG2	1:A:607:ARG:HH21	1.66	0.61
1:A:365:LYS:HB2	3:A:878:HOH:O	2.00	0.61
1:B:118:LEU:H	1:B:118:LEU:HD23	1.66	0.60
1:A:19:CYS:O	1:A:686:LEU:HD21	2.00	0.60
1:B:494:THR:CG2	1:B:497:SER:H	2.14	0.60
1:B:483:GLU:HG3	1:B:484:GLN:N	2.17	0.60
1:A:397:ASP:O	1:A:401:THR:HG22	2.02	0.59
1:B:170:THR:HB	3:B:861:HOH:O	2.00	0.59
1:A:441:PRO:HB3	1:A:530:PHE:CZ	2.37	0.59
1:B:566:GLN:CG	1:B:569:MET:HG2	2.32	0.59
1:A:580:LEU:HD23	1:A:587:VAL:HG23	1.84	0.59
1:A:607:ARG:HD3	3:A:876:HOH:O	2.04	0.58
1:A:118:LEU:HD23	1:A:118:LEU:H	1.69	0.57
1:A:388:ALA:HA	1:A:412:VAL:HG11	1.85	0.57
1:A:535:ALA:O	1:A:539:ILE:HG13	2.03	0.57
1:A:77:GLN:HE22	1:B:687:LEU:HD13	1.69	0.57
1:A:194:SER:CB	1:A:290:ILE:HG21	2.34	0.57
1:A:479:PRO:HB2	1:A:623:ARG:NH2	2.19	0.57
1:B:452:LEU:HG	1:B:453:LEU:HD23	1.87	0.57
1:B:483:GLU:HG3	1:B:484:GLN:H	1.69	0.57
1:B:223:GLU:HB2	1:B:224:PRO:HD2	1.87	0.57
1:A:271:ASN:ND2	1:A:273:HIS:HB2	2.18	0.57
1:A:678:ARG:HG3	1:A:687:LEU:HD11	1.87	0.57
1:B:387:PRO:HB3	2:D:2:VAL:HG11	1.87	0.57
1:A:536:GLU:HG2	1:A:607:ARG:NH2	2.20	0.56
1:A:130:SER:HB2	3:A:881:HOH:O	2.05	0.56
1:B:256:GLN:O	1:B:260:GLU:HG3	2.04	0.56
1:B:368:PHE:CD2	1:B:368:PHE:O	2.58	0.56
1:B:443:PHE:O	1:B:447:VAL:HG23	2.05	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:706:GLU:H	1:A:706:GLU:CD	2.08	0.56
1:A:84:LEU:HD11	1:A:122:LYS:HB3	1.88	0.56
1:A:304:LYS:CE	1:A:372:ASP:HB2	2.36	0.56
1:B:409:LEU:O	1:B:412:VAL:HG12	2.06	0.55
1:A:555:GLU:OE2	1:A:666:LYS:HD2	2.06	0.55
1:B:409:LEU:HB2	1:B:412:VAL:HG12	1.87	0.55
1:B:387:PRO:HB3	2:D:2:VAL:CG1	2.36	0.55
1:B:621:PHE:CE2	1:B:625:LEU:HD11	2.42	0.55
1:A:158:LEU:HD23	1:A:168:ILE:HD11	1.88	0.55
1:A:112:THR:HG23	3:A:867:HOH:O	2.06	0.55
1:B:76:ARG:HD3	1:B:86:GLU:OE1	2.07	0.55
1:A:589:ILE:HG21	1:A:658:LEU:HD11	1.89	0.54
1:A:368:PHE:O	1:A:368:PHE:CD2	2.61	0.54
1:B:357:LEU:HD13	1:B:359:TRP:CZ2	2.42	0.54
1:B:535:ALA:O	1:B:538:VAL:HG22	2.07	0.54
1:B:706:GLU:CD	1:B:706:GLU:H	2.11	0.54
1:B:568:HIS:CD2	2:D:4:PRO:HD3	2.43	0.54
1:A:31:ARG:HB3	1:A:684:VAL:CG1	2.38	0.54
1:B:648:THR:HG23	1:B:650:ALA:H	1.72	0.53
1:B:388:ALA:HB1	1:B:413:LEU:HD11	1.90	0.53
1:B:494:THR:HG22	1:B:497:SER:H	1.73	0.53
1:A:463:GLN:NE2	1:A:467:GLY:HA2	2.23	0.53
1:A:67:PHE:HA	1:A:70:GLN:O	2.08	0.53
1:A:226:LEU:HD12	1:A:287:GLN:HE22	1.73	0.53
1:B:377:ASP:OD2	1:B:411:ASN:HB3	2.09	0.53
1:B:696:LEU:HD23	1:B:696:LEU:O	2.09	0.53
1:A:247:THR:HG22	3:A:810:HOH:O	2.10	0.52
1:A:271:ASN:ND2	1:A:273:HIS:H	2.06	0.52
1:A:419:THR:HA	1:A:423:LYS:HE3	1.91	0.52
1:B:346:LEU:HG	1:B:452:LEU:HD23	1.92	0.52
1:B:466:LYS:HG3	1:B:468:ALA:H	1.75	0.52
1:A:476:VAL:HG12	1:A:485:ILE:HD13	1.92	0.52
1:B:398:LEU:HA	1:B:401:THR:HG22	1.91	0.52
1:B:536:GLU:HB2	3:B:818:HOH:O	2.10	0.52
1:A:274:GLN:O	1:A:277:MET:HG2	2.10	0.52
1:B:278:LEU:O	1:B:282:ILE:HG13	2.09	0.52
1:A:358:PRO:HB3	1:A:619:GLU:HG3	1.92	0.51
1:A:376:LEU:HD22	1:A:407:VAL:CG1	2.41	0.51
1:B:198:THR:HG21	3:B:862:HOH:O	2.10	0.51
1:A:568:HIS:NE2	2:C:4:PRO:HD3	2.26	0.51
1:B:26:LEU:HB2	1:B:31:ARG:HD3	1.93	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:516:LEU:HD11	1:A:546:MET:HG2	1.93	0.51
1:B:469:PHE:HB3	1:B:471:PHE:CD1	2.46	0.51
1:B:136:HIS:HB3	1:B:139:GLU:CG	2.40	0.51
1:A:17:LEU:HD21	1:A:378:VAL:HB	1.92	0.51
1:B:516:LEU:HD22	1:B:543:TRP:CD1	2.46	0.50
1:A:136:HIS:HB3	1:A:139:GLU:OE2	2.11	0.50
1:A:225:SER:CB	1:A:248:ARG:HH22	2.23	0.50
1:B:535:ALA:O	1:B:539:ILE:HG13	2.12	0.50
1:A:409:LEU:HB2	1:A:412:VAL:HG12	1.93	0.50
1:B:462:VAL:HG23	1:B:470:ASN:HD21	1.75	0.50
1:A:316:GLU:OE1	1:A:316:GLU:HA	2.11	0.50
1:B:60:TYR:C	1:B:60:TYR:CD2	2.84	0.50
1:A:648:THR:HG23	1:A:650:ALA:H	1.77	0.50
1:B:425:THR:O	1:B:426:PHE:HB2	2.12	0.50
1:A:139:GLU:H	1:A:139:GLU:CD	2.13	0.50
1:A:689:TYR:CZ	1:A:699:SER:HA	2.47	0.50
1:B:473:GLN:H	1:B:473:GLN:CD	2.15	0.50
1:B:44:GLY:HA3	1:B:328:PHE:CE2	2.47	0.49
1:B:253:PRO:O	1:B:256:GLN:HB3	2.12	0.49
1:B:716:THR:O	1:B:720:THR:HG23	2.12	0.49
1:A:555:GLU:O	1:A:555:GLU:HG2	2.12	0.49
1:A:589:ILE:CD1	1:A:603:VAL:HG13	2.42	0.49
1:A:378:VAL:HG22	1:A:409:LEU:HD22	1.94	0.49
1:B:42:TRP:CD2	1:B:703:ARG:HD3	2.47	0.49
1:A:161:LEU:HA	1:A:168:ILE:O	2.13	0.49
1:A:502:ILE:HD13	1:A:638:ARG:HG2	1.93	0.49
1:B:300:TRP:HH2	1:B:392:ILE:HG13	1.78	0.49
1:B:160:HIS:HB3	3:B:838:HOH:O	2.12	0.49
1:B:365:LYS:N	1:B:459:LYS:HB2	2.27	0.49
1:A:568:HIS:O	1:A:572:ARG:HG3	2.13	0.49
1:A:44:GLY:HA3	1:A:328:PHE:CE2	2.48	0.48
1:A:220:LEU:O	1:A:248:ARG:HG3	2.14	0.48
1:B:471:PHE:HD1	1:B:471:PHE:H	1.60	0.48
1:A:158:LEU:CD2	1:A:168:ILE:HD11	2.43	0.48
1:B:259:VAL:O	1:B:263:GLU:HG2	2.13	0.48
1:A:335:VAL:HA	1:A:376:LEU:HD12	1.95	0.48
1:B:409:LEU:O	1:B:413:LEU:HD13	2.13	0.48
1:A:260:GLU:O	1:A:263:GLU:HG2	2.14	0.48
1:A:376:LEU:HD22	1:A:407:VAL:HG13	1.96	0.48
1:B:489:TYR:CE1	1:B:498:LYS:HD3	2.49	0.48
1:A:476:VAL:HG12	1:A:485:ILE:CD1	2.44	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:4:THR:HG23	1:A:666:LYS:NZ	2.29	0.47
1:B:566:GLN:HG2	1:B:569:MET:HG2	1.95	0.47
1:B:476:VAL:HG12	1:B:485:ILE:HD13	1.96	0.47
1:B:427:LEU:CD1	1:B:548:ARG:HD2	2.44	0.47
1:A:525:LEU:HD13	1:A:535:ALA:HB1	1.95	0.47
1:B:160:HIS:N	1:B:160:HIS:CD2	2.82	0.47
1:A:556:PHE:CD1	1:A:569:MET:HG3	2.50	0.47
1:A:466:LYS:CG	1:A:467:GLY:H	2.19	0.47
1:B:30:GLU:OE2	1:B:307:ILE:HD12	2.14	0.47
1:B:56:ALA:HB3	1:B:57:PRO:HD3	1.95	0.47
1:A:419:THR:HA	1:A:423:LYS:CE	2.45	0.47
1:A:431:ASP:HB3	1:A:544:LEU:HD21	1.96	0.47
1:A:119:PRO:HB2	1:A:122:LYS:CG	2.45	0.46
1:A:316:GLU:HG2	1:A:329:GLU:OE2	2.15	0.46
1:A:6:TYR:O	1:A:114:PHE:HA	2.15	0.46
1:A:76:ARG:HB2	1:A:89:TYR:CE2	2.50	0.46
1:A:713:GLU:O	1:A:717:GLN:HG2	2.16	0.46
1:B:19:CYS:O	1:B:686:LEU:CD2	2.62	0.46
1:A:453:LEU:HD13	1:A:518:LEU:HD13	1.97	0.46
1:A:680:GLU:HB2	1:A:683:ASP:OD1	2.15	0.46
1:B:119:PRO:HB2	1:B:122:LYS:HG2	1.98	0.46
1:B:273:HIS:HB3	1:B:303:ASP:HB2	1.96	0.46
1:B:43:TYR:CD2	1:B:257:LYS:HB3	2.50	0.46
1:B:229:GLU:H	1:B:229:GLU:HG2	1.54	0.46
1:B:230:VAL:HG21	1:B:287:GLN:O	2.16	0.46
1:A:252:ALA:HB3	1:A:253:PRO:HD3	1.97	0.46
1:A:673:VAL:HG11	1:A:689:TYR:HB2	1.97	0.46
1:B:689:TYR:CZ	1:B:699:SER:HA	2.50	0.46
1:B:471:PHE:CD1	1:B:471:PHE:N	2.84	0.46
1:A:536:GLU:OE1	1:A:537:ASP:N	2.49	0.46
1:B:20:ARG:O	1:B:23:PHE:HB3	2.15	0.46
1:B:109:PHE:CD2	1:B:669:ARG:HD2	2.51	0.46
1:A:466:LYS:CG	1:A:467:GLY:N	2.79	0.46
1:A:351:GLU:HB2	1:A:368:PHE:CE2	2.51	0.45
1:A:371:PRO:HB2	1:A:406:ASN:ND2	2.30	0.45
1:A:483:GLU:HG2	1:A:484:GLN:N	2.27	0.45
1:B:462:VAL:HG12	1:B:463:GLN:N	2.32	0.45
1:B:439:LYS:O	1:B:439:LYS:HD3	2.15	0.45
1:B:221:GLY:H	1:B:223:GLU:CD	2.20	0.45
1:B:663:LEU:O	1:B:666:LYS:HE2	2.15	0.45
1:A:156:PRO:HA	1:A:159:ARG:HG3	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:172:PHE:HA	1:B:200:LEU:O	2.16	0.45
1:A:342:LYS:HE3	1:A:343:PHE:CE1	2.51	0.45
1:A:419:THR:O	1:A:419:THR:CG2	2.64	0.45
1:A:227:ASP:O	1:A:228:SER:HB3	2.17	0.45
1:A:460:LEU:HD23	1:A:489:TYR:CZ	2.52	0.45
1:B:113:LYS:HG2	1:B:114:PHE:N	2.30	0.45
1:A:411:ASN:O	1:A:415:VAL:HG23	2.17	0.45
1:B:367:LYS:O	1:B:368:PHE:HB3	2.17	0.45
1:A:387:PRO:O	1:A:409:LEU:HD12	2.17	0.45
1:B:266:LYS:NZ	1:B:279:ALA:HB2	2.30	0.45
1:A:453:LEU:HD13	1:A:518:LEU:CD1	2.47	0.45
1:B:5:GLN:HG2	1:B:666:LYS:NZ	2.30	0.45
1:B:106:TYR:CE2	1:B:113:LYS:HB2	2.50	0.45
1:B:415:VAL:HG13	1:B:670:LYS:HE2	1.98	0.45
1:B:371:PRO:O	1:B:405:LYS:HA	2.17	0.45
1:B:351:GLU:O	1:B:354:LEU:HB2	2.17	0.44
1:B:472:ASP:O	1:B:476:VAL:HG23	2.17	0.44
1:B:409:LEU:HB2	1:B:412:VAL:CG1	2.47	0.44
1:B:131:GLU:O	1:B:135:GLN:HG3	2.18	0.44
1:B:476:VAL:HG12	1:B:485:ILE:CD1	2.47	0.44
1:A:260:GLU:O	1:A:264:LYS:HD3	2.18	0.44
1:B:469:PHE:HB3	1:B:471:PHE:CE1	2.52	0.44
1:A:154:LEU:HD23	1:A:154:LEU:HA	1.84	0.44
1:B:460:LEU:N	1:B:460:LEU:HD12	2.32	0.44
1:B:516:LEU:HD21	1:B:543:TRP:HA	2.00	0.44
1:B:139:GLU:CD	1:B:139:GLU:H	2.20	0.44
1:B:194:SER:HB3	1:B:290:ILE:HG21	1.99	0.44
1:A:71:ASP:OD2	1:A:74:GLN:HG3	2.17	0.44
1:A:420:GLN:OE1	1:A:423:LYS:HE2	2.18	0.44
1:A:510:ARG:O	1:A:514:VAL:HG13	2.18	0.44
1:A:652:PRO:HG2	1:A:653:GLU:OE1	2.18	0.44
1:A:703:ARG:HG2	1:A:704:PHE:CZ	2.53	0.44
1:B:388:ALA:HB1	1:B:413:LEU:CD1	2.48	0.44
1:B:521:HIS:HA	1:B:522:PRO:HD3	1.85	0.44
1:B:249:GLY:O	1:B:252:ALA:HB2	2.18	0.44
1:A:357:LEU:HD21	1:A:518:LEU:HD11	2.00	0.43
1:A:445:VAL:O	1:A:449:LEU:HD13	2.18	0.43
1:B:11:ASP:OD1	1:B:11:ASP:N	2.50	0.43
1:B:537:ASP:O	1:B:541:VAL:HG23	2.18	0.43
1:B:580:LEU:HD23	1:B:587:VAL:HG23	2.00	0.43
1:A:119:PRO:HB2	1:A:122:LYS:HG2	1.99	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:473:GLN:HG2	1:A:474:GLU:N	2.32	0.43
1:B:703:ARG:HG2	1:B:704:PHE:CE2	2.52	0.43
1:A:661:THR:O	1:A:665:ARG:HG3	2.17	0.43
1:A:680:GLU:HB2	1:A:683:ASP:CG	2.38	0.43
1:A:489:TYR:CE1	1:A:498:LYS:HD3	2.54	0.43
1:B:284:SER:HB2	1:B:292:ALA:HB3	2.01	0.43
1:A:77:GLN:HG2	3:B:850:HOH:O	2.19	0.43
1:B:556:PHE:CD1	1:B:569:MET:HG3	2.53	0.43
1:A:221:GLY:C	1:A:223:GLU:H	2.21	0.43
1:A:378:VAL:CG2	1:A:409:LEU:HD22	2.49	0.43
1:B:417:TYR:O	1:B:419:THR:HG22	2.18	0.43
1:B:424:LEU:HD23	1:B:424:LEU:HA	1.90	0.43
1:B:478:ASN:HB3	1:B:481:THR:OG1	2.18	0.43
1:A:77:GLN:HE21	1:B:687:LEU:HD22	1.82	0.43
1:A:521:HIS:CE1	1:A:523:GLN:HB3	2.54	0.42
1:B:358:PRO:CB	1:B:619:GLU:HG3	2.46	0.42
1:B:613:VAL:O	1:B:616:PRO:HD2	2.19	0.42
1:B:33:TYR:CZ	1:B:37:LEU:HD11	2.54	0.42
1:B:374:THR:OG1	1:B:376:LEU:HD11	2.18	0.42
1:B:417:TYR:CE2	1:B:440:GLY:HA3	2.55	0.42
1:B:194:SER:HB3	1:B:290:ILE:HG12	2.00	0.42
1:B:388:ALA:HA	1:B:412:VAL:HG11	2.00	0.42
1:B:452:LEU:HG	1:B:453:LEU:CD2	2.49	0.42
1:B:494:THR:HG23	1:B:496:ASP:N	2.34	0.42
1:A:252:ALA:HB3	1:A:253:PRO:CD	2.50	0.42
1:B:426:PHE:HB3	1:B:603:VAL:HG23	2.00	0.42
1:B:466:LYS:HE3	1:B:466:LYS:HB2	1.83	0.42
1:B:679:LEU:HD12	1:B:679:LEU:HA	1.86	0.42
1:A:335:VAL:HG12	1:A:376:LEU:HD11	2.01	0.42
1:B:494:THR:HG23	1:B:497:SER:H	1.83	0.42
1:B:536:GLU:OE1	1:B:537:ASP:N	2.53	0.42
1:B:666:LYS:HE2	1:B:666:LYS:HB3	1.77	0.42
1:A:568:HIS:CE1	2:C:4:PRO:HD3	2.55	0.42
1:A:621:PHE:CE2	1:A:625:LEU:HD11	2.55	0.42
1:B:155:GLU:HA	1:B:156:PRO:HD3	1.91	0.42
1:A:19:CYS:O	1:A:686:LEU:CD2	2.68	0.42
1:A:271:ASN:HD22	1:A:273:HIS:H	1.66	0.42
1:A:568:HIS:CD2	2:C:4:PRO:HD3	2.55	0.41
1:B:255:LEU:HD23	1:B:255:LEU:HA	1.86	0.41
1:B:446:GLN:O	1:B:450:HIS:HB2	2.20	0.41
1:A:469:PHE:HE1	1:A:488:TRP:CE2	2.38	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:121:GLU:HG2	1:B:122:LYS:N	2.35	0.41
1:B:188:LEU:HD13	1:B:195:ALA:HB2	2.01	0.41
1:B:316:GLU:HB3	1:B:318:TYR:CD1	2.55	0.41
1:A:607:ARG:H	1:A:607:ARG:HG2	1.73	0.41
1:A:679:LEU:HD12	1:A:679:LEU:HA	1.92	0.41
1:B:602:ARG:HD3	1:B:602:ARG:HA	1.92	0.41
1:A:461:PHE:HB3	1:A:471:PHE:CE1	2.55	0.41
1:B:510:ARG:O	1:B:514:VAL:HG13	2.21	0.41
1:B:566:GLN:HB2	3:B:765:HOH:O	2.20	0.41
1:B:661:THR:O	1:B:665:ARG:HG2	2.20	0.41
1:B:226:LEU:HB3	1:B:227:ASP:H	1.77	0.41
1:A:294:LYS:HE3	1:A:395:TYR:CD1	2.56	0.41
1:A:373:PHE:HD2	1:A:374:THR:N	2.19	0.41
1:A:460:LEU:HD23	1:A:489:TYR:CE2	2.56	0.41
1:A:508:GLU:HG2	1:A:568:HIS:CD2	2.54	0.41
1:A:551:LEU:CD1	1:A:658:LEU:HD13	2.50	0.41
1:B:252:ALA:HB3	1:B:253:PRO:HD3	2.02	0.41
1:B:459:LYS:C	1:B:460:LEU:HD12	2.40	0.41
1:A:473:GLN:CD	1:A:473:GLN:H	2.23	0.41
1:A:487:SER:HB2	1:A:631:THR:HB	2.02	0.41
1:A:506:TYR:C	1:A:506:TYR:CD2	2.94	0.41
1:A:540:TYR:CD1	1:A:607:ARG:HB3	2.56	0.41
1:B:45:GLY:O	1:B:48:VAL:HB	2.21	0.41
1:B:233:LYS:HG2	3:B:855:HOH:O	2.21	0.41
1:B:371:PRO:HB3	1:B:404:PHE:CE1	2.55	0.41
1:B:649:ASP:OD1	1:B:654:CYS:HB3	2.21	0.41
2:D:2:VAL:CG1	2:D:3:TYR:N	2.84	0.41
1:A:575:ILE:O	1:A:579:LEU:HG	2.21	0.41
1:B:67:PHE:HA	1:B:70:GLN:O	2.21	0.41
1:B:136:HIS:HB3	1:B:139:GLU:HG2	2.02	0.40
1:B:424:LEU:HD21	1:B:435:TYR:CE1	2.56	0.40
1:B:560:GLU:H	1:B:560:GLU:HG3	1.40	0.40
1:B:573:PHE:CE2	1:B:647:VAL:HG22	2.56	0.40
1:A:337:LYS:HE3	3:A:837:HOH:O	2.21	0.40
1:A:461:PHE:O	1:A:488:TRP:HB2	2.22	0.40
1:A:677:THR:HA	1:A:685:GLN:O	2.21	0.40
1:B:42:TRP:HE3	3:B:859:HOH:O	2.04	0.40
1:B:159:ARG:CB	1:B:160:HIS:HD2	2.34	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	722/726 (99%)	694 (96%)	27 (4%)	1 (0%)	51	68
1	B	722/726 (99%)	697 (96%)	25 (4%)	0	100	100
2	C	3/5 (60%)	3 (100%)	0	0	100	100
2	D	3/5 (60%)	3 (100%)	0	0	100	100
All	All	1450/1462 (99%)	1397 (96%)	52 (4%)	1 (0%)	51	68

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	223	GLU

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	608/609 (100%)	583 (96%)	25 (4%)	30	48
1	B	608/609 (100%)	580 (95%)	28 (5%)	27	43
2	C	5/5 (100%)	5 (100%)	0	100	100
2	D	5/5 (100%)	5 (100%)	0	100	100
All	All	1226/1228 (100%)	1173 (96%)	53 (4%)	29	46

All (53) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	3	ASP
1	A	112	THR
1	A	160	HIS
1	A	250	ASP
1	A	317	SER
1	A	369	LEU
1	A	373	PHE
1	A	419	THR
1	A	443	PHE
1	A	497	SER
1	A	504	SER
1	A	506	TYR
1	A	514	VAL
1	A	523	GLN
1	A	531	GLU
1	A	536	GLU
1	A	538	VAL
1	A	577	ARG
1	A	587	VAL
1	A	634	VAL
1	A	649	ASP
1	A	706	GLU
1	A	707	ASP
1	A	713	GLU
1	A	724	ARG
1	B	15	SER
1	B	16	SER
1	B	19	CYS
1	B	31	ARG
1	B	66	LEU
1	B	87	GLU
1	B	139	GLU
1	B	196	TYR
1	B	198	THR
1	B	226	LEU
1	B	238	GLU
1	B	254	ILE
1	B	264	LYS
1	B	290	ILE
1	B	373	PHE
1	B	378	VAL
1	B	396	ASP
1	B	419	THR

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Mol	Chain	Res	Type
1	B	433	ASP
1	B	443	PHE
1	B	471	PHE
1	B	523	GLN
1	B	536	GLU
1	B	560	GLU
1	B	566	GLN
1	B	587	VAL
1	B	624	ARG
1	B	649	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (11) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	77	GLN
1	A	271	ASN
1	A	287	GLN
1	A	302	GLN
1	A	473	GLN
1	B	5	GLN
1	B	90	GLN
1	B	160	HIS
1	B	192	ASN
1	B	484	GLN
1	B	626	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)

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)

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 (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	724/726 (99%)	-0.15	23 (3%) 47 46	8, 27, 57, 88	0
1	B	724/726 (99%)	0.12	45 (6%) 20 19	14, 39, 71, 102	0
2	C	5/5 (100%)	-0.20	0 100 100	24, 28, 28, 33	0
2	D	5/5 (100%)	-0.29	0 100 100	32, 34, 37, 41	0
All	All	1458/1462 (99%)	-0.02	68 (4%) 31 30	8, 32, 66, 102	0

All (68) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	467	GLY	7.5
1	A	224	PRO	7.2
1	B	682	SER	7.0
1	B	475	THR	6.8
1	A	467	GLY	6.1
1	B	466	LYS	5.9
1	B	208	GLY	5.4
1	A	206	GLY	5.2
1	B	204	VAL	4.7
1	B	469	PHE	4.3
1	B	474	GLU	4.2
1	A	207	GLU	4.1
1	A	418	ALA	4.0
1	B	465	GLU	3.9
1	B	206	GLY	3.7
1	A	226	LEU	3.7
1	A	475	THR	3.7
1	A	466	LYS	3.6
1	B	165	LYS	3.6
1	B	207	GLU	3.6
1	B	419	THR	3.6

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Mol	Chain	Res	Type	RSRZ
1	A	205	ASP	3.6
1	A	225	SER	3.5
1	B	477	ILE	3.4
1	A	681	GLY	3.4
1	B	205	ASP	3.4
1	B	244	PHE	3.3
1	B	473	GLN	3.2
1	A	464	ASP	3.2
1	B	210	PRO	3.2
1	A	473	GLN	3.1
1	B	242	SER	3.1
1	A	419	THR	3.0
1	B	241	GLY	2.9
1	A	472	ASP	2.8
1	B	417	TYR	2.8
1	B	189	ASP	2.8
1	B	595	SER	2.7
1	A	208	GLY	2.6
1	A	204	VAL	2.6
1	B	487	SER	2.6
1	B	484	GLN	2.5
1	B	238	GLU	2.5
1	B	369	LEU	2.5
1	B	227	ASP	2.5
1	B	418	ALA	2.5
1	B	603	VAL	2.4
1	B	211	TYR	2.4
1	B	483	GLU	2.4
1	B	462	VAL	2.4
1	A	165	LYS	2.4
1	B	463	GLN	2.3
1	B	464	ASP	2.3
1	A	491	SER	2.3
1	B	237	TYR	2.2
1	A	682	SER	2.2
1	B	491	SER	2.2
1	B	164	GLY	2.2
1	B	482	GLY	2.2
1	A	239	PHE	2.2
1	B	212	TYR	2.1
1	B	636	GLY	2.1
1	A	465	GLU	2.1

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Mol	Chain	Res	Type	RSRZ
1	B	240	ARG	2.1
1	B	200	LEU	2.1
1	A	3	ASP	2.0
1	B	183	LEU	2.0
1	B	367	LYS	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)

There are no ligands in this entry.

6.5 Other polymers (i)

There are no such residues in this entry.