Full wwPDB X-ray Structure Validation Report (i)

Jun 13, 2024 – 11:33 AM EDT

PDB ID	:	1OEY
Title	:	Heterodimer of p40phox and p67phox PB1 domains from human NADPH oxidase
Authors	:	Wilson, M.I.; Gill, D.J.; Perisic, O.; Quinn, M.T.; Williams, R.L.
Deposited on	:	2003-04-02
Resolution	:	2.00 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 (i)) were used in the production of this report:

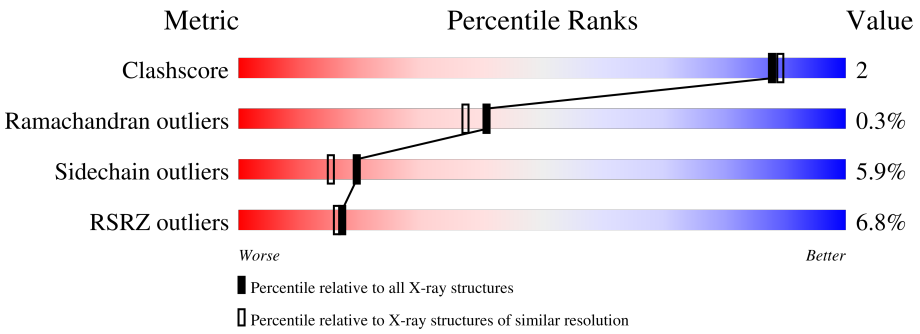
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36.2
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36.2

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 2.00 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	141614	9178 (2.00-2.00)
Ramachandran outliers	138981	9054 (2.00-2.00)
Sidechain outliers	138945	9053 (2.00-2.00)
RSRZ outliers	127900	7900 (2.00-2.00)

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	83	7%, 86%, 12%, ••
1	B	83	16%, 82%, 8%, •, 7%
1	C	83	13%, 77%, 16%, 7%
1	D	83	5%, 76%, 17%, ••, 5%
2	J	107	7%, 90%, 8%, •
2	K	107	2%, 86%, 11%, •

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Mol	Chain	Length	Quality of chain
2	L	107	2% 83% 8% • 7%
2	M	107	2% 82% 8% • 8%

2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 6382 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 NEUTROPHIL CYTOSOL FACTOR 2.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
			Total	C	N	O	S	Se			
1	A	82	674	428	116	124	2	4	0	0	0
1	B	77	638	408	108	117	2	3	19	0	0
1	C	77	641	409	109	118	2	3	7	0	0
1	D	79	654	417	111	120	2	4	8	0	0

- Molecule 2 is a protein called NEUTROPHIL CYTOSOL FACTOR 4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	Se			
2	J	105	884	559	154	168	3	6	0	0
2	K	104	874	553	151	167	3	10	0	0
2	L	99	835	528	144	160	3	0	0	0
2	M	98	839	531	147	159	2	0	1	0

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
J	242	VAL	CYS	engineered mutation	UNP Q15080
K	242	VAL	CYS	engineered mutation	UNP Q15080
L	242	VAL	CYS	engineered mutation	UNP Q15080
M	242	VAL	CYS	engineered mutation	UNP Q15080

- Molecule 3 is water.

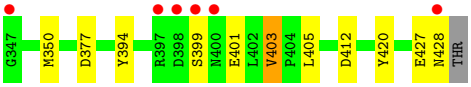
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
3	A	46	46	46	0	0
			Total	O		
3	B	16	16	16	0	0
			Total	O		
3	C	9	9	9	0	0
			Total	O		
3	D	18	18	18	0	0
			Total	O		
3	J	64	64	64	0	0
			Total	O		
3	K	59	59	59	0	0
			Total	O		
3	L	57	57	57	0	0
			Total	O		
3	M	74	74	74	0	0

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.

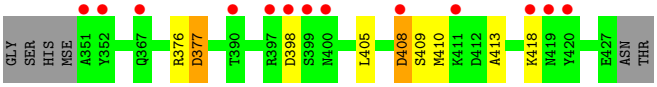
• Molecule 1: NEUTROPHIL CYTOSOL FACTOR 2

Chain A:



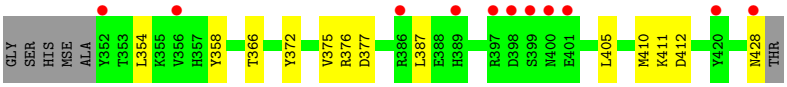
• Molecule 1: NEUTROPHIL CYTOSOL FACTOR 2

Chain B:



• Molecule 1: NEUTROPHIL CYTOSOL FACTOR 2

Chain C:

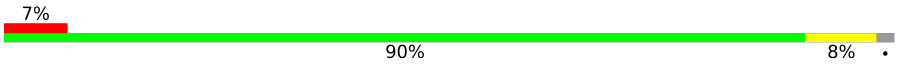


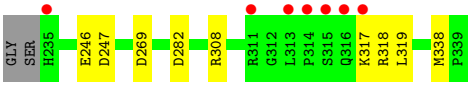
• Molecule 1: NEUTROPHIL CYTOSOL FACTOR 2

Chain D:

• Molecule 2: NEUTROPHIL CYTOSOL FACTOR 4

Chain J:



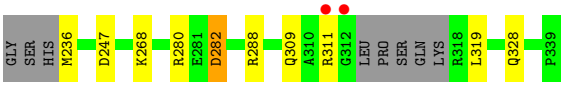


• Molecule 2: NEUTROPHIL CYTOSOL FACTOR 4

Chain K:

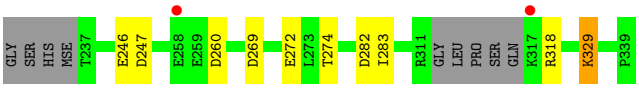
- Molecule 2: NEUTROPHIL CYTOSOL FACTOR 4

Chain L:



- Molecule 2: NEUTROPHIL CYTOSOL FACTOR 4

Chain M:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 64	Depositor
Cell constants a, b, c, α, β, γ	151.42Å 151.42Å 68.32Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	100.00 – 2.00 24.90 – 2.00	Depositor EDS
% Data completeness (in resolution range)	97.7 (100.00-2.00) 84.6 (24.90-2.00)	Depositor EDS
R_{merge}	0.15	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.92 (at 1.99Å)	Xtriage
Refinement program	REFMAC 5.1.24	Depositor
R, R_{free}	0.210 , 0.252 0.210 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å^2)	23.0	Xtriage
Anisotropy	0.100	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.37 , 46.5	EDS
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.31$	Xtriage
Estimated twinning fraction	0.035 for h,-h-k,-l	Xtriage
F_o,F_c correlation	0.93	EDS
Total number of atoms	6382	wwPDB-VP
Average B, all atoms (Å^2)	19.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 7.91% 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)

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	0.61	0/686	0.82	2/920 (0.2%)
1	B	0.53	0/650	0.80	3/874 (0.3%)
1	C	0.55	0/653	0.77	2/878 (0.2%)
1	D	0.49	0/666	0.75	3/895 (0.3%)
2	J	0.66	0/898	0.90	3/1210 (0.2%)
2	K	0.64	0/888	0.96	6/1198 (0.5%)
2	L	0.65	0/847	0.88	2/1141 (0.2%)
2	M	0.61	0/855	0.91	4/1151 (0.3%)
All	All	0.60	0/6143	0.86	25/8267 (0.3%)

There are no bond length outliers.

All (25) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	J	282	ASP	CB-CG-OD2	6.59	124.23	118.30
2	K	300	ASP	CB-CG-OD2	6.47	124.13	118.30
2	K	288	ARG	NE-CZ-NH2	-6.43	117.09	120.30
2	M	260	ASP	CB-CG-OD2	6.37	124.03	118.30
2	L	282	ASP	CB-CG-OD2	6.11	123.80	118.30
1	B	408	ASP	CB-CG-OD2	5.96	123.67	118.30
1	B	377	ASP	CB-CG-OD2	5.88	123.59	118.30
2	L	247	ASP	CB-CG-OD2	5.66	123.39	118.30
1	A	377	ASP	CB-CG-OD2	5.60	123.34	118.30
1	B	398	ASP	CB-CG-OD2	5.59	123.33	118.30
2	M	247	ASP	CB-CG-OD2	5.51	123.26	118.30
2	J	269	ASP	CB-CG-OD2	5.49	123.24	118.30
2	K	288	ARG	NE-CZ-NH1	5.44	123.02	120.30
1	C	377	ASP	CB-CG-OD2	5.43	123.19	118.30
2	K	302	ASP	CB-CG-OD2	5.43	123.19	118.30
2	M	282	ASP	CB-CG-OD2	5.42	123.18	118.30
1	D	377	ASP	CB-CG-OD2	5.36	123.13	118.30
2	J	247	ASP	CB-CG-OD2	5.33	123.10	118.30
2	K	330	ASP	CB-CG-OD2	5.32	123.09	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	412	ASP	CB-CG-OD2	5.31	123.08	118.30
1	C	412	ASP	CB-CG-OD2	5.31	123.08	118.30
1	D	412	ASP	CB-CG-OD2	5.24	123.02	118.30
2	K	247	ASP	CB-CG-OD2	5.22	123.00	118.30
1	D	398	ASP	CB-CG-OD2	5.05	122.85	118.30
2	M	269	ASP	CB-CG-OD2	5.02	122.82	118.30

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	674	0	674	3	0
1	B	638	0	644	1	0
1	C	641	0	645	6	0
1	D	654	0	659	3	0
2	J	884	0	878	1	0
2	K	874	0	871	4	0
2	L	835	0	826	1	0
2	M	839	0	836	7	0
3	A	46	0	0	0	0
3	B	16	0	0	0	0
3	C	9	0	0	0	0
3	D	18	0	0	0	0
3	J	64	0	0	0	0
3	K	59	0	0	0	0
3	L	57	0	0	0	0
3	M	74	0	0	1	0
All	All	6382	0	6033	24	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 2.

All (24) 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)
2:J:338:MSE:SE	2:J:338:MSE:CE	2.16	1.43
1:C:372:TYR:HA	1:C:410:MSE:CE	2.05	0.85
1:C:372:TYR:HA	1:C:410:MSE:HE2	1.66	0.77
1:C:372:TYR:HA	1:C:410:MSE:HE3	1.72	0.69
2:M:274:THR:HG21	2:M:283:ILE:CD1	2.27	0.65
2:L:280:ARG:HD2	2:L:282:ASP:OD1	1.99	0.62
2:M:274:THR:HG21	2:M:283:ILE:HD12	1.86	0.58
1:A:427:GLU:O	1:A:428:ASN:HB2	2.03	0.57
1:D:386:ARG:O	1:D:390:THR:HG23	2.06	0.55
2:K:279:GLN:HE22	2:M:329:LYS:HE3	1.72	0.54
2:M:272:GLU:HG3	3:M:2027:HOH:O	2.06	0.54
2:M:274:THR:CG2	2:M:283:ILE:CD1	2.86	0.53
1:C:354:LEU:HD13	1:C:366:THR:HG21	1.91	0.52
2:K:279:GLN:NE2	2:M:329:LYS:HE3	2.29	0.48
1:D:396:PRO:O	1:D:398:ASP:N	2.47	0.47
1:A:394:TYR:CE2	1:A:403:VAL:HG12	2.51	0.45
2:K:255:ILE:HG12	2:K:277:GLU:HG2	1.99	0.45
1:D:354:LEU:HD13	1:D:366:THR:HG21	2.00	0.44
1:A:350:MSE:HG3	1:A:420:TYR:CE1	2.53	0.44
2:M:274:THR:CG2	2:M:283:ILE:HD11	2.50	0.42
2:K:326:ILE:HD12	2:K:326:ILE:N	2.35	0.42
1:B:410:MSE:HE3	1:B:413:ALA:HB3	2.01	0.41
1:C:354:LEU:HD21	1:C:375:VAL:HG13	2.03	0.41
1:C:358:TYR:CD1	1:C:428:ASN:HB3	2.55	0.41

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	80/83 (96%)	78 (98%)	2 (2%)	0	100 100
1	B	75/83 (90%)	73 (97%)	2 (3%)	0	100 100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	C	75/83 (90%)	71 (95%)	4 (5%)	0	100	100
1	D	77/83 (93%)	71 (92%)	5 (6%)	1 (1%)	12	6
2	J	103/107 (96%)	101 (98%)	2 (2%)	0	100	100
2	K	102/107 (95%)	101 (99%)	1 (1%)	0	100	100
2	L	95/107 (89%)	93 (98%)	2 (2%)	0	100	100
2	M	95/107 (89%)	93 (98%)	1 (1%)	1 (1%)	14	8
All	All	702/760 (92%)	681 (97%)	19 (3%)	2 (0%)	41	37

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	397	ARG
2	M	318	ARG

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	77/74 (104%)	73 (95%)	4 (5%)	23	19
1	B	73/74 (99%)	67 (92%)	6 (8%)	11	7
1	C	74/74 (100%)	70 (95%)	4 (5%)	22	18
1	D	75/74 (101%)	66 (88%)	9 (12%)	5	2
2	J	98/96 (102%)	93 (95%)	5 (5%)	24	19
2	K	97/96 (101%)	94 (97%)	3 (3%)	40	40
2	L	92/96 (96%)	85 (92%)	7 (8%)	13	8
2	M	93/96 (97%)	91 (98%)	2 (2%)	52	55
All	All	679/680 (100%)	639 (94%)	40 (6%)	19	15

All (40) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	399	SER
1	A	401	GLU
1	A	403	VAL
1	A	405	LEU
1	B	376	ARG
1	B	377	ASP
1	B	405	LEU
1	B	408	ASP
1	B	409	SER
1	B	418	LYS
1	C	376	ARG
1	C	387	LEU
1	C	405	LEU
1	C	411	LYS
1	D	354	LEU
1	D	388	GLU
1	D	393	SER
1	D	398	ASP
1	D	399	SER
1	D	405	LEU
1	D	418	LYS
1	D	427	GLU
1	D	428	ASN
2	J	246	GLU
2	J	308	ARG
2	J	317	LYS
2	J	318	ARG
2	J	319	LEU
2	K	309	GLN
2	K	317	LYS
2	K	323	LYS
2	L	236	MSE
2	L	268	LYS
2	L	288	ARG
2	L	309	GLN
2	L	311	ARG
2	L	319	LEU
2	L	328	GLN
2	M	246	GLU
2	M	329	LYS

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

Mol	Chain	Res	Type
1	A	419	ASN
1	B	400	ASN
2	K	279	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	78/83 (93%)	0.33	6 (7%)	13	12	5, 17, 31, 37	1 (1%)
1	B	74/83 (89%)	0.91	13 (17%)	1	1	12, 29, 39, 45	4 (5%)
1	C	74/83 (89%)	1.02	11 (14%)	2	2	15, 28, 39, 43	2 (2%)
1	D	74/83 (89%)	0.55	4 (5%)	25	24	10, 25, 35, 43	0
2	J	102/107 (95%)	0.33	7 (6%)	16	16	4, 10, 34, 46	1 (0%)
2	K	101/107 (94%)	0.13	2 (1%)	65	63	5, 11, 24, 31	3 (2%)
2	L	96/107 (89%)	0.12	2 (2%)	63	62	5, 13, 28, 43	0
2	M	96/107 (89%)	0.01	2 (2%)	63	62	3, 9, 21, 40	0
All	All	695/760 (91%)	0.39	47 (6%)	17	16	3, 16, 36, 46	11 (1%)

All (47) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	J	316	GLN	9.5
1	D	398	ASP	7.3
2	J	314	PRO	7.0
2	J	311	ARG	6.7
1	C	398	ASP	6.0
1	C	400	ASN	5.7
2	J	313	LEU	5.5
2	J	315	SER	5.4
1	A	398	ASP	5.2
1	C	397	ARG	5.0
1	D	399	SER	4.6
2	J	235	HIS	4.4
1	A	428	ASN	4.4
1	A	347	GLY	4.3
2	L	311	ARG	4.3
1	B	398	ASP	4.2

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Mol	Chain	Res	Type	RSRZ
2	K	314	PRO	4.1
1	C	428	ASN	3.8
1	B	418	LYS	3.7
1	A	397	ARG	3.7
1	B	411	LYS	3.7
1	A	400	ASN	3.4
1	B	400	ASN	3.3
1	B	408	ASP	3.3
1	B	390	THR	3.2
1	B	351	ALA	3.1
1	C	386	ARG	3.1
1	C	420	TYR	3.1
1	B	419	ASN	3.0
2	K	315	SER	2.9
1	C	352	TYR	2.8
1	B	352	TYR	2.7
1	C	401	GLU	2.7
1	C	399	SER	2.6
1	B	399	SER	2.6
1	D	397	ARG	2.6
1	C	389	HIS	2.5
1	A	399	SER	2.4
1	D	400	ASN	2.4
1	B	420	TYR	2.4
1	B	367	GLN	2.4
2	L	312	GLY	2.4
2	M	317	LYS	2.3
1	B	397	ARG	2.3
1	C	356	VAL	2.3
2	M	258	GLU	2.1
2	J	317	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.